The LS-STAG immersed boundary/cut-cell method for non-Newtonian flows in quasi-3D geometries

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Résumé :

*La méthode LS-STAG est une méthode de type frontières immergées/*cut-cell *pour les écoulements visqueux incompressibles, basée sur la méthode MAC sur grilles cartésiennes décalées, telle que la frontière irrégulière du domaine est représente par sa fonction level-set. La version 2D de la méthode LS-STAG est maintenant bien éprouvée, et cette présentation portera sur son extension aux géométries 3D avec symétrie de translation dans la troisième direction (appelées par la suite géométries quasi-3D). La discrétisation dans les 3 types de* cut-cells *d'un maillage quasi-3D sont obtenues en suivant les principes de la discrétisation energy-conserving de Cheny & Botella (*J. Comput. Phys. *Vol. 229, 1043-1076, 2010). Nous présenterons des applications de la méthode à l'écoulement de fluides non-Newtoniens dans une conduite circulaire à expansion brusque, pour laquelle des expériences ont été réalisées dans notre équipe. Finalement, les performances du code LS-STAG dans un environnement de calcul intensif seront discutées.*

Abstract :

The LS-STAG method is an immersed boundary/cut-cell method for viscous incompressible flows based on the staggered MAC arrangement for Cartesian grids, where the irregular boundary is sharply represented by its level-set function. The 2D version of the LS-STAG method is now well-established, and this talk presents its extension to 3D geometries with translational symmetry in the z direction (subsequently called quasi-3D *configurations), which can be viewed as an intermediate step before fully 3D geometries, where both numerical and HPC implementation issues are tackled at this stage of development. The discretization in the 3 basic types of quasi-3D cut-cells is performed by following the principles of the energy-conserving discretization of Cheny & Botella (*J. Comput. Phys. *Vol. 229, 1043-1076, 2010). We will present applications on the flow of non-Newtonian fluids in a circular duct with sudden expansion, for which experimental results performed in our team are available. Finally, the performance of the LS-STAG code on high-performance parallel computers will be discussed.*

Keywords : Computational fluid dynamics, Immersed boundary method, Cut-cell method, Incompressible flows, non-Newtonian fluids, 3D geometries, High performance computing

Advanced computational fluid dynamics (CFD) applications concern flows in highly irregular three-dimensional geometries, whose process of grid generation, from the early stage of CAD design to final volume meshing, is very time-consuming and requires highly trained users. Typical unstructured body-conformal meshes are made of elements (cells of heaxaedral, tetraedral shape, ...) with irregular connectivity, which makes the solution algorithms extremely memory and CPU intensive. Moreover, it is difficult to assess the quality of the grid (smooth, undistorted cells properly clustered at the wall, ...), which may negatively impact the convergence and accuracy of the numerical solution.

In contrast, cut-cell/immersed boundary CFD codes (see [1] for a review) are based on Cartesian methods which are extremely robust and optimized, and thus requires only a fraction of the computer resources of an unstructured code. Cartesian grid generation is greatly simplified compared to the body-conformal approach, and the grid regularity and quality is not significantly impacted by the complexity of the geometry. Moreover, the computation of flows with moving boundaries can be performed on fixed grids, without the domain remeshing which is required by body-conformal methods.

The major difficulty of traditional IB methods is the treatment of the cut-cells (cells of irregular shape which are formed by the intersection of the Cartesian mesh with the immersed boundary). Classical IB methods such as the *momentum forcing method* [1] discard the discretization of flow equations in the cut-cells, and use special interpolations instead. Thus, strict conservation of mass is not observed, which leads to non-divergence free velocities or non-physical presssure oscillations in the vicinity of the immersed boundary [2, 3]. On the other hand, cut-cell methods aim for discretizing the flow equations in cut-cells by *ad hoc* treatments, whose major drawback is the loss of the 5-points structure (in 2D) of Cartesian methods. Moreover, these methods rely on cell-merging techniques for which 3D extension is known to be nontrivial [1]. Therefore, the development of an accurate and cost-effective 3D solver based upon the IB/cut-cell approach is still a challenging task.

