Massively Parallel Large-Eddy Simulations of Primary Atomization on Adaptive Unstructured Meshes. Interface capturing algorithm and multiscale coupling perspectives

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Abstract This work presents a robust and efficient procedure to simulate turbulent incompressible interfacial liquid-gas flows on massively-distributed dynamically-adapted unstructured meshes in complex geometries. The present strategy extends the Accurate Conservative Level Set (ACLS) / Ghost-Fluid interface-capturing framework of Desjardins et al. (2008) and Chiodi et al. (2017) to unstructured grids, and combines it with an isotropic Adaptive Mesh Refinement (AMR) technique for triangular and tetrahedral meshes. The computational cost of the ACLS method is reduced by using a narrow-band to compute level set variables only in a restricted region around the liquid-gas interface. In the ACLS method, the interface is defined as the isosurface of a hyperbolic tangent function, which is transported by the fluid, and then reshaped using a reinitialization equation. Several forms of this reinitialization exist: the original form proposed by Desjardins et al. involves numerical estimation of the hyperbolic tangent gradient, which is susceptible to induce spurious deformation of the interface, especially on unstructured meshes. Chiodi et al. proposed a new form, which much better preserves the interface shape. The implementation of this new equation on unstructured grids is not straightforward and thus requires special attention. In this work, a robust implementation of this new form for unstructured meshes is proposed and implemented in the YALES2 low-Mach flow solver. In order to compute interface normals and curvature, the signed-distance function is reconstructed in parallel at nodes in the narrow band using the second-order Geometric-Projection Marker Method (GPMM) of Janodet et al. (2019). Spatial convergence and physical meaning of the overall procedure are demonstrated through classical interface transport tests and canonical two-phase flow simulations, respectively. Then, to point out the large computational gain using dynamic mesh refinement, two Large-Eddy Simulations (LES) of atomizing liquid jets are presented, namely a water jet in quiescent air from a low-pressure compound nozzle and a high-pressure kerosene jet in air crossflow. Both simulations are validated against experiments, demonstrating the potential of the overall procedure to accurately and efficiently handle primary atomization with large-density ratios using unstructured grids. Eventually, the ongoing developments and perspectives of a multiscale coupling of the Eulerian interface-capturing ACLS/AMR technique with a Lagrangian Point-Particle (LPP) modeling of the small droplets are discussed.

Keywords Multiphase flows · Atomization · Unstructured grids · Incompressible flow LES · Conservative Level Set · Adaptive Mesh Refinement · Multiscale modeling

1 Introduction

Multiphase flows are ubiquitous in nature and in industrial systems, and understanding the formation of sprays is crucial for designing complex injection technologies. More specifically, turbulent primary atomization is of first importance in aeronautical combustors, into which fuel is injected

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in liquid form, goes under atomization, evaporation, turbulent mixing and eventually combustion. All these physical processes are strongly dependent, and thus improving numerical predictions of pollutant formation requires deep numerical insights into atomization. This process designates the evolution of large liquid structures into small droplets and thus governs the liquid droplet distribution in the combustor and the subsequent evaporation. Realistic industrial injector geometries for atomization simulations are very complex, including sharp edges and narrow corners, which hinders the meshing task with cartesian grids: the use of unstructured meshes is thus well suited for this type of simulations. The atomization process involves a wide range of time and space scales, which leads to important calculation costs. Thus, the use of dynamic mesh adaptation for unstructured meshes is particularly helpful for simulating industrial liquid-gas flow problems, as it allows implicit interface dynamics calculation in complex geometries at a reasonable cost. To capture the interface on unstructured grids, the Accurate Conservative Level Set (ACLS) method is used, which accurately predicts the interface dynamics while conserving liquid mass. This work presents a massively parallel algorithm for complex turbulent spray simulations on unstructured grids. A narrow band around the liquid-gas interface is built to compute interface features only in the area of interest, allowing significant computational savings. The various parts of the procedure implemented in the YALES2 unstructured low-Mach number code are first presented, whose accuracy and computational performance are assessed on classical interface transport test cases. Then, the break-up of a turbulent liquid jet from a triple-disk injector and of a liquid jet in cross-flow are shown at various resolutions, demonstrating the accessibility to jet instabilities with 3D unstructured meshes. The results are validated against experiments performed in the same conditions. Eventually, the perspectives of coupling the present Eulerian method with a Lagrangian Point-Particle model to treat the small droplets are discussed.

