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PAVING THE (RIGHT) WAY FOR DNS AND LES ON UNSTRUCTURED GRIDS: (FULLY) CONSERVATIVE COLLOCATED/STAGGERED DISCRETIZATIONS

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Abstract. The essence of turbulence are the smallest scales of motion. They result from a subtle balance between convective transport and diffusive dissipation. Mathematically, these terms are governed by two differential operators differing in symmetry: the convective operator is skew-symmetric whereas the diffusive is symmetric and positive-definite. On the other hand, accuracy and stability need to be reconciled for simulations of turbulent flows in complex geometries. With this in mind, a fully-conservative discretization method for general unstructured grids was proposed in Ref. [1]: it exactly preserves the symmetries of the underlying differential operators on collocated grids. Hence, unlike other formulations, the discrete convective operator transports energy from a resolved scale of motion to other resolved scales without dissipating energy, as it should do from a physical point-of-view. Therefore, we think that apart from being a right approach for large-scale DNSs of turbulence, it also forms a solid basis for testing subgrid scale LES models. In this work, we will explore the possibility to build up staggered formulations based on the set of discrete operators defined for collocated meshes.

1 Introduction

We consider the simulation of turbulent, incompressible flows of Newtonian fluids. Under these assumptions, the dimensionless governing equations in primitive variables read

$$\partial_t \boldsymbol{u} + (\boldsymbol{u} \cdot \nabla)\boldsymbol{u} = \nu \nabla^2 \boldsymbol{u} - \nabla p, \qquad \nabla \cdot \boldsymbol{u} = 0, \tag{1}$$

where $\boldsymbol{u}$ is the velocity field, p is the kinematic pressure and ν is the kinematic viscosity. The basic physical properties of the Navier-Stokes (NS) equations (1) can be deduced from the symmetries of the differential operators. In a discrete sense, it suffices to retain such operator symmetries to preserve the analogous (invariant) properties of the continuous equations [2]. However, for unstructured meshes, it is still a common argument that accuracy should take precedence over the properties of the operators. Contrary to this, our philosophy is that operator symmetries are critical to the dynamics of turbulence

