ON A HIGH-ORDER ENERGY-PRESERVING UNCONDITIONALLY STABLE DISCRETIZATION ON COLLOCATED UNSTRUCTURED GRIDS

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Abstract

In this work, an energy-preserving unconditionally stable fractional step method on collocated unstructured grids is presented. Its formulation is based on preserving the underlying symmetries of the differential operators. This formulation was proven to be unconditionally stable even for highly distorted meshes in Santos et al (2021,2022). However, it was second-order accurate for Cartesian meshes. Within this context, new insights of higher order accurate operators are presented. This high-order formulation is based on a Richardson Extrapolation.

1 Introduction

General purpose CFD codes such as OpenFOAM or ANSYS-Fluent rely on a finite-volume (stencil) discretization over unstructured meshes formulation to solve Navier-Stokes equations due to its simplicity. The stencil formulations solve the discretized equations with an algorithm that goes cell by cell, computing the desired quantities. Alternatively, algebraic formulations preserve them in matrix-vector form, and compute the desired quantities by using these matrices and vectors.

A collocated fully-conservative algebraic symmetry-preserving formulation of incompressible Navier-Stokes equations was proposed by Trias et al (2014). Assuming n control volumes and m faces:

$$\Omega \frac{d\mathbf{u}_c}{dt} + \mathbf{C}(\mathbf{u}_s)\mathbf{u}_c = \mathbf{D}\mathbf{u}_c - \Omega \mathbf{G}_c p_c, \quad (1)$$

$$\mathbf{M}\mathbf{u}_s = \mathbf{0}_c, \quad (2)$$

where $\mathbf{u}_c \in \mathbb{R}^{3n}$ and $\mathbf{p}_c \in \mathbb{R}^n$ are the cell-centered velocity and the cell-centered pressure, respectively. The face-centered quantities, such as $\mathbf{u}_s \in \mathbb{R}^m$ are related to the cell-centered quantities via an interpolation operator $\Gamma_{c\to s} \in \mathbb{R}^{m\times 3n}$:

$$\mathbf{u}_s = \Gamma_{c\to s}\mathbf{u}_c. \quad (3)$$

Finally, $\Omega \in \mathbb{R}^{3n\times 3n}$ is a diagonal matrix containing the cell volumes, $\mathbf{C}(\mathbf{u}_s) \in \mathbb{R}^{3n\times 3n}$ is the discrete convective operator, $\mathbf{D} \in \mathbb{R}^{3n\times 3n}$ is the discrete diffusive operator, $\mathbf{G}_c \in \mathbb{R}^{3n\times n}$ is the cell-to-cell discrete gradient operator and $\mathbf{M} \in \mathbb{R}^{n\times m}$ is the face-to-cell discrete divergence operator. The velocity correction after applying the Fractional Step Method (FSM) to the Navier-Stokes equations reads:

$$\mathbf{u}_c^{n+1} = \mathbf{u}_c^{p} - \Gamma_{s\to c}\mathbf{G}p_c^{n+1}, \quad (4)$$

where $\Gamma_{s\to c} \in \mathbb{R}^{3n\times m}$ is the face-to-cell interpolator, which is related to the cell-to-face interpolator via the volume matrices $\Gamma_{s\to c} = \Omega^{-1}\Gamma_{c\to s}\Omega_s$, and $\mathbf{G} \in \mathbb{R}^{m\times n}$ is the cell-to-face gradient operator.

Only five discrete operators are needed to formulate these equations: the cell-centered and staggered control volumes (diagonal matrices), Ω_c and Ω_s, the face normal vectors, N_s, the scalar cell-to-face interpolation, $\Pi_{c\to s}$ and the cell-to-face divergence operator, $\mathbf{M}$. For more details of these operators and its construction, the reader is referred to Trias et al (2014). Due to its simplicity, these operators can be easily builded in existing codes, such as OpenFOAM, see Komen et al (2021).

2 An energy-preserving unconditionally stable FSM

From our perspective, respecting the symmetries of these differential operators is crutial in order to respect the physical structure of the equations. For example, constructing $\mathbf{G} = -\Omega_s^{-1}\mathbf{M}^T$ is essential to preserve kinetic energy as in Trias et al (2014), but it is also mimicking the symmetries of the continuos level operators.