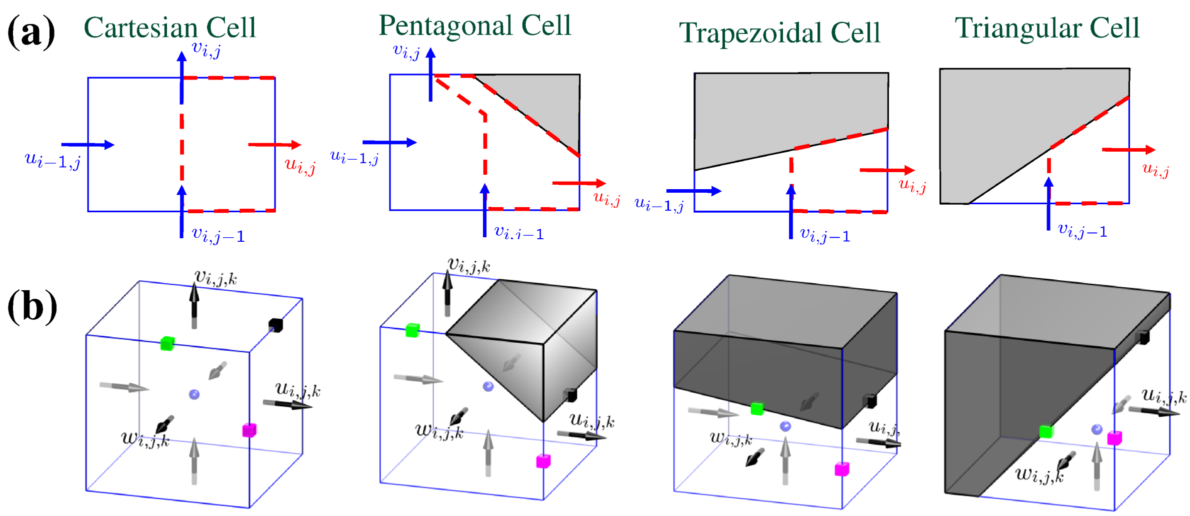

FIGURE 1 – Cartesian cell and 3 basic types of cut-cells present in the LS-STAG mesh in 2D (a) and quasi-3D (b). For the quasi-3D mesh, the velocities are discretized at cell faces, pressure and normal stresses at cell center (•), shear stresses at edge centers : $\frac{\partial u}{\partial y}$, $\frac{\partial v}{\partial x}$ (■), $\frac{\partial u}{\partial z}$, $\frac{\partial w}{\partial x}$ (■) and $\frac{\partial v}{\partial z}$, $\frac{\partial w}{\partial y}$ (■).

In Refs. [4, 5] we have developed an innovative cut-cell discretization for 2D incompressible flows called "LS-STAG" (*Level-Set, STAGgered*), which is based on the classical MAC method for Cartesian staggered grids, where the irregular boundary is sharply represented by its level-set function. In the three basic types of 2D cut-cells (pentagonal, trapezoidal and triangular, see Fig. 1(a)), the discretization is designed such as the global invariants of the flow (total mass, momentum and kinetic energy) are preserved at the discrete level. The LS-STAG discretization in the cut-cells is consistent with the MAC discretization used in Cartesian fluid cells, and has the ability to preserve the 5-point Cartesian structure of the stencil, resulting in a highly computationally efficient method. We have successfully applied the LS-STAG method to Newtonian flows at moderate Reynolds number in fixed and moving geometries [5], pseudoplastic flows [6], and viscoelastic flows [7, 8]. In addition, we mention that the LS-STAG discretization has also been implemented in the ship hydrodynamics software COMFLOW [9] for the handling of irregular geometries, and has been extended to the computation of coupled aeroelastic problems [10] and turbulent flows with RANS modelling [11].

