Development and analysis of a Lagrange-Remap sharp interface solver for stable and accurate atomization computations

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Abstract

This work focuses on a Lagrange-Remap approach developed for free surface flows and involving two recent improvements which are presented: first, a second order un-split Coupled Level Set and Volume-of-Fluid interface capturing method designed for arbitrary grids [1], and second, a robust and conservative flow solver for incompressible Navier-Stokes equations in the presence of an liquid/gas interface [2]. The resulting approach is shown to be stable at high density ratios without any filtering or artificial viscosity, and the interface capturing scheme to be second order accurate. In addition, the method is shown to have excellent mass and momentum conservation properties on a selection of test cases.

Introduction

Propulsion engines often rely on the combustion of high energy-density liquid fuel to meet weight and volume restrictions. The efficiency of the conversion and the emission of harmful pollutants depends directly on the mixing of the fuel and oxidizer, which itself results from a cascade of mechanisms initiated by the atomization of a coherent liquid stream. Despite existing investigations on varying nozzle designs, the effects of viscosity, surface tension, turbulence, flow structure and cavitation on the atomizer performance are still poorly understood. The challenges found in experimental studies caused by the multi-scale and multi-physics aspects of such flows has promoted the development of numerical strategies to simulate the atomization process.

These techniques however also face challenges, which need to be overcome for them to have acceptable accuracy. In particular, the sensitivity of the atomization mechanism to the turbulence generated by the internal injector geometry suggests energy conserving schemes as an ideal discretization strategy. In sharp interface methods however, the zero-thickness interface assumption results in a shock, where the density may vary by orders of magnitude. In such regions, centered schemes are known to be numerically unstable. Instead of filtering or adding numerical viscosity, the presented work relies on the blending of an energy conserving discretization with a geometric Lagrangian-Eulerian solver in the interface vicinity. This novel strategy builds upon a recently developed un-split Volume-of-Fluid scheme coupled to a classical Level Set method [1], which are introduced along with standard test cases.

Since the pioneering work of Rudman [3] on incompressible solvers for high density ratio two-phase flows, momentum conservative formulations have been shown [4, 5] to be more accurate and stable than discretizations based on the non-conservative form of the Navier-Stokes equations. The presented work extends this idea to design a Ghost Fluid [6] prediction/correction algorithm which is 'almost' momentum conservative. While small (third order), the introduced momentum error is required for the convective transport term to be monotonicity preserving at the interface. This property guarantees the flow solver to remain stable, even at extreme density ratios. Away from the interface, in order to conserve kinetic energy, a centered scheme developed for staggered arrangement [7] is used.

The proposed discretizations of the convective and pressure terms are furthermore combined to a harmonic averaging of the viscosity in the interface vicinity, and a balanced force treatment of the surface tension forces. The resulting framework is shown to also give satisfactory results for viscous and capillary flows.

Various academic test cases are then used to illustrate the accuracy and robustness of the proposed framework, and the applicability to more realistic cases is discussed.

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Interface Capturing

The numerical representation of two immiscible fluids requires appropriate treatment of their respective thermodynamic properties (density ρ, viscosity μ and surface tension σ). In interface capturing methods, this is done by advecting a marker function φ with the fluid velocity,

$$\frac{\partial \varphi}{\partial t} + \mathbf{u} \cdot \nabla \varphi = 0. \tag{1}$$

The two most widespread interface capturing schemes, namely the Level Set and the Volume-of-Fluid methods, consist in transporting a distance and indicator function respectively. While Level Set methods [8] are known to provide excellent geometric accuracy, they perform poorly when it comes to mass conservation. Volume-of-Fluid [9] methods on the other hand perform inversely. Hence, the method used in this work [1] combines a classical high-order Level Set method with a fully unstructured and second order Volume-of-Fluid transport.

The main challenge in Volume-of-Fluid methods is the explicit representation of the interface front required to limit numerical diffusion. The use of Strang dimensional splitting however lead to the development of a variety of split Volume-of-Fluid method of reasonable complexities. For realistic problems such as the primary atomization of a jet, the splitting has been known to enhance numerical breakup of under-resolved structures (Flotsam/Jetsam). This lead to the development of the Hybrid Lagrangian-Eulerian Method (HyLEM) presented in [1].

In HyLEM, the unsplit Volume-of-Fluid transport relies on a two-step Lagrange-Remap procedure based on the weak form of transport equation 1. For any material control volume $\Omega(t)$, one can write,

$$\frac{\mathrm{d}}{\mathrm{d}t} \int_{\Omega(t)} f(\mathbf{x}, t)\, d\mathcal{V} = -\int_{\Sigma(t)} \frac{\dot{\omega}}{\rho^{\text{liq}}}\, d\mathcal{S} + \int_{\Omega(t)} f\,(\nabla \cdot \mathbf{u})\, d\mathcal{V}. \tag{2}$$

For incompressible media and in the absence of mass transfer across the interface, the velocity field is solenoidal and the evaporation rate,

$$\dot{\omega} = \rho^{\text{liq}} \left(\mathbf{u}^{\text{liq}} - \mathbf{w}\right) \cdot \mathbf{n}_{\text{I}} = \rho^{\text{gas}} \left(\mathbf{u}^{\text{gas}} - \mathbf{w}\right) \cdot \mathbf{n}_{\text{I}}, \tag{3}$$

is null. In these conditions, liquid volume fraction is therefore conserved over any material control volume.