The utility of an algebraic formulation can be found, as an example, in Santos et al (2021,2022). In these works, the matrix-vector formulation is used in order to study the stability of the solution in terms of the pressure gradient interpolation in collocated frameworks. To do so, the eigenvalues of $\mathbf{L} - \mathbf{L}_c$ were deeply studied ($\mathbf{L} = \mathbf{MG} \in \mathbb{R}^{n\times n}$ is the compact

Laplacian operator whereas $\mathbf{L}_c = \mathbf{M}\Gamma_{c\to s}\Gamma_{s\to c}\mathbf{G} \in \mathbb{R}^{n\times n}$ is the collocated wide-stencil Laplacian operator), and the cell-to-face interpolation that leads to an unconditionally stable FSM turned out to be:

$$\Pi_{c\to s} = \Delta_s^{-1}\Delta_{sc}^T \in \mathbb{R}^{m\times n}, \tag{5}$$

where $\Delta_s \in \mathbb{R}^{m\times m}$ is a diagonal matrix containing the projected distances between two adjacent control volumes, and $\Delta_{sc} \in \mathbb{R}^{n\times m}$ is a matrix containing the projected distance between a cell node and its corresponding face. For details, the reader is referred to Santos et al (2021,2022).

3 Towards a high-order formulation

High-order formulations are usually preferred over low-order ones due to computational power reasons: they have better accuracy for the same mesh resolution and higher arithmetic intensity. A high-order (staggered) discretization over structured meshes of Navier-Stokes equations can be found in Verstappen and Veldman (2003). This discretization relies on the possibilty of building coarser meshes using bigger control volumes and then eliminate the leading term error by a Richardson Extrapolation.

However, this formulation cannot be extended to unstructured meshes due to the impossibility of building these coarser meshes. In this work, preliminary results in constructing high-order operators are presented. This new formulation does not require to build coarser meshes (directly) using bigger control volumes, but it is based on a Richardson extrapolation with a pseudo-control volume constructed with the collocated velocities. Alternatively, other methodologies such as compact schemes (see De Angelis et al (2018) and Hokpunna (2010) for staggered grids), could be considered.

Fig. 1 shows a typical collocated arrengements, where all the variables are located at the cell center. Considering that the cell center is the point (x_i, y_i) and that the mesh size is h, we define, for Cartesian meshes:

- Control volume:
  $[x_i - h/2, x_i + h/2] \times [y_i - h/2, y_i + h/2]$
- Pseudo-control volume:
  $[x_i - h, x_i + h] \times [y_i - h, y_i + h]$

Suppose a quantity A is approximated by means of a method $A(h)$ that depends on a parameter h, and that this method has order n, that is:

$$A = A(h) + Ch^n + O(h^{n+1}). \tag{6}$$

One example of a Richardson extrapolation, such as the one used by Verstappen and Veldman (2003), is the following one:

$$R(h,t) = \frac{t^n A(h/t) - A(h)}{t^n - 1} = A + O(h^{n+1}), \tag{7}$$

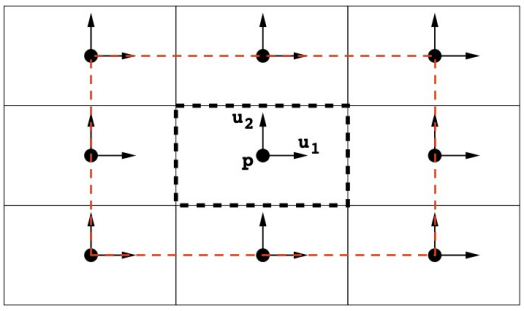

Figure 1: Collocated mesh scheme. Black dashed line shows a typical control volume. Red dashed line shows a pseudo-control volume.

where h/t is a new step size that depends on the previous step size h. It is remarkable that $R(h,t)$, has a higher order error estimation. In the work by Verstappen and Veldman (2003) a parameter of $t = 3$ was selected due to the nature of the staggered grid configuration.