2 Algorithms

2.1 Accurate Conservative Level Set framework

In the Accurate Conservative Level Set (ACLS) framework [1], the liquid-gas interface Γ is represented using a hyperbolic tangent profile: $\psi(\mathbf{x},t) = \frac{1}{2}\left(\tanh\left(\frac{\phi(\mathbf{x},t)}{2\varepsilon}\right)+1\right)$ where the parameter ε sets the thickness of the profile, and $\phi(\mathbf{x},t) = \pm|\mathbf{x}(t) - \mathbf{x}_\Gamma(t)|$ is the signed-distance function. Using ψ, the interface is located at the iso-level 1/2: $\Gamma(t) = \{\mathbf{x} \in \mathbb{R}^3 | \, \psi(\mathbf{x},t) = 1/2\}$. Assuming the flow velocity field $\mathbf{u}$ is divergence free, the scalar ψ is advected by the fluid and then reshaped using the reformulated reinitialization equation of [2]:

$$\frac{\partial \psi}{\partial \tau} = \boldsymbol{\nabla} \cdot \left(\frac{1}{4\cosh^2\left(\phi_{\text{map}}/2\varepsilon\right)} \left(|\boldsymbol{\nabla}\phi_{\text{map}} \cdot \mathbf{n}| - 1\right) \mathbf{n} \right) \tag{1}$$

where τ is a pseudo-time, $\mathbf{n}$ is the interface normal $\mathbf{n} = \boldsymbol{\nabla}\phi/|\boldsymbol{\nabla}\phi|$, and $\phi_{\text{map}} = \varepsilon \ln\left(\psi/(1-\psi)\right)$ is an analytical signed-distance function, mapped for $\psi \in]0;1[$. The signed-distance function ϕ is reconstructed at nodes in the narrow band around the interface using a Geometric-Projection Marker Method (GPMM), firstly introduced in [3], to estimate the smallest distance to the interface. The mean curvature κ is computed directly from ϕ using Goldman's formula [4].

2.2 Isotropic dynamic mesh adaptation strategy

To resolve the small physical scales at the interface on tetrahedral grids at a moderate cost, an isotropic Adaptive Mesh Refinement (AMR) technique is used [5], employing the MMG library [6]. Special attention is needed when coupling AMR with ACLS to avoid liquid mass loss, so that the interface never encounters cell-size gradients. Thus, the mesh is refined around the interface based on the distance $\mathcal{D} = |\phi|$ to it, so that Γ always stays in a protected region of constant cell size Δx_{min} (Fig. 1). This metric evolution ensures that the remeshing process always occurs upwind and downwind of the interface but never at the interface itself to avoid any interpolation error at the interface. The width of this region is $2N_p\Delta x_{\text{min}}$, with N_p a user-defined parameter, set between 6 and 12. Away from this area, the metric follows a linear law until it reaches the maximum cell size Δx_{init}. The adaptation process is triggered automatically when the interface approaches the edge of the protected region, leading to considerable computational savings in remeshing.

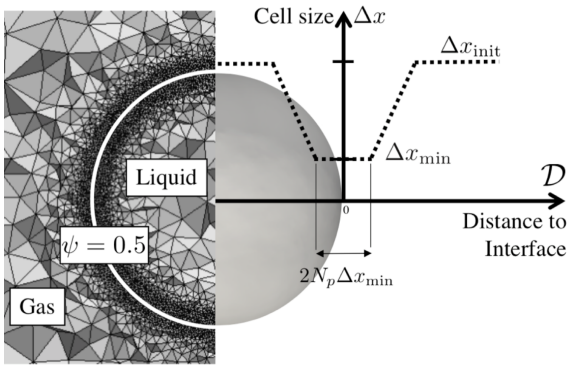

Fig. 1 Adaptive mesh refinement strategy: refinement based on the distance $\mathcal{D}$ to the interface.

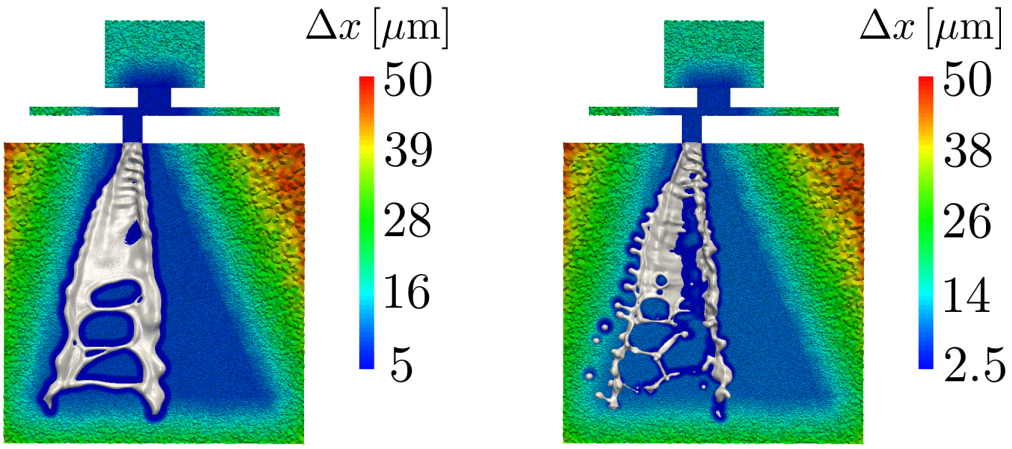

Fig. 2 Interface topology along with tetrahedral cell size distribution in the mid-plane.

