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A MASSIVELY PARALLEL ACCURATE CONSERVATIVE LEVEL SET ALGORITHM FOR PRIMARY ATOMIZATION ON ADAPTIVE UNSTRUCTURED GRIDS

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Abstract. Accurate and efficient simulations of 3D liquid-gas flows are of first importance in many industrial applications, such as fuel injection in aeronautical combustors. In this context, it is mandatory to handle complex geometries. The use of unstructured grids for two-phase flow modeling fulfills this requirement and paves the way to isotropic adaptive mesh refinement. This work presents a narrow-band Accurate Conservative Level-Set (ACLS)/ghost-fluid algorithm combined with dynamic mesh adaptation. This strategy enables the resolution of small physical scales at the liquid-gas interface at an affordable cost. In the accurate conservative level set framework, the interface is defined as the iso-contour of a hyperbolic tangent function, which is advected by the fluid, and then reshaped using a reinitialization equation. Several forms of this reinitialization exist: the original ACLS form proposed by Desjardins et al. involves numerical estimation of the hyperbolic tangent gradient, which is susceptible to induce artificial deformation of the interface, especially on unstructured meshes. A new form has been recently proposed by Chiodi et al., which takes advantage of the classical distance level set while much better preserving the interface shape. A robust implementation of this new form on unstructured meshes is proposed and implemented in the YALES2 incompressible flow solver. In order to compute interface normals and curvature, the classical signed-distance function is reconstructed at nodes in the narrow band around the interface using a Geometric-Projection Multiple-Marker method (GPMM), to compute the smallest distance to the interface by exact geometric projection to the closest surface elements. To show the spatial convergence and efficiency of the overall procedure, especially the significant computational gain using adaptive mesh refinement, LES simulations of water injection in air from a low-pressure compound nozzle at various resolutions are presented: the flow inside the injector is fully computed along with the atomization demonstrating the strong potential of the proposed method.

1 INTRODUCTION

The atomization process in two-phase flows 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 [1] is particularly helpful for simulating industrial liquid-gas flow problems, as it allows implicit interface dynamics calculation in complex geometries at a reasonable cost [2]. To capture the interface, the Accurate Conservative Level Set (ACLS) method is used, which accurately predicts the interface dynamics while conserving liquid mass [3]. 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 [4] are first presented, whose accuracy and computational performance are checked on classical interface transport test cases. Eventually, the break-up of a turbulent liquid jet from a triple-disk injector is shown at various resolutions, demonstrating the accessibility of a deep numerical insight of jet instabilities with 3D unstructured meshes. Results are validated against the experiment of [5].

2 ALGORITHMS

2.1 Accurate Conservative Level Set

In the ACLS framework [3], the interface Γ is represented as a specific iso-contour of an hyperbolic tangent profile $\psi(\mathbf{x}, t) = \frac{1}{2} \left(\tanh \left(\frac{\phi(\mathbf{x}, t)}{2\epsilon} \right) + 1 \right)$, where 2ϵ is the thickness of the profile, and $\phi = \pm|\mathbf{x} - \mathbf{x}_\Gamma|$ is the signed-distance function. The interface is located at $\Gamma = \{\mathbf{x} \in \mathbb{R}^3 / \psi(\mathbf{x}, t) = 0.5\}$. Assuming the flow velocity \mathbf{u} is divergence free, the scalar ψ is advected by the fluid in conservative form, and then reshaped using the reformulated reinitialization equation of [6]:

$$\frac{\partial \psi}{\partial \tau} = \nabla \cdot \left[\frac{1}{4 \cosh^2 \left(\frac{\phi_{\text{map}}}{2\epsilon} \right)} (|\nabla \phi_{\text{map}} \cdot \mathbf{n}| - |\mathbf{n}|) \mathbf{n} \right], \quad (1)$$

where τ is a pseudo-time, $\phi_{\text{map}} = \epsilon \ln(\psi/(1-\psi))$ is an analytical signed-distance function mapped for $\psi \in]0; 1[$, and $\mathbf{n} = \nabla \phi / |\nabla \phi|$ is the interface normal. More details regarding the unstructured discretization of Eq. 1 can be found in [7].

2.2 Isotropic Adaptive Mesh Refinement 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 [1]. 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). The width of this region is $2N_p \Delta x_{\text{min}}$, with N_p a

user-defined parameter, usually set between 6 and 12. Away from this area, the metric evolution follows a linear law until it reaches the maximum cell size Δx_{init} , allowing only smooth and controlled cell-size gradients in the domain. The adaptation process is triggered automatically when the interface approaches the edge of the protected region, leading to considerable computational savings in remeshing.