In this work, a parameter of $t = 2$ will be selected in order to be able to eliminate the leading term error of the divergence operator by means of linearly combining the divergence of a control volume and the divergence of the associated pseudo-control volume. A notation relating continuous and discrete differential operators will be used for the sake of simplicity. What is meant by this notation, present for example in Eq.(8), is that the local error of the discretized operator, when applied to a discrete field, is of order $O(h^n)$. The left hand side of the equation shows the continuous operator, the first term of the right hand side shows the discrete operator, and the last term is the order of the local error. Doing that, the Richardson Extrapolation becomes:

$$\nabla\cdot = \frac{4\Omega^{-1}\mathbf{M} - \tilde{\Omega}^{-1}\tilde{\mathbf{M}}}{3} + O(h^4), \tag{8}$$

where Ω and $\mathbf{M}$ are the volume matrix and the discrete divergence operator, respectively, and $\tilde{\Omega}$ and $\tilde{\mathbf{M}}$ are the volume matrix of the pseudo-control volumes and the discrete divergence computed at the pseudo-control volumes, respectively. This relation can also be proven using the fact that, for Cartesian meshes, and assuming a mid-point integration rule for approximating the integrals:

$$\nabla\cdot = \Omega^{-1}\mathbf{M} + O(h^2), \tag{9}$$

$$\nabla\cdot = \tilde{\Omega}^{-1}\tilde{\mathbf{M}} + 4O(h^2). \tag{10}$$

One easy way to obtain Eq. (10) from Eq. (9) is realizing that the jump in step size from the control volume to the pseudo-control volume in this case is $h \to 2h$. Now, combining (4Eq.(9)-Eq.(10))/3, the leading term error is eliminated. The fact that the order of the error is reduced to 4 and not to 3 is because some symmetries present in Cartesian meshes, and can be proved by means of the mid-point integration rule

applied to the discretized divergence theorem. These symmetries are the same that cancel out the first order error term in Eq.(9) for Cartesian meshes. They are not found in triangular grids, for example, whose discrete divergence has order 1.

In order to illustrate this idea, the divergence of a test function ($u = (Acos(ax + 1)sin(by + 2), Bsin(ax + 3)cos(by + 4))$ was computed for a Cartesian grid of constant mesh size h. Fig. 2 shows the error of the discrete divergence **M** computed in a control volume as a function of h. Order 2 is found for Eq.(9) and order 4 is found for Eq.(10). In this example, it is assumed that the discrete velocity is known at cell-centers and at the faces.

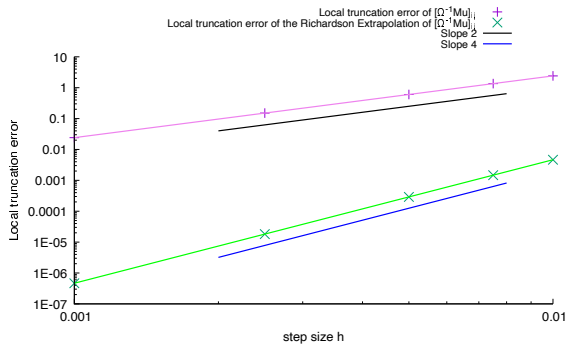

Figure 2: Local truncation error of the discrete divergence **M** operator. Order 2 is found for the discrete divergence and order 4 is found for the Richardson Extrapolation.

Collocated arrangement

In Fig. 2, it is shown that the order of the error of the Richardson Extrapolation is 4. However, this is only true if we assume that the velocities at the cell-center and at the faces are known. Unfortunately, this is not the case for collocated arrangements. The velocities at the cell-center are known, but the face velocity needs to be interpolated. Testing the same procedure with a Cartesian mesh of constant step size h leads to the result shown in Fig. 3.

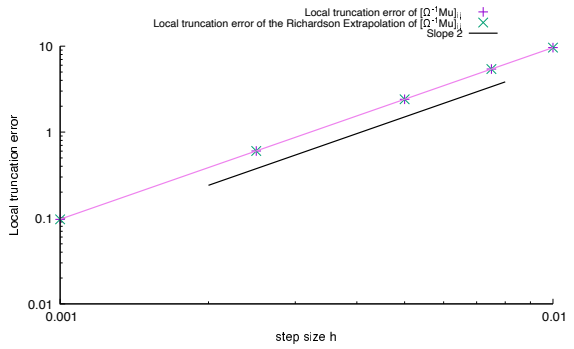

Figure 3: Local truncation error of the discrete divergence **M** operator. Order 2 is found for the discrete divergence and order 4 is found for the Richardson Extrapolation.