3 LES of a low-pressure water jet from a compound nozzle

This study follows the experiments of [7] and the simulations of [8]. A single low-pressure compound nozzle is considered: three off-centered cylinders are superimposed from which water is injected in quiescent air at Reynolds number Re = 3653, based on the discharge orifice diameter $d_{\text{inj}} = 180\mu$m, and liquid Weber number $\text{We}_{\text{l}} = 1061$. The injector induces non-axial velocity components, and a double-vortex flow is formed. In these physical conditions, primary atomization is mainly driven by capillary effects such as ligament breakup and jet forming by bubble burst, and enhanced by liquid turbulence. As the injector geometry strongly conditions the primary breakup process, the unsteady resolution of the internal flow is important [8]. In this work, the whole flow is computed by the mean of one Large-Eddy Simulation (LES), from the internal flow to the primary atomization process. The LES turbulence model is the dynamic Smagorinsky model [9,10]. Adaptive tetrahedral meshes are used and two resolutions are investigated: $\Delta x_{\min} = 5\mu$m and $\Delta x_{\min} = 2.5\mu$m. The jet morphology and angle are studied, and compared to the ones of [8]. The jet topology in the 2.5μm case, displayed in Fig. 2 (b), is close to the one obtained by the DNS simulation at 1.44μm of [8]. Furthermore, the cost of the simulation is moderate: the same run on a static grid requires 1.62B cells, versus 141M in the present work. With the adaptive grid 915,531CPUh are used for 1ms of physical time.

4 LES of a high-pressure kerosene jet in crossflow

In order to test the capabilities of the algorithm for resolving atomization in aeronautical injection systems, a non-reactive liquid kerosene jet in crossflow (JICF) injection has been simulated. Liquid is injected through a nozzle into a plenum where a stream of air flows in the perpendicular direction to the liquid (the crossflow). Then, the jet bends towards the air direction and atomizes

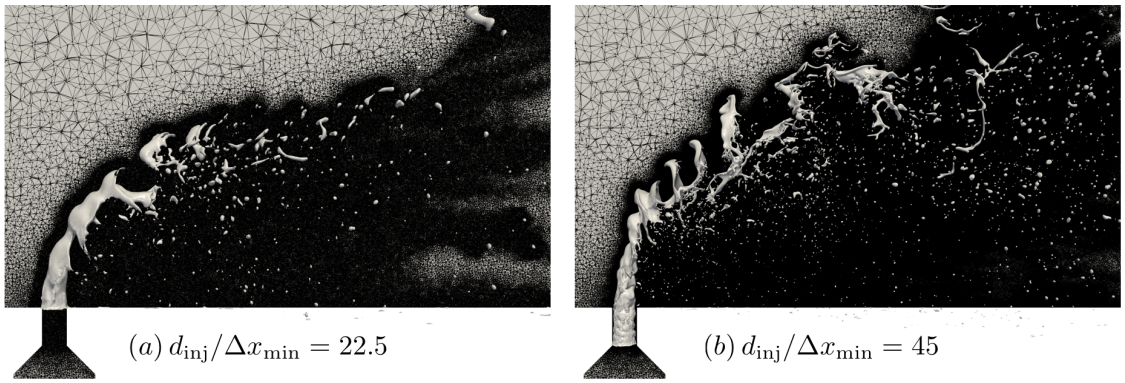

Fig. 3 Interface topology along with tetrahedral cells at time instant $t = 0.3$ms. q = 6. $\text{We}_g = 1470$.

due to the aerodynamic interaction. The chosen configuration is the experimental test-bench by Becker and Hassa [11], which consists of a kerosene JICF injected into a high-pressure environment representative of the ambient conditions found within aeronautical gas turbines. Two operating points studied experimentally by [11] are simulated. They are given by the kinetic energy ratio $\text{q} = \rho_l u_l^2 / \rho_g u_g^2$ and gaseous Weber number $\text{We}_g = \rho_g u_g^2 d_{\text{inj}} / \sigma$. In this study, q = 6 for both operating points and $\text{We}_g = 830$ or 1470. Two interface resolutions are considered for both operating points: $\Delta x_{\min} = 20\mu$m and 10μm, corresponding to $d_{\text{inj}}/\Delta x_{\min} = 22.5$ and 45 respectively. For these four LES, a dynamic Smagorinsky closure is used for modeling the unresolved turbulence scales [9,10]. The interface topology and grid for operating point $\text{We}_g = 1470$ at the two investigated resolutions can be seen in Fig. 3. The jet trajectories for both operating points are studied and are in good agreement with the experimental correlation of Becker [11].

5 Conclusion and perspectives

Adaptive mesh refinement allows significant computational savings: highly-resolved flows in complex geometries using unstructured meshes are now accessible. This is a major step forward for the computation of realistic industrial flows. In order to further increase the gain in computational cost, small and round droplets will soon be treated using a Lagrangian Point Particle (LPP) two-way model, allowing local coarsening of the mesh. This Eulerian-Lagrangian coupling would thus result in much cheaper simulations at equivalent resolutions. Eventually, this multiscale approach would pave the way to both extremely-resolved liquid jet cores using unstructured meshes and accurate droplet statistics far from the injector.

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