An energy-preserving unconditionally stable fractional step method for DNS/LES on collocated unstructured grids

D. Santos, F.X. Trias, G. Colomer, and A. Oliva

1 Introduction

A finite-volume discretization over unstructured meshes is the most used formulation to solve Navier-Stokes equations by many general purpose CFD packages codes such as OpenFOAM or ANSYS-Fluent. These codes work with collocated stencil formulations, that is, once the equations are discretized, an algorithm goes cell by cell computing the required quantities.

On the other hand, algebraic formulations maintain the discrete equations in matrix-vector form, and compute the required quantities by using matrices and vectors. A collocated fully-conservative algebraic symmetry-preserving formulation of incompressible Navier-Stokes equations was proposed by Trias et. al. [1]. 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 staggered 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

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the face-to-cell discrete divergence operator. The velocity correction after applying the Fractional Step Method (FSM) to the Navier-Stokes equations reads:

$$\mathbf{u}_c^{n+1} = \mathbf{u}_c^p - \Gamma_{s\rightarrow c}\mathbf{G}p^{n+1}, \tag{4}$$

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

All the operators needed to formulate the equations can be constructed using only five discrete ones: 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, $\Pi_{c\rightarrow s}$ and the cell-to-face divergence operator, $\mathbf{M}$. For more details of these operators and its construction see [1]. Due to its simplicity, these operators can be easily builded in existing codes, such as OpenFOAM [2]. However, as it was shown in [3], this code introduces a large amount of numerical dissipation. In our opinion, this is not an appropiate approach for DNS and LES simulations since this artificial dissipation interferes with the subtle balance between convective transport and physical dissipation. Hence, reliable numerical methods for DNS/LES must be free of numerical dissipation (or, at least, have a small amount), and unconditionally stable, i.e. simulations must be stable regardless of the mesh quality and resolution.

2 An energy-preserving unconditionally stable FSM

2.1 Conservation of energy

Left-multiplying eq. (1) by $\mathbf{u}_c^T$ and summing the result with its transpose we obtain the global discrete kinetic energy equation:

$$\begin{aligned}\frac{d}{dt}||\mathbf{u}_c||^2 = &-\mathbf{u}_c^T(\mathbf{C}(\mathbf{u}_s)+\mathbf{C}(\mathbf{u}_s)^T)\mathbf{u}_c - \mathbf{u}_c^T(\mathbf{D}+\mathbf{D}^T)\mathbf{u}_c \\ &- \mathbf{u}_c^T\Omega\mathbf{G}_c p_c - p_c^T\mathbf{G}_c^T\Omega\mathbf{u}_c. \end{aligned}\tag{5}$$

Respecting the symmetries of these differential operators is crutial in order to respect the physical structure of the equations. In absence of diffusion, that is $\mathbf{D} = \mathbf{0}$, energy must be preserved. This will happen, if and only if, the convective operator is skew-symmetric and $\mathbf{G} = -\Omega_s^{-1}\mathbf{M}^T$ [1]. These two conditions are also mimicking the symmetries of the continuous level operators [4]. So, we do not only have physical arguments to do so, but also mathematical ones. In fact, mathematical arguments (continuous symmetry-preserving), directly imply discrete symmetry-preserving and automatically conservation of energy, but the converse is not true.

The turbulence phenomenon arises from a balance between convective transport and diffusive dissipation. These two physical processes are described (in its discrete form) by $\mathbf{C}(\mathbf{u}_s)$ and $\mathbf{D}$, respectively. At continuous level, the convective operator is skew-symmetric, and the diffusive operator is symmetric and negative-definite. If we retain these properties at the discrete level (namely $\mathbf{C}(\mathbf{u}_s)$ being a skew-symmetric matrix, $\mathbf{D}$ being a symmetric negative-definite matrix and $\mathbf{G} = -\Omega_s^{-1}\mathbf{M}^T$), the discrete convective operator is going to transport energy from resolved scales of motion to others without dissipating energy, as one should expect.