Now, order 2 is also found for the Richardson Extrapolation. This feature comes from the fact that the interpolation used for computing the velocity at the faces is second order. Thus, the previous Richardson Extrapolation is not able to eliminate the second order error. Possible solutions are:

- Using a fourth order interpolation to interpolate from cells to faces.
- Taking into account that for the first pseudo-control volume, we also know the velocities at the vertex, so we can apply Trapezoidal's rule instead of the mid-point rule.
- Using a second pseudo-control volume of mesh size $4h$ and combining the solutions to eliminate the leading term error.

The first option was the chosen one in Verstappen and Veldman (2003) for staggered grids and would work the same for collocated configurations. The second option was not able to provide better accuracy. So, let us explore the third option, which can exploit some features of the collocated arrangement.

Double Richardson Extrapolation for the Divergence operator

Let us assume the divergence of a collocated quantity, for example the velocity, wants to be calculated at a control volume located at $[x_i - h/2, x_i + h/2] \times [y_i - h/2, y_i + h/2]$. Let us consider the following pseudo-control volumes:

- Pseudo-control volume 1:
  $[x_i - h, x_i + h] \times [y_i - h, y_i + h]$
- Pseudo-control volume 2:
  $[x_i - 2h, x_i + 2h] \times [y_i - 2h, y_i + 2h]$

This pseudo-control volumes have already the velocity at the faces, so doing the same procedure like in Eq.(8) the leading term error can be eliminated. Fig. 4 shows the results for the double Richardson Extrapolation:

Again, order 4 is recovered for the double Richardson Extrapolation, while order 2 is found for the discrete divergence computed with a second order interpolation at the faces of the control volume. It is remarkable that no direct interpolation was needed to obtain order 4, so this procedure does not require to compute interpolations due to the natural arrangement of a collocated grid.

Convective operator

Let us assume a scalar quantity f is convected through a velocity field $\mathbf{U} = [u, v]$. The (discrete) convective operator applied to the discretized (collocated) field in divergence form f_c reads:

$$\mathbf{C}_c(\mathbf{u}_s) f_c = \mathbf{M} U_f \Pi_{c \to s} f_c, \tag{11}$$

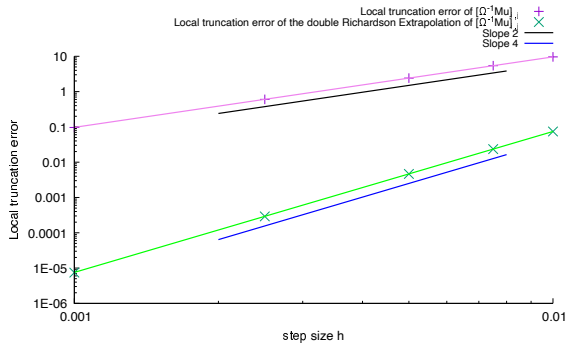

Figure 4: Local truncation error of the discrete divergence $\mathbf{M}$ operator. Order 2 is found for the discrete divergence and order 4 is found for the double Richardson Extrapolation.

where $\mathbf{u}_s$ is the staggered velocity, U_f is a diagonal matrix containing the staggered velocities, and $\Pi_{c\to s} f_c$ is the interpolation from cells to faces of the convected quantity. Typically, $\Pi_{c\to s}$ is selected to be a mid-point interpolation, in order to retain the skew-symmetry at the discrete level.

Now, let us define the double Richardson Extrapolation divergence matrix as $\mathbf{M}_{2R}$. Observe that now, when computing the convection of a cell-centered quantity f_c:

$$\tilde{\mathbf{C}}_c(u_s) f_c = \mathbf{M}_{2R} U_f f_f, \tag{12}$$

where now an interpolation is not needed anymore because the quantities are at the faces of the pseudo-control volumes.

