WORKSHOP
Direct and Large-Eddy Simulation 13
October 26th-29th 2022, Udine, Italy

AN ENERGY-PRESERVING UNCONDITIONALLY STABLE FRACTIONAL STEP METHOD FOR DNS/LES ON COLLOCATED UNSTRUCTURED GRIDS

D. Santos, F.X. Trias, G. Colomer, A. Oliva
[1] Heat and Mass Transfer Technological Center (CTTC)
Technical University of Catalonia, C/Colom 11, 08222 Terrassa (Barcelona), Spain
daniel.santos.serrano@upc.edu
francesc.xavier.trias@upc.edu
guillem.colomer@upc.edu
asensio.oliva@upc.edu

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 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 equations in matrix-vector form, and compute the required 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. in [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 the face-to-cell discrete divergence operator. The velocity correction after applying the Fractional Step Method (FSM) to the Navier-Stokes equations reads:

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

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.

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, $\Pi_{c\to s}$ and the cell-to-face divergence operator, $\mathbf{M}$. For more details of these operators and its construction, the reader is referred to [1]. Due to its simplicity, these operators can be easily builded in existing codes, such as OpenFOAM [2].

The most popular open-source code used to solve Navier-Stokes equations with LES modelization is OpenFOAM due to its stability and robustness. 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 an small amount), and, of course, unconditionally stable, i.e. simulations must be stable regardless of the mesh quality and resolution.

AN ENERGY-PRESERVING UNCONDITIONALLY STABLE FSM

From our point of view, respecting the symmetries of these differential operators is crutial in order to respect the physical structure of the equations. For example, constructing $\mathbf{G} = -\Omega_s\mathbf{M}^T$ is essential to preserve kinetic energy [1], but it is also mimicking the symmetries of the continuos level operators. So, we do not only have physical arguments to do so, but also mathematical ones.

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 $\mathbf{G} = -\Omega_s\mathbf{M}^T$), the discrete convective operator is going to transport energy from resolved scales of motion to others without dissipating energy, as one should expect.

The utility of an algebraic formulation can be found, as an example, in [4]. 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 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 [4].

With the construction of a reduced set of (algebraic) kernels, these matrix operators can be constructed, along with basic operations like matrix-vector product, and we can solve the equations numerically using proper solvers.

PRELIMINARY RESULTS

In order to check the stability of the method, some tests have been carried out with very coarse and very bad quality meshes. Figures 1 and 2 show an example of an air-filled ($Pr = 0.71$) differentially heated cavity with aspect ratio 2 at Rayleigh number (based on the cavity height) of 10^6, respecting the symmetries of the operators and using (5) to interpolate the pressure gradient:

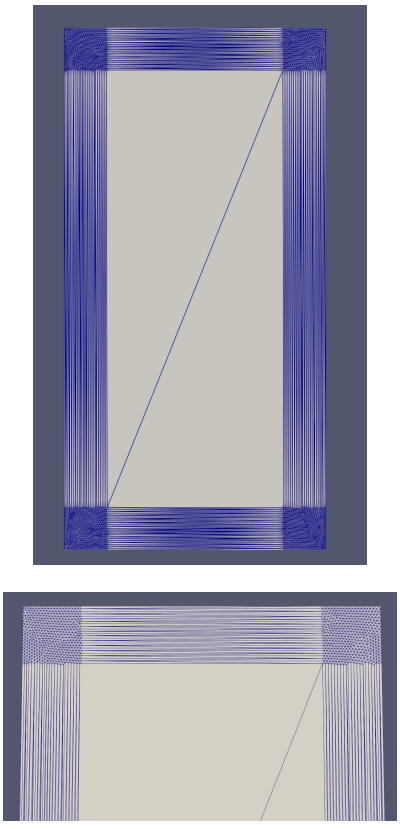

Figure 1: (Top) Test mesh used to check the stability of the method. (Bottom) Zoom at the top part of the mesh.

As you can see in Fig. 2, the method is stable, giving us results and not blowing up the simulation. As we can expect with such a bad quality mesh, the accuracy is not going to be very high. It is worth to mention that trying other interpolations for the pressure gradient, such as using $\frac{1}{2}$ weights will blow up the simulation from the very beginning.

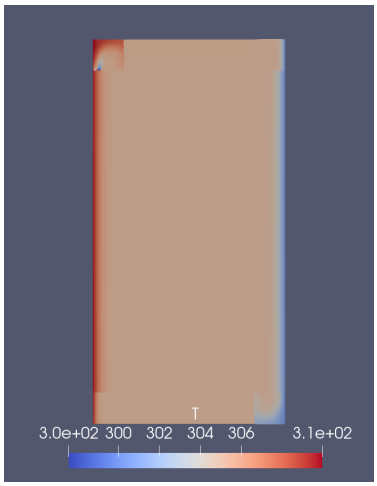

Figure 2: Temperature distribution obtained for $Ra = 10^6$.

CONCLUSIONS AND FUTURE WORK

Respecting the symmetries of the differential operators at the discrete level is essential to retain invariances from the continuos level and preserve kinetic energy. Furthermore, the interpolation of the pressure gradient from faces to cells should be done with the correct interpolator (5) to obtain stable solutions. The aim of this work is to solve Navier-Stokes equations (1,2), from an algebraic point of view, while preserving the symmetries of the differential operators [1] and interpolating in the proper way the pressure gradient [4]. To do so, we plan to study a set of DNS/LES cases (Rayleigh-Bénard convection, Channel Flow...). The accuracy and the preservation of energy due to the introduction of this new interpolation will be tested. All the simulations will be carried out on a new CFD code based on the fully-portable algebra-based HPC^2 framework [5].

REFERENCES

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

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

[3]Komen, E.M.J, Camilo, L.H., Shams, A., Geurts, B.J., Koren, B.: *A quantification method for numerical dissipation in quasi-DNS and under-resolved DNS, and effects of numerical dissipation in quasi-DNS and under-resolved DNS of turbulent channel flows. Journal of Computational Physics, 345:565-595*, (2017).

[4]Santos, D., Muela J., Valle, N., Trias, F.X.: On the Interpolation Problem for the Poisson Equation on Collocated Meshes. *14th WCCM-ECCOMAS Congress 2020, DOI: 10.23967/wccm-eccomas.2020.257*, July 2020 (postponed to January 2021 due to COVID19 pandemic)

[5]Álvarez, X., Gorobets, A., Trias, F.X.: *A hierarchical parallel implementation for heterogeneous computing. Application to algebra-based CFD simulations on hybrid supercomputers. Computers & Fluids, 214:104768*, (2021).