2.2 Stability of the pressure gradient interpolation

Due to the fact that the pressure gradient is computed at the faces and we need to interpolate it back to the cells in order to correct our (collocated) velocity (see eq. 4), this interpolation can lead us to some instability issues (see eq. 5). This problem was studied in [5], thus showing the utility of an algebraic formulation. In that work, the matrix-vector formulation is used in order to study the stability of the solution in terms of the pressure gradient interpolation. 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 so-called collocated wide-stencil Laplacian operator), and the cell-to-face interpolation that leads to an unconditionally stable FSM turned out to be the volume weighted:

$$\Pi_{c\to s} = \Delta_s^{-1}\Delta_{sc}^T \in \mathbb{R}^{m\times n}, \tag{6}$$

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 [5].

3 Test case: turbulent channel flow at $Re_\tau = 395$

In this section, the robustness and the accuracy of the method is tested in a channel flow at $Re_\tau = 395$, using different meshes. The domain chosen to carry out the simulations is the same as in Moser et. al. [7]: $2\pi x 2 x\pi$. All the meshes had a y^+ around 1. Other interpolations used in our work are the midpoint interpolation ($\frac{1}{2}$ interpolation coefficients) and the linear interpolation.

3.1 Accuracy of the interpolator in high quality meshes

The mesh shown in Figure 1 was chosen to test the accuracy. It is stretched towards y-direction. Figures 2 and 3 show the normalised mean velocity (in wall units) and the $< u'v' >$ component of the Reynolds stress tensor. We compare the results obtained against the DNS data obtained by Moser et. al.[7]. The results are very similar for the three interpolators. We expected this because for regular Cartesian meshes all three interpolators collapse to the same one (midpoint), and if the stretching is very soft, the mesh is almost regular and Cartesian (locally).

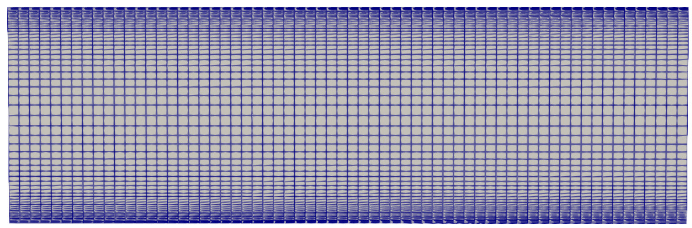

Fig. 1 64x64x64 mesh used to test our method with different interpolators.

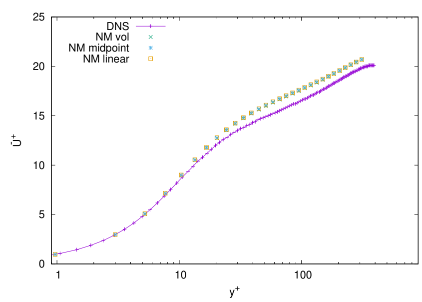

Fig. 2 Normalised mean velocity profile in wall units for channel flow at $Re_\tau = 395$.

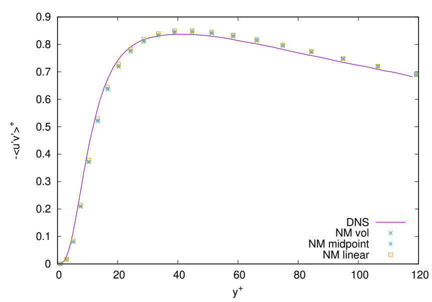

Fig. 3 Normalised turbulent shear stress profile $- < u'v' >$ in wall units at $Re_\tau = 395$.

3.2 Robustness in distorted meshes

Figure 4 shows the mesh chosen to test the robustness of the method. It is stretched towards the beginning and the end, while having very long control volumes in the center. As expected with this kind of meshes, the results are not even qualitatively good (turbulence is not even triggered, the control volumes in the center filter any kind of eddy), but the only one that converges to a solution is the volume weighted, while the others were unstable.