Continuing with the previous numerical example, Fig. 5 shows the order of convergence of the collocated convective operator:

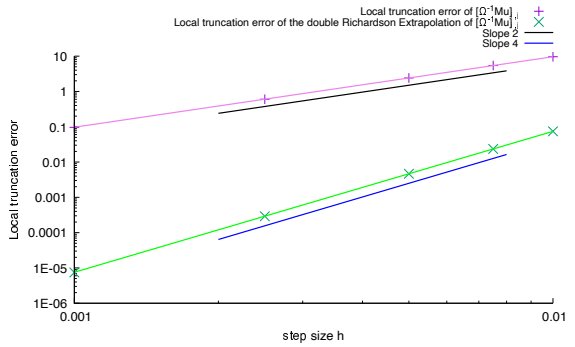

Figure 5: Local truncation error of the discrete collocated convective operator $\mathbf{C}_c(\mathbf{u}_s)$. Order 2 is found for the typical discretization and order 4 is found for the double Richardson Extrapolation.

Algebraic representation of the Double Richardson Extrapolation

In general, for collocated arrangements, the discrete divergence matrix can be written as:

$$\mathbf{M} = T_{s\to c} A_f, \tag{13}$$

where $T_{s\to c} \in \mathbb{R}^{m\times n}$ is the incidence matrix from faces to cells, m is the number of faces and n the number of cells, and A_f is a diagonal matrix containing face areas. Then, this matrix is multiplied by a vector containing face-quantities in order to obtain an approximation of the divergence of this field.

However, taking into account, for example, Eq.(12), our new discrete divergence operator is acting in a pseudo-control volume space. The face-quantities of this pseudo-grid are cell-centered quantities in our collocated grid. So, it seems more convenient to rewrite our operators in terms of collocated quantities, because no interpolations are needed in this new formulation. Let us write the Double Richardson Extrapolation divergence matrix as:

$$\mathbf{M}_{2R} = T_{\bar{c}\to c} A_c, \tag{14}$$

where $T_{\bar{c}\to c} \in \mathbb{R}^{n\times m\cdot n}$ is an incidence matrix from cells to cells and $A_c \in \mathbb{R}^{m\cdot n\times m\cdot n}$ is a diagonal matrix containing weighted-face areas. This divergence will be applied to a vector space of dimension $m \cdot n$, containing the collocated vectorial quantities.

In order to illustrate the construction of this matrix, let us consider Fig. 6. For simplicity, only two directions will be shown. The other directions are analogous.

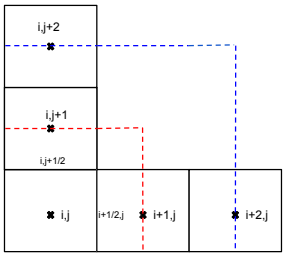

Figure 6: Collocated mesh scheme. Red dashed line shows the first pseudo-control volume and blue dashed line shows the second pseudo-control volume.

For this example, the number of control volumes is 5: $(i,j), (i+1,j), (i+2,j), (i,j+1), (i,j+2)$; and the number of faces is 2: $(i+1/2,j)$ and $(i,j+1/2)$.

$$A_c = \begin{bmatrix} \vec{A}_{f1} & & & & & & \\ & 2\vec{A}_{f1} & & & & & \\ & & 4\vec{A}_{f1} & & & & \\ & & & \vec{A}_{f2} & & & \\ & & & & 2\vec{A}_{f2} & & \\ & & & & & 4\vec{A}_{f2} & \\ & & & & & & \ldots \end{bmatrix},$$

where each area is multiplied by the normal vector to that face. Then, this matrix will be multiplied by the cell-center vectorial quantity, for example the velocity:

$$u_c = \begin{bmatrix} \vec{u_{i,j}} \\ \vec{u_{i+1,j}} \\ \vec{u_{i+2,j}} \\ \vec{u_{i,j}} \\ \vec{u_{i,j+1}} \\ \vec{u_{i,j+2}} \\ ... \end{bmatrix}$$

At this point, matrix $T_{\bar{c}\to c}$ should do the sumation over the faces of the pseudo-control volumes with the appropriate weights:

$$T_{\bar{c}\to c} = \begin{bmatrix} 0 & \frac{4}{3} & -\frac{1}{3} & 0 & \frac{4}{3} & -\frac{1}{3} & ... \\ & & & ... & & & \end{bmatrix}$$

Note that $\mathbf{M}_{2R} = T_{\bar{c}\to c} A_c$ gives Eq.(8) for the two pseudo-control volumes (the dividing volumes can be included in A_c matrix).

