Parallel implementation of k-exact Finite Volume Reconstruction on Unstructured Grids

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ABSTRACT

The quest for high-order accurate finite volume schemes for convection dominated flows remains an important challenge. Whereas second-order accuracy is sufficient to calculate strong discontinuities, CFD applications in industrial context such as jet noise predictions, LES modelling, internal flow applications with thermochemistry, require high-order accurate schemes. For this reason designing finite volume schemes on general grids using high-order reconstructions has become a scientific objective for industrial CFD codes.

Keeping the paradigm of one unknown per cell, the question can be reframed into two subproblems. The first one is purely mathematical and is an interpolation problem: it consists in selecting high-order local interpolants based on the knowledge of averaged values on a certain neighborhood. The second problem is algorithmic: high-order local interpolants require accessing data beyond the direct neighborhood thus giving a prohibitive computing complexity specifically on parallel computers.

Such questions were being addressed by several authors since more than 20 years. It has been early recognized [1] that high-order polynomial interpolation on non cartesian grids lead to stability problems. Such problems were intensively studied in the framework of adaptive reconstruction stencil selection (ENO or WENO schemes [7]). Other approaches include non polynomial functions such as RBF or splines [2].

The present contribution is the continuation of preceding studies devoted to the design of high-order centered polynomial reconstructions [5, 6]. This contribution takes place within the CEDRE project at ONERA. [1] Here we focus on the second problem namely the data access in irregular (finite-volume) grids for parallelism issues.

Specifically consider a cell α of a general grid together with cells β in the direct neighborhood of α. We show that it is possible to access high-order derivatives at the barycenter x_α by accessing data in the direct neighborhood only.

A reconstruction in cell α is a linear application mapping the cell averages $\overline{u}_\beta$ of u for β in a small neighborhood of cell α onto a polynomial w of degree k. It is called *k-exact* [3, 4] if the restrictions of w and u to the cell α coincide whenever u is a polynomial of degree k. If w has the same averaged value as u over cell α then the reconstruction is *conservative*. Let $\mathbb{W}_\alpha = \{\beta_1, \ldots, \beta_m\}$ be the cells of the neighborhood used for reconstruction in cell α, with $m = \sharp\mathbb{W}_\alpha$ and $\alpha \in \mathbb{W}_\alpha$, and write $\overline{\mathrm{u}}_{\mathbb{W}_\alpha} = (\overline{u}_{\beta_1}, \ldots, \overline{u}_{\beta_m})$. A polynomial w of degree k is uniquely determined by its mean value over cell α and its k non-vanishing derivatives $D^{(l)}w$, $1 \leq l \leq k$, at the barycenter $\boldsymbol{x}_\alpha$ of cell

[1]CEDRE is a multiphysics multisolver 3D code of ONERA / DSNA (Châtillon, FRANCE) for applications in aerothermochemistry and propulsion.

α. Any k-exact conservative reconstruction is therefore given by k linear applications $w_\alpha^{(l)}$ that must satisfy for all polynomials u of degree k

$$w_\alpha^{(l)}\left(\overline{\mathrm{u}}_{\mathbb{W}_\alpha}\right) = w_\alpha^{(l)}\left(\left(\overline{u}_{\beta_1}, \ldots, \overline{u}_{\beta_m}\right)\right) = D^{(l)}u\Big|_{\boldsymbol{x}_\alpha} \quad , \; 1 \le l \le k \; . \tag{1}$$

The values $w_\alpha^{(l)}$ are typically calculated using least squares. This requires $m \ge \binom{k+d}{d}$ which gives a lower bound for the size m of the neighborhood $\mathbb{W}_\alpha$ in the case where the reconstruction order $k \ge 2$.

The recursive algorithm that is suggested proceeds as follows: let $\mathbb{W}_\alpha = \{\beta_1, \ldots, \beta_m\}$ be the neighborhood of cell α for 1-exact reconstruction. This is typically the direct neighborhood. Let $j \in \{1, \ldots, k\}$ and assume that for each $\beta \in \mathbb{W}_\alpha$ there is a $w_\beta^{(j)}$ satisfying the identity (1) at cell β. We claim that there exists a linear operator denoted by $\mathfrak{J}_\alpha^{(j+1)}$ depending on the geometry of the grid such that for all polynomials u of degree $j+1$

$$\mathfrak{J}_\alpha^{(j+1)}\left(D^{(j+1)}u\Big|_{\boldsymbol{x}_\alpha}\right) = \left(w_{\beta_1}^{(j)}\left(\overline{\mathrm{u}}_{\mathbb{W}_{\beta_1}}\right) - w_\alpha^{(j)}\left(\overline{\mathrm{u}}_{\mathbb{W}_\alpha}\right), \ldots, w_{\beta_m}^{(j)}\left(\overline{\mathrm{u}}_{\mathbb{W}_{\beta_m}}\right) - w_\alpha^{(j)}\left(\overline{\mathrm{u}}_{\mathbb{W}_\alpha}\right)\right) \; . \tag{2}$$

Identity (2) means that the derivatives of order $j+1$ of u at x_α are implicitely expressed in terms of the difference of derivatives of order j. Therefore assuming that the operator $\mathfrak{J}_\alpha^{(j+1)}$ in (2) has a left inverse $\mathfrak{D}_\alpha^{(j+1)}$ and taking the left multiplication on the right side of (2) by $\mathfrak{D}_\alpha^{(j+1)}$ allows to define a derivative $w_\alpha^{(j+1)}$. We insist on the fact that this calculation only requires values of $w_\beta^{(j)}$ for $\beta \in \mathbb{W}_\alpha$.

The core of the reconstruction algorithm is now as follows: starting from a predicted value of the first-order derivative $w_\beta^{(1)}$, one first computes the second-order derivative $w_\beta^{(2)}$, then the third-order derivative $w_\beta^{(3)}$ and so on. *This recursive algorithm avoids accessing large neighborhoods thus drastically reducing the complexity of the reconstruction.*

It can be established that the inverse $\mathfrak{D}_\alpha^{(j+1)}$ exists in the case of an uniform cartesian grids. Furthermore numerical evidence indicates that $\mathfrak{D}_\alpha^{(j+1)}$ also exists on tetrahedral as well as on polyhedral grids [5]. The order of accuracy of the resulting approximation has been numerically assessed for the linear advection equation on unstructured 3D grids for reconstruction order $k = 2$ and $k = 3$ [5].

Further CFD test problems including the propagation of an isentropic vortex will be presented.

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