Figure 5 shows a less distorted mesh, that could be used in daily simulations. Even for this (not so bad) mesh, the linear interpolation is not able to trigger turbulence. For the midpoint and the volume weighted interpolations, the results are very

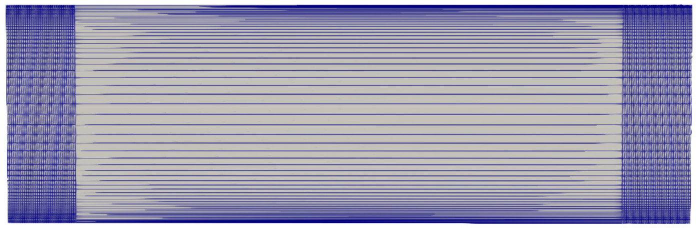

Fig. 4 Highly distorted mesh used to test the robustness of the method. Maximum aspect ratio is 250.

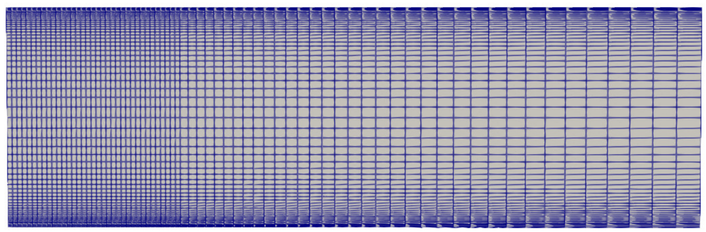

Fig. 5 Mesh which starts growing the control volumes at 1/3 of total length. Maximum aspect ratio is 5.

similar, as shown in Figures 6 and 7 (results obtained with linear interpolation are so inaccurate that are not shown here):

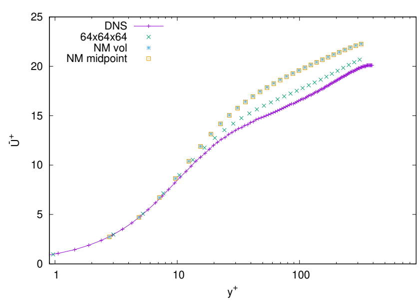

Fig. 6 Normalised mean velocity profile in wall units for channel flow at $Re_\tau = 395$.

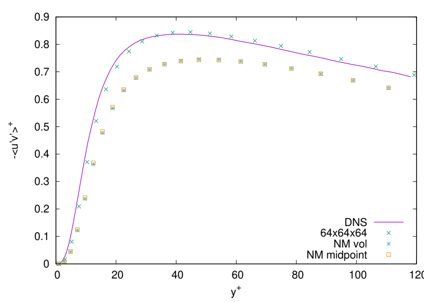

Fig. 7 Normalised turbulent shear stress profile $- < u'v' >$ in wall units at $Re_\tau = 395$.

As expected, results are worse than those obtained with a regular Cartesian mesh, but they are still reasonable. What can be surprising is that the midpoint and the volume weighted interpolators seem to give the same results, while the linear interpolation, although it is converging, gives very bad results. A possible explanation of this fact, taking into account also the results of section 3.2, is that while we start stretching the mesh, the results are similar, until some point where the linear interpolation starts failing, but the other two still give similar results. Then, under more stretching, the midpoint fails while the volume weighted is unconditionally stable.

4 Conclusions and future work

An energy-preserving unconditionally stable fractional step method on collocated grids has been presented. Three interpolators have been tested for the pressure gradient: volume weighted, linear and midpoint. All three seem to have the same accuracy in high quality meshes. When distorting the mesh, the first one that loses accuracy and eventually blows up is the linear. The midpoint seems to be more stable than the linear, but it is still blowing up in highly distorted meshes, and the volume weighted is unconditionally stable.

Future and ongoing work related to our method would be to test the accuracy of the solution when varying progressively the distortion of the mesh, and to test it on unstructured meshes. Furthermore, it would be also interesting to test the preservation of energy using different interpolators.

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