The purpose of this communication is to present a progress report towards a fully 3D LS-STAG code, totally optimized for high-performance computing. One of the major difficulty in cut-cell discretization for 3D geometries is the large number of cases to consider : we have enumerated 16 different cut-cells in 3D whereas there are only 3 in 2D, see Fig. 1(a)). In order to mitigate this issue, we first consider building the LS-STAG discretization for 3D configurations with translational symmetry in the z direction (subsequently called *quasi-3D* configurations), where are only present the 4 types of cells depicted in Fig. 1(b). This intermediate step towards the fully 3D implementation can be applied to a wide variety of canonical flows (Taylor-Couette flow, flow past cylinder of arbitrary cross section shape, abrupt planar/axisymmetric contraction flow, ...) and is regarded as the keystone for the full 3D solver, since both numerical and HPC implementation issues are tackled at this stage of development. In quasi-3D geometries, only extruded 2D cut-cells are present, which enables us to easily extend the principles of the energy-conserving discretization of Ref. [5] to the cut-cells of Fig. 1(b) : the discretization of the continuity equation, pressure gradient, convective fluxes, normal stresses are straightforward extensions of the 2D LS-STAG formulas. The discretization of shear stresses terms such as $\partial w/\partial x$ and $\partial w/\partial y$, which were absent from the 2D case, needs further attention. These terms are tentatively discretized with the formula proposed by van der Heiden *et al.* [9]. Preliminary computations of the quasi-3D LS-STAG method for benchmark confined cylinder flows were presented in Ref. [12].

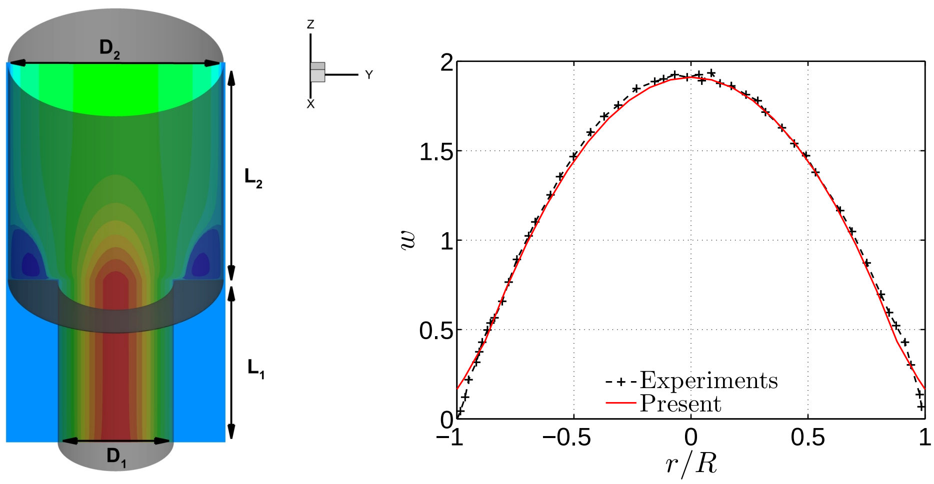

FIGURE 2 – At left : flow in a cylinder duct with sudden expansion at $Re = 273$. At right : axial velocity profile at $z/D_1 = -0.9$ obtained with the LS-STAG method and comparison with the experimental results of [13].

In this talk, we will present the extension of the quasi-3D LS-STAG method to the computation of pseudoplastic flows, where the stress tensor takes the form $\boldsymbol{\tau} = \eta(\dot{\gamma})\boldsymbol{D}$ and the viscosity η is modelled by popular non-Newtonian laws such as the power-law or Cross models. The crucial part for taking into account shear-thinning or shear-thickening effects is the accurate computation of the shear rate $\dot{\gamma} = \sqrt{\frac{1}{2}\boldsymbol{D} : \boldsymbol{D}}$ in the vicinity of the immersed boundary, since the velocity gradients appear at different locations inside a cut-cell (see Fig. 1(b)). To perform this, we had to adapt to the 3D staggering the special interpolations developed in [6] for 2D pseudoplatic flows. The accuracy of the discretization will be evaluated on Poiseuille pipe flow, and we will present preliminary results on the flow of xanthan fluids in a circular duct with sudden expansion (see Fig. 2), for which MRI [1] velocity measurements performed in our group [13] are available.

Finally, we will discuss the HPC optimization of the LS-STAG code, which is made necessary by the the large computational resources required by 3D computations. The principal issue in the optimization of a Cartesian code for incompressible flows is the parallelisation of the iterative solution of linear systems, most notably the Poisson pressure equation. For that purpose, the LS-STAG quasi-3D code has been developed in an MPI parallel environment on the HPC cluster of the *Université de Lorraine*, and the linear systems are solved with the multigrid and Krylov solvers of the Hypre library [14]. The parallel implementation will be discussed and results on its scalability properties will be presented.

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