It is remarkable that this matrix construction can be done for non-regular structured and unstructured meshes. The extension to non-regular structured meshes is straightforward. The extension to unstructured meshes can be done by means of the following algorithm:

- Select a control volume (i, j) and one of its faces f.
- Select the corresponding neighbour of (i, j) regarding f, $neigh(i, j, f)$ as first pseudo-volume quantity.
- For the second pseudo-volume quantity, compute the maximum of $n_f \cdot n_{neigh(i,j,f)}$, where n_f is the normal face vector of f and $n_{neigh(i,j,f)}$. Select the neighbour of this face as the second pseudo-volume quantity.

Doing that, the formulation collapses to the proposed for the regular Cartesian grid, which is fourth order. No work has been done in this direction, so nothing can be say about the order of convergence for non-regular structured and unstructured grids. However, this algorithm is a good starting point in order to implement the procedure in general purpose codes.

Gradient and Laplacian operator

In order to extend the formulation to the Navier-Stokes equations, the gradient operator and the Laplacian operator are needed. To do so, and in order to preserve the underlying symmetries of the differential operators, the gradient operator is defined as:

$$\mathbf{G}_{2R} = -\tilde{\Omega}^{-1} \mathbf{M}_{2R}^T, \tag{15}$$

where $\tilde{\Omega} = (4\Omega_2 - \Omega_3)/3$, following the suggestion of Vertsappen and Veldman (2003), being Ω_2 and Ω_3 the diagonal matrices containing the pseudo-control volumes. However, more work has to be done in order to coordinate the dimensions of $\mathbf{M}_{2R}$ and $\mathbf{G}_{2R}$, to construct the gradient in order to be part of $\mathbb{R}^{n\times n}$.

From this point, the construction of the Laplacian operator would be:

$$\mathbf{L}_{2R} = \mathbf{G}_{2R}\mathbf{M}_{2R}. \tag{16}$$

4 Conclusions

An energy-preserving unconditionally stable fractional step method was presented in this work. From that point, an extension to a high-order formulation has been proposed. Even though this extension has not been achieved for the complete Navier-Stokes equations, a fourth order divergence and convective operator has been suggested. Theoretical derivation has been done for this operators, and numerical examples have been provided in order to test the order of convergence. Finally, an algebraic representation has been purposed, along with a general algorithm to compute the discrete divergence matrix for general meshes.

The extension to Navier-Stokes equations relies on the possibility of computing a proper symmetry-preserving gradient. More work need to be done in this direction. Once the gradient is computed, the Laplacian operator is straightforward.

Acknowledgments

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References

Santos, D., Muela J., Valle, N., Trias, F.X. (2021), On the Interpolation Problem for the Poisson Equation on Collocated Meshes, *14th WCCM-ECCOMAS Congress* (postponed to January 2021 due to COVID19 pandemic).

Santos, D., Trias, F.X., Colomer, G., Pérez-Sergarra, C.D. (2022), An energy-preserving unconditionally stable fractional step method on collocated grids, *8th European Congress on Computational Methods in Applied Sciences and Engineering, ECCOMAS 2022*, Oslo.

Trias, F.X., Lehmkuhl, O., Oliva, A., Pérez-Segarra, C.D., and Verstappen, R.W.C.P. (2014), Symmetry-preserving discretization of Navier-Stokes equations on collocated unstructured meshes, *Journal of Computational Physics*, 258:246–267.

Komen, E., Hopman, J.A., Frederix, E.M.A., Trias, F.X., and Verstappen, R.W.C.P. (2021), A symmetry-preserving second-order time-accurate PISO-based method, *Computers & Fluids*, 225:104979.

Verstappen, R.W.C.P., Veldman, A.E.P. (2003), Symmetry-preserving discretization of turbulent flow, *Journal of Computational Physics*, 187(1), 343-368.

De Angelis, E.M, Coppola, G., Capuano, F., De Luca, L. (2018), Derivation of New Staggered Compact Schemes

with Application to Navier-Stokes Equations, *Applied sciences (Basel)*, 29 Juny 2018, vol. 8, núm. 7, p. 1-24.

Hokpunna, A., Manhart, M. (2010), Compact fourth-order finite volume method for numerical solutions of Navier–Stokes equations on staggered grids, *Journal of Computational Physics*, Volume 229, Issue 20, pp. 7545-7570