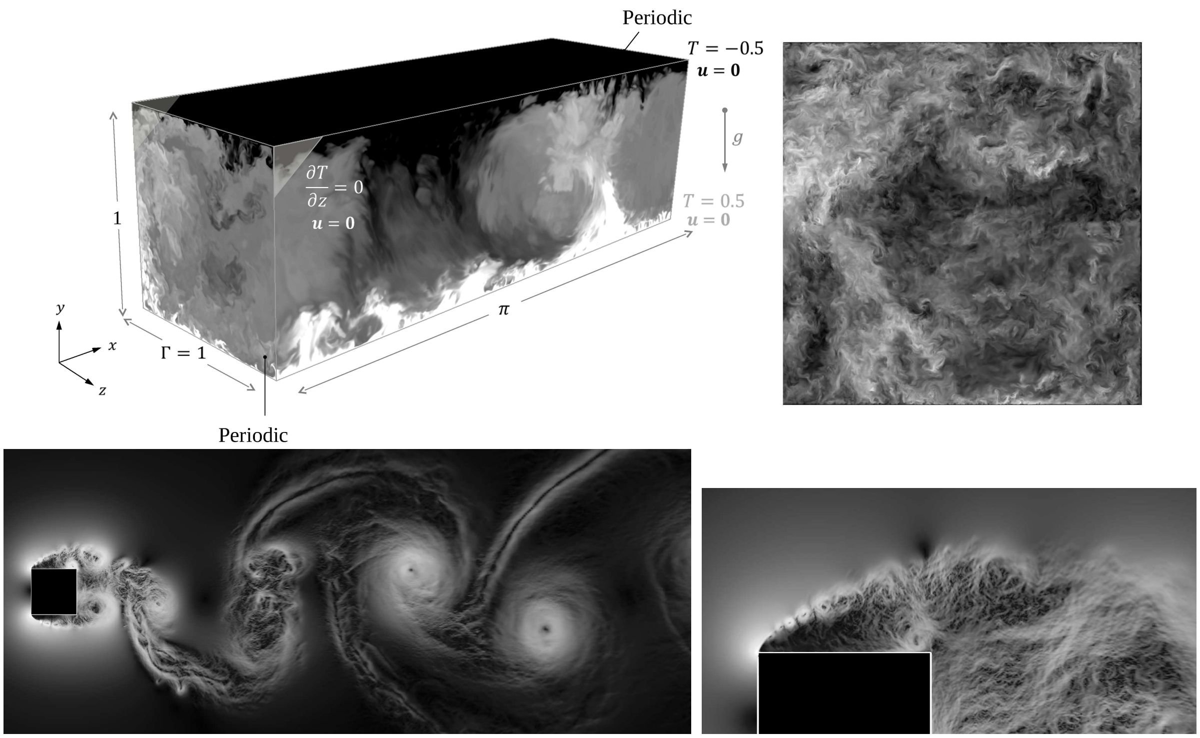

Figure 1: Examples of DNSs computed using symmetry-preserving discretizations. Top: air-filled ($Pr = 0.7$) Rayleigh-Bénard configuration studied in Ref. [3]. Instantaneous temperature field at $Ra = 10^{10}$ (left) and instantaneous velocity magnitude at $Ra = 10^{11}$ (right) for a span-wise cross section are shown. The later was computed on 8192 CPU cores of the MareNostrum 4 supercomputer on a mesh of 5.7 billion grid points. Bottom: DNS of the turbulent flow around a square cylinder at $Re = 22000$ computed on 784 CPU cores of the MareNostrum 3 supercomputer on a mesh of 323 million grid points [4] .

and must be preserved [1, 2]. Namely, the convective operator is represented by a skew-symmetric coefficient matrix and the diffusive operator by a symmetric, positive-definite matrix. These ideas are briefly revised in the next section. Then, their extension to unstructured meshes is discussed in the last section.

2 Starting point: staggered Cartesian meshes

The fully conservative discretization of the incompressible NS equations (1) is briefly described in this section. Otherwise stated, we follow the same operator-based notation than in [2]. The symmetry properties of the underlying differential operators are preserved: the convective operator is represented by a skew-symmetric matrix and the diffusive operator by a symmetric positive-definite matrix. In short, the temporal evolution of the spatially discrete staggered velocity vector, $\boldsymbol{u}_s \in \mathbb{R}^m$, is governed by the following operator-based finite-volume discretization of Eqs.(1)

$$\Omega_s \frac{d\boldsymbol{u}_s}{dt} + \mathsf{C}\left(\boldsymbol{u}_s\right)\boldsymbol{u}_s + \mathsf{D}\boldsymbol{u}_s - \mathsf{M}^T\boldsymbol{p}_c = \boldsymbol{0}_s, \qquad \mathsf{M}\boldsymbol{u}_s = \boldsymbol{0}_c, \tag{2}$$

where $\boldsymbol{p}_c \in \mathbb{R}^n$ is the cell-centered pressure scalar field. The dimension of these vectors, n and m, are the number of control volumes and faces on the computational domain, respectively. The sub-indices c and s refer to whether the variables are cell-centered or staggered at the faces. The diffusive matrix, $\mathsf{D} \in \mathbb{R}^{m\times m}$ represents the integral of the diffusive flux $-(\mu/\rho)\nabla \boldsymbol{u}\cdot\boldsymbol{n}$ through the faces. Like the underlying differential operator, $\nabla^2 = \nabla\cdot\nabla$, the diffusive operator consists of the product of a divergence matrix, $\mathsf{M}_s \in \mathbb{R}^{m\times m}$, and a gradient matrix. The divergence is discretized and the discrete gradient becomes the transpose of the discrete divergence (multiplied by a diagonal scaling). This construction leads to a symmetric, positive-definite, approximation of the diffusive operator given by $\mathsf{D} = \nu \mathsf{M}_s \Omega_v^{-1} \mathsf{M}_s^T$, where $\Omega_v \in \mathbb{R}^{m\times m}$ is a diagonal matrix containing the sizes of the control volumes associated with the faces of the velocity control volumes. The previous equation corresponds to Eq.(37) in [2]. For further details about the discretization of the diffusive operator the reader is referred to this work. The matrix $\mathsf{M} \in \mathbb{R}^{n\times m}$ is the face-to-center discrete divergence operator whereas the integral of the gradient operator is given by the transpose of M. The diagonal matrix, $\Omega_s \in \mathbb{R}^{m\times m}$, describes the sizes of the staggered control volumes and the approximate convective flux is discretized as in [2]. The resulting convective matrix, $\mathsf{C}(\boldsymbol{u}_s) \in \mathbb{R}^{m\times m}$, is skew-symmetric, *i.e.*

$$\mathsf{C}(\boldsymbol{u}_s) + \mathsf{C}^T(\boldsymbol{u}_s) = \mathsf{0}. \tag{3}$$

