Optimally Weighted LSKUM for Compressible flows

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ABSTRACT

The robustness and accuracy of the meshfree least squares kinetic upwind method (LSKUM) depends on the condition number of the weighted least-squares matrix associated with the approximation of spatial derivatives. In computational domains with a highly stretched or anisotropic distribution of points, the least-squares matrix experiences high condition numbers, which results in either loss of accuracy or code divergence. This paper presents the development of optimally weighted LSKUM with minimal conditioning. The optimal weights that result in minimal condition numbers are found using discrete adjoints based on algorithmic differentiation. Numerical results have shown that the LSKUM with optimal weights yielded a more accurate solution than the current strategies for weights.

Keywords: Meshfree, LSKUM, weighted least-squares, condition number, discrete adjoints, AD

1 Introduction

The Least Squares Kinetic Upwind Method (LSKUM) [1, 2] is a meshfree method that belongs to the family of kinetic theory-based upwind schemes for the numerical solution of fluid flow problems. It requires a distribution of points around the configuration of interest and a set of neighbours for each point. In meshfree terminology, the point distribution is often known as the cloud of points, while the set of neighbours is referred to as connectivity or stencil. The point cloud can be obtained from simple or chimera grid generation algorithms, quadtree, or even advancing front methods [3]. The basic idea of LSKUM is to first introduce upwinding in the governing Euler or Navier-Stokes equations through the Kinetic Flux Vector Splitting (KFVS) scheme [4]. Later, the spatial derivatives at each point are approximated using the least-squares or weighted least-squares principle with suitable connectivity information. Over the past two decades, the LSKUM based meshfree CFD codes have been successfully used for computing flows around realistic configurations [5, 6, 7, 8].

A variant of LSKUM that is particularly interesting to us is the weighted LSKUM (W-LSKUM) [2]. In W-LSKUM, for each point in the domain, weights are assigned to its neighbours. The spatial derivatives are then approximated using weighted least-squares. Central to the robustness of the meshfree W-LSKUM solver is the well-conditioning of the weighted least-squares matrix. In general, the least-squares matrix with uniform weights $(w_i = 1)$ experiences high condition numbers in highly stretched or anisotropic distribution of points [5]. High condition numbers incur numerical instabilities, resulting in either loss of accuracy or code divergence. To avoid code divergence due to ill-conditioning, various strategies have been proposed regarding the choice of weights.

In one line of research [5, 8], the weights to the neighbours are chosen as $w_i = 1/d_i^2$. Here, d_i is the Cartesian distance between the point of interest P_0 and its neighbour P_i. Compared to $w_i = 1$, this choice of weights will result in minimum truncation error as they ensure the locality of the derivative. Furthermore, on highly stretched point distributions, use of weights as a decreasing function of distance reduces the condition numbers considerably. In another work [9], weights are chosen in such a way that the least-squares matrix becomes diagonal or the upwind direction becomes an eigendirection of the least-squares matrix. This approach results in a non-zero determinant of the least-squares matrix, which prevents the code divergence. However, in both the approaches, the condition numbers thus obtained may not be minimal and therefore the choice of weights are not optimal. The objective of this research is to find the optimal distribution of weights that yield a robust and accurate W-LSKUM solver with minimal conditioning.

2 Optimally Weighted Meshfree LSKUM

The Euler equations that govern the inviscid fluid flows can be obtained by taking moments of the Boltzmann equation with the velocity distribution function being the Maxwellian. In two-dimensions, these equations can be related in the inner product form as

$$\frac{\partial U}{\partial t}+\frac{\partial Gx}{\partial x}+\frac{\partial Gy}{\partial y}=\left\langle \Psi, \frac{\partial F}{\partial t}+v_1\frac{\partial F}{\partial x}+v_2\frac{\partial F}{\partial y}\right\rangle=0 \tag{1}$$

Here, U is the conserved vector, Gx and Gy are the flux vectors along the coordinate directions x and y respectively. F is the Maxwellian velocity distribution function and Ψ is the moment function vector. v_1 and v_2 are the molecular velocities along the coordinates x and y, respectively. Using Courant-Issacson-Rees (CIR) splitting of molecular velocities, an upwind scheme for the Boltzmann equation can be constructed as

$$\frac{\partial F}{\partial t}+\frac{v_1+|v_1|}{2}\frac{\partial F}{\partial x}+\frac{v_1-|v_1|}{2}\frac{\partial F}{\partial x}+\frac{v_2+|v_2|}{2}\frac{\partial F}{\partial y}+\frac{v_2-|v_2|}{2}\frac{\partial F}{\partial y}=0 \tag{2}$$

Using the weighted least-squares principle, the first-order accurate approximations for the spatial derivatives F_x and F_y at a point P_0 are given by the solution of the linear system

$$\begin{bmatrix}\sum w_i\Delta x_i^2 & \sum w_i\Delta x_i\Delta y_i\\ \sum w_i\Delta x_i\Delta y_i & \sum w_i\Delta y_i^2\end{bmatrix}\begin{bmatrix}F_x\\ F_y\end{bmatrix}_{P_0}=\begin{bmatrix}\sum w_i\Delta x_i\Delta F_i\\ \sum w_i\Delta y_i\Delta F_i\end{bmatrix}_{P_i\in N(P_0)} \tag{3}$$