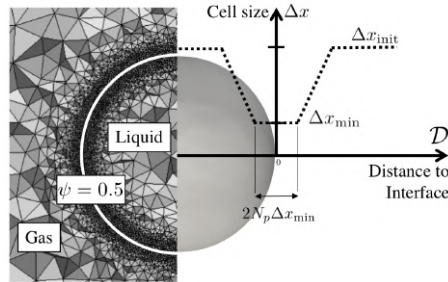


Figure 1: Adaptive mesh refinement strategy

3 LARGE-EDDY SIMULATION OF A LOW-PRESSURE COMPOUND NOZZLE

Atomization simulations of a water jet from a triple-disk injector [5, 8] in air on adaptive unstructured meshes are shown in this section. The geometry consists of three disks superimposed, with an outlet diameter of $d = 180\mu\text{m}$. The Reynolds number is $\text{Re} = 3653$ and the liquid Weber number is $\text{We}_l = 1061$. Interface contours can be seen in Fig. 2 for two mesh resolutions: $5\mu\text{m}$ and $2.5\mu\text{m}$. It is clearly observed that the jet instabilities are much more resolved in the finest case. The cell size distribution and ψ -field for the

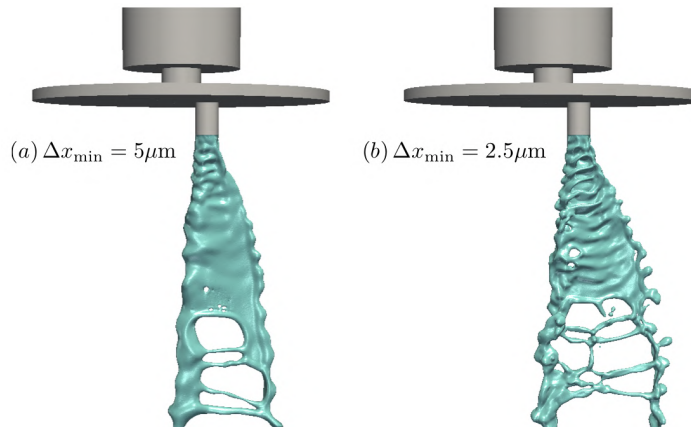


Figure 2: Interface contours for $\Delta x_{\text{min}} = 5\mu\text{m}$ (a) and $\Delta x_{\text{min}} = 2.5\mu\text{m}$ (b)

finest case $\Delta x_{\text{min}} = 2.5\mu\text{m}$ are presented in Fig. 3 (a) and (b), respectively. In order to assess the computational costs of the runs, a reduced computational time is calculated as $\text{RCT} = \text{Wall time}[\mu\text{s}]N_{\text{cores}}/N_{\text{iter}}/N_{\text{cv}}$. Results are presented in table 1 along with other simulation parameters. Previously obtained results on static meshes are also displayed for comparison. Huge computational gains in mesh size and necessary number of cores are observed between static and adaptive meshes.

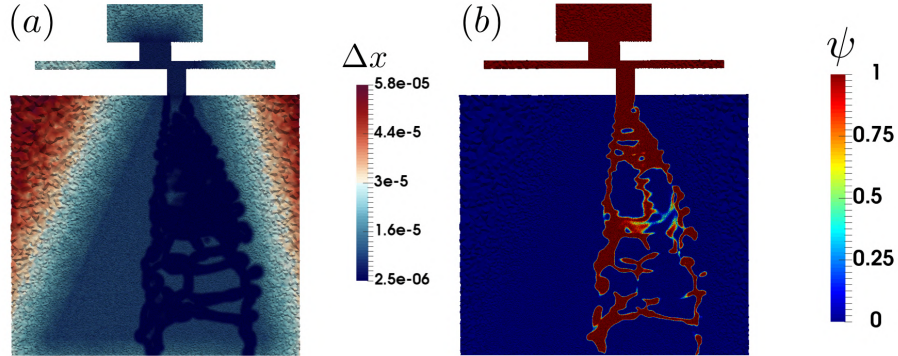


Figure 3: Cell size distribution Δx (a) and ACLS function ψ (b) for the case $\Delta x_{\min} = 2.5\mu\text{m}$

Table 1: Atomization from a triple-disk injector - Simulation parameters

| $\Delta x_{\min} [\mu\text{m}]$ | Static mesh | | Adaptive mesh | | | |
|---------------------------------|--------------------|--------------------|--------------------|--------------------|-------|---------------------------------|
| | N_{cores} | N_{cells} | N_{cores} | N_{cells} | RCT | CPU time [h]/physical time [ms] |
| 5 | 2048 | 200M | 576 | 43M | 513.4 | 55,296 |
| 2.5 | 8192 | 1.62B | 1400 | 135M | 586.1 | 840,000 |

4 CONCLUSIONS 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 could 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 even cheaper simulations.

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