In a discrete setting, the skew-symmetry of $\mathsf{C}(\boldsymbol{u}_s)$ implies that

$$\mathsf{C}(\boldsymbol{u}_s)\,\boldsymbol{v}_s \cdot \boldsymbol{w}_s = \boldsymbol{v}_s \cdot \mathsf{C}^T(\boldsymbol{u}_s)\,\boldsymbol{w}_s = -\boldsymbol{v}_s \cdot \mathsf{C}(\boldsymbol{u}_s)\,\boldsymbol{w}_s, \tag{4}$$

for any discrete velocity vectors $\boldsymbol{u}_s$ (if $\mathsf{M}\boldsymbol{u}_s = \boldsymbol{0}_c$), $\boldsymbol{v}_s$ and $\boldsymbol{w}_s$. Then, the evolution of the discrete energy, $\|\boldsymbol{u}_s\|^2 = \boldsymbol{u}_s \cdot \Omega_s \boldsymbol{u}_s$, is governed by

$$\frac{d}{dt}\|\boldsymbol{u}_s\|^2 = -\boldsymbol{u}_s \cdot \left(\mathsf{D} + \mathsf{D}^T\right)\boldsymbol{u}_s < 0, \tag{5}$$

where the convective and pressure gradient contributions cancel because of Eq.(3) and the incompressibility constraint, $\mathsf{M}\boldsymbol{u}_s = \boldsymbol{0}_c$, respectively. Therefore, even for coarse grids, the energy of the resolved scales of motion is convected in a stable manner, *i.e.* the discrete convective operator transports energy from a resolved scale of motion to other resolved scales without dissipating any energy, as it should be from a physical point-of-view. It is noteworthy to mention that in the last decade, many DNS reference results have been successfully generated using this type of discretization (see Figure 1, for example).

3 Unstructured meshes. Collocated or staggered?

Accuracy and stability need to be reconciled for numerical simulations of turbulent flows around complex configurations. With this in mind, a fully-conservative discretization method for general unstructured grids was proposed in Ref. [1]: it exactly preserves the symmetries of the underlying differential operators on a collocated mesh. In summary, and following the same notation than in Ref. [1], the method is based on a set of five basic operators: the cell-centered and staggered control volumes (diagonal matrices), Ω_c and Ω_s, the matrix containing the face normal vectors, N_s, the cell-to-face scalar field interpolation, $\Pi_{c \rightarrow s}$ and the cell-to-face divergence operator, M. Once these operators are constructed, the rest follows straightforwardly from them. Therefore, the proposed method constitutes a robust and easy-to-implement approach to solve incompressible turbulent flows in complex configurations that can be easily implemented in already existing codes such as OpenFOAM® [5]. However, any pressure-correction method on collocated grids suffer from the same drawbacks: the cell-centered velocity field is not exactly incompressible and some artificial dissipation is inevitable introduced. Conversely, the projection of a staggered velocity onto a divergence-free space is a well-posed problem: it can be uniquely decomposed into a solenoidal vector and the gradient of a scalar (pressure) field. This can be easily done without introducing any dissipation as it should be from a physical point-of-view. In this work, we will explore the possibility to build up staggered formulations based on the above mentioned reduced set of discrete operators. Hence, the proposed method constitutes a robust and easy-to-implement approach to solve incompressible turbulent flows in complex configurations. Moreover, we also consider that the symmetry-preserving discretization method presented here forms an excellent starting point for LES. Namely, the energy of the resolved scales of motion is convected in a stable manner: that is, the discrete convective operator transports energy from a resolved scale of motion to other resolved scales without dissipating any energy, as it should do from a physical point-of-view.

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