Here, $N(P_0)$ is the set of neighbours or connectivity of the point P_0. Taking Ψ - moments of eq. (2) along with the formulae in eq. (3), we get the semi-discrete form of the meshfree weighted least-squares kinetic upwind method (W-LSKUM) for $2D$ Euler equations, given by

$$\frac{dU}{dt}+\frac{\partial Gx^+}{\partial x}+\frac{\partial Gx^-}{\partial x}+\frac{\partial Gy^+}{\partial y}+\frac{\partial Gy^-}{\partial y}=0 \tag{4}$$

Here, $Gx^{\pm}$ and $Gy^{\pm}$ are the kinetic split fluxes [4] along x and y directions, respectively. The first-order accurate least-squares formulae for the split flux derivatives are given by

$$\frac{\partial Gx^{\pm}}{\partial x}=\frac{1}{|A|}\begin{vmatrix}\sum w_i\Delta x_i\Delta Gx_i^{\pm} & \sum w_i\Delta x_i\Delta y_i\\ \sum w_i\Delta y_i\Delta Gx_i^{\pm} & \sum w_i\Delta y_i^2\end{vmatrix},\quad \frac{\partial Gy^{\pm}}{\partial y}=\frac{1}{|A|}\begin{vmatrix}\sum w_i\Delta x_i^2 & \sum w_i\Delta x_i\Delta Gy_i^{\pm}\\ \sum w_i\Delta x_i\Delta y_i & \sum w_i\Delta y_i\Delta Gy_i^{\pm}\end{vmatrix} \tag{5}$$

The derivatives of the split fluxes $Gx^{\pm}$ are evaluated using the split stencils $N_x^{\pm}(P_0)$, defined by

$$N_x^+(P_0)=\{P_i\in N(P_0)\mid x_{P_i}-x_{P_0}\le 0\},\quad N_x^-(P_0)=\{P_i\in N(P_0)\mid x_{P_i}-x_{P_0}\ge 0\} \tag{6}$$

Similarly, the spatial derivatives of the split fluxes $Gy^{\pm}$ are evaluated using appropriate split stencils. The state-update formula for the steady-state flow problems is constructed using the implicit LUSGS algorithm and local time stepping. Second-order accurate spatial approximations is obtained using the defect correction procedure with the entropy variables [2, 10].

The robustness of the meshfree W-LSKUM solver depends on the condition number of the weighted least-squares matrix present in the linear system in eq. (3). Connectivity due to the highly anisotropic or stretched distribution of points can make the least-squares matrix highly ill-conditioned. Large condition numbers may greatly amplify the effect of noise in $\sum w_i\Delta x_i\Delta Gx_i^{\pm}$, $\sum w_i\Delta y_i\Delta Gx_i^{\pm}$, $\sum w_i\Delta x_i\Delta Gy_i^{\pm}$ and $\sum w_i\Delta y_i\Delta Gy_i^{\pm}$, leading to loss of accuracy in the approximation of split flux derivatives. The robustness of the meshfree W-LSKUM solver can be enhanced if we can make the condition number of the least-squares matrix close to unity by suitably choosing the weights.

In the present work, this objective is achieved by posing the minimisation of the condition number as an optimal control problem. The objective function is defined as a function of the condition number of the weighted least-squares matrix. The control variables are the weights assigned to the neighbours of the point of interest. The constraints are that the weights must be positive. The optimisation problem at a point P_0 can be formulated as

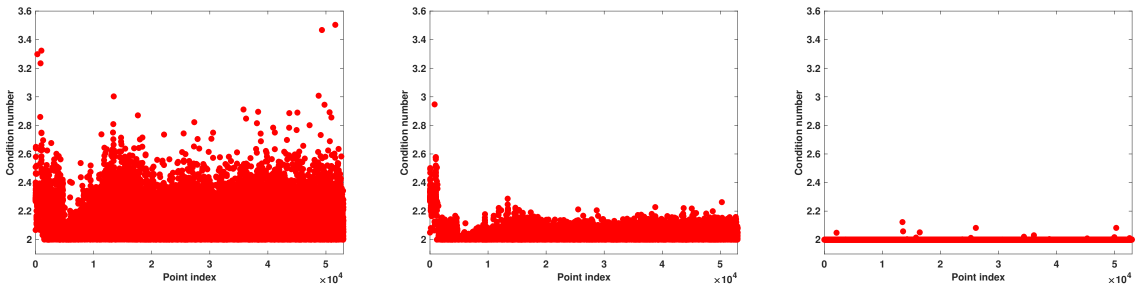
$$\begin{aligned}&\text{Minimise} && J=\frac{1}{2}\left(\|A\|\|A^{-1}\|-1\right)^2_{P_0}\\ &\text{subject to} && w_i>0,\ P_i\in N(P_0)\end{aligned} \tag{7}$$

Here, $\|A\|\|A^{-1}\|$ is the condition number and $\|A\|$ is the Frobenius norm of the weighted least-squares matrix associated with the point P_0. The optimal distribution of weights that minimise the condition number is found using a gradient descent algorithm. The sensitivities of the objective function with respect to the weights are evaluated using the discrete adjoint approach based on algorithmic differentiation (AD). Note that, at each point in the computational domain, optimal weights are required for the full and split stencils.

3 Results and Discussion

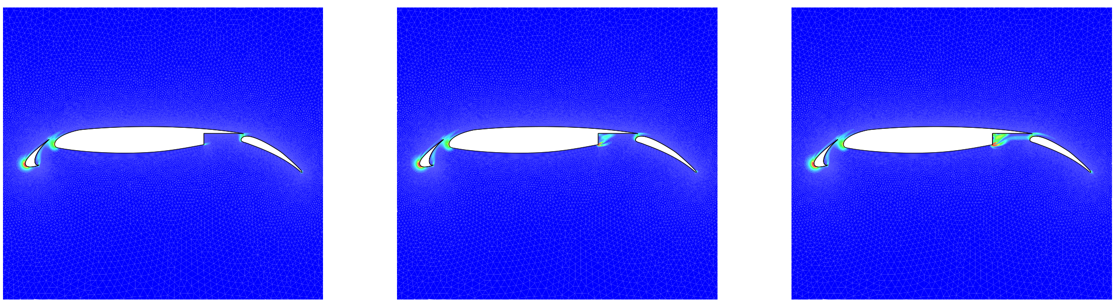
The optimally weighted LSKUM solver is applied to the test case of a subsonic flow past the McDonnell Douglas Aerospace (MDA) 30P-30N three-element high-lift configuration. Numerical simulations are performed with a freestream Mach number, $M_\infty = 0.2$, and angle of attack, $\alpha = 16^o$. The computational domain consists of $52,997$ points. The main airfoil has 696 points, while the slat and flap contain 298 points each.

Figure 1 shows a comparison of the condition numbers of the weighted least-squares matrix associated with the full stencil for all points in the computational domain. We observe that the optimal weights resulted in minimal condition numbers compared to the weights $w_i = 1.0$ and $w_i = 1/d_i^2$. Figure 2 shows the contours of the Frobenius norm of the velocity gradient tensor. These plots show that the optimally weighted LSKUM computes the velocity gradients more accurately and thus resulted in maximum enstrophy, as shown in Table 1. An increase in enstrophy has generated more vorticity, which yielded more lift. The surface pressure distribution plots in Figure 3 and coefficient of lift in Table 1 demonstrate the ability of optimally weighted LSKUM in then accurate computation of C_p distribution and lift coefficient. The residue plot in Figure 4 shows that the optimal weights resulted in more convergence of the flow solution.



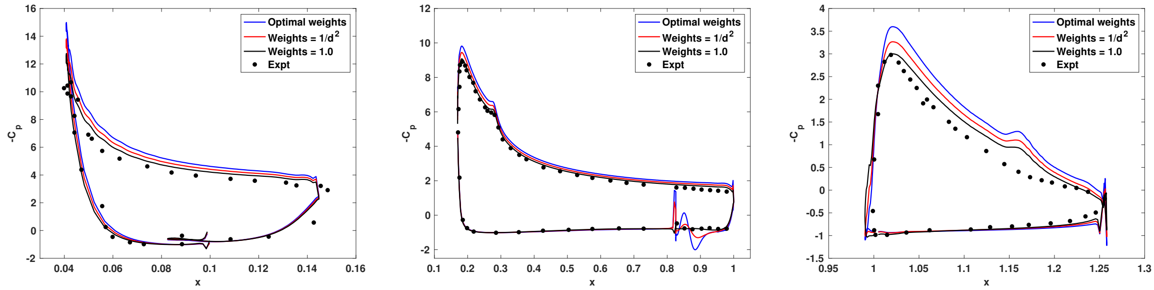
(a) Using weights $w_i = 1$ (b) Using weights $w_i = 1/d_i^2$ (c) Using optimal weights

Figure 1: Condition numbers of the weighted least-squares matrix associated with the full stencil.



(a) Using weights $w_i = 1$ (b) Using weights $w_i = 1/d_i^2$ (c) Using optimal weights

Figure 2: Contours of the Frobenius norm of the velocity gradient tensor based on W-LSKUM with different weights.



(a) C_p distribution on the slat (b) C_p distribution on the airfoil (c) C_p distribution on the flap

Figure 3: A comparison of the C_p-distribution based on W-LSKUM with different weights.

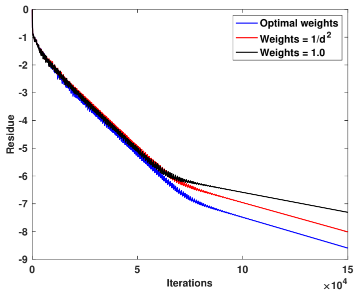


Figure 4: Comparison of the residual history based on W-LSKUM with different weights.

Weights	Lift	Enstrophy
1.0	3.6237	2.0523
$1/d^2$	3.7807	2.7262
Optimal	3.9456	4.1087

Table 1: Lift coefficient and enstrophy based on W-LSKUM with different weights.

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