In order to solve 2 over a computational mesh, HyLEM proceeds as follows: at time n, all cells $\mathcal{E}^n$ are transported forward in time with the flow velocity. The new cell $\mathcal{L}^{n+1}$ represents the exact same material control volume defined over cell $\mathcal{E}^n$, but at time $n+1$. From 2, the volume fraction over both cells is therefore the same. Since the control volumes $\mathcal{L}^{n+1}$ do not match the mesh cells $\mathcal{E}^{n+1}$, the information has to be transferred from one to another: this is called remapping.

A similar algorithm was also derived in [1] by following the characteristics of equation 1 backward in time, as opposed to forward in time in the previously described algorithm. In this paper, these variants will be referred to as Backward and Forward Euler respectively, and their combination (arithmetic average) as trapezoidal rule.

The advection equation effectively solved for either Backward or Forward advection by HyLEM is a discrete equivalent of,

$$\frac{\mathrm{d}}{\mathrm{d}t} \left(\frac{\int_{\Omega(t)} f(\mathbf{x}, t)\, d\mathcal{V}}{\int_{\Omega(t)} d\mathcal{V}} \right) = 0. \tag{4}$$

While equation 2 is analytically equivalent to equation 4 for incompressible flows with no phase change, they are not at the discrete level. On the one hand, a discretization starting off equation 2 leads to a conservative form of the transport equation, but which does not guarantee boundedness ($0 \leq f \leq 1$). On the other hand, a discretization based on equation 4 leads to a volume fraction field bounded at all time but which is not conserved. Although both conservation and boundedness are necessary, they are challenging to combine in a three-dimensional non-diffusive fashion. Deforming a three dimensional mesh while enforcing exact local volume conservation is indeed a tedious task.

In addition, another reason to favor the bounded form 4 over the conservative form 2 follows from the stability requirements for convective term in the momentum equation 8, as shown in the following section. From interface reconstruction to remapping step, all operations in the HyLEM method rely on a polyhedral library. By combining piecewise linear reconstruction of the interface and robust polyhedra intersection and volume computations, it was shown [1] to conserve mass exactly for linear velocity fields.

Lagrange-Remap Incompressible Flow Solver

Governing Equations

The proposed method follows the one-fluid formulation, where both liquid and gas phases are considered as a single fluid with varying thermodynamic properties. Such an approach involves specific treatment of the Rankine-Hugoniot jump conditions,

$$\begin{cases} \left[\!\left[\rho\left(\mathbf{u}-\mathbf{w}\right)\cdot\mathbf{n}_{\mathrm{I}}\right]\!\right]_{\mathrm{I}}=0, \\ \left[\!\left[p\mathbf{n}_{\mathrm{I}}-\tau\cdot\mathbf{n}_{\mathrm{I}}+\rho\mathbf{u}\left(\mathbf{u}-\mathbf{w}\right)\cdot\mathbf{n}_{\mathrm{I}}\right]\!\right]_{\mathrm{I}}=\sigma\kappa\mathbf{n}_{\mathrm{I}}, \end{cases} \tag{5}$$

where κ denotes the interface curvature, computed in the present work from a Level Set function. Early one-fluid solvers for two-phase flows were derived from the discretization of the non-conservative form of the incompressible Navier-Stokes equations,

$$\begin{cases} \rho\left[\dfrac{\partial\mathbf{u}}{\partial t}+\left(\mathbf{u}\cdot\nabla\right)\mathbf{u}\right]=-\nabla p+\nabla\cdot\tau+\rho\mathbf{b}, \\ \nabla\cdot\mathbf{u}=0. \end{cases} \tag{6}$$

where, in the absence of mass transfer across the interface, the convective term can be treated in the same fashion as in a single phase solver to predict the updated velocity $\mathbf{u}^{*}$. The pressure correction step would then typically take the form,

$$\nabla\cdot\left(\frac{1}{\rho}\nabla p\right)=\frac{\nabla\cdot\mathbf{u}^{*}}{\Delta t}. \tag{7}$$

Later on [3], the non-conservative treatment of the convective term in the momentum equation was found to be inaccurate, especially at high density ratio. Various attempts to solve the conservative form,

$$\frac{\partial\left(\rho\mathbf{u}\right)}{\partial t}+\nabla\cdot\left(\rho\mathbf{u}\otimes\mathbf{u}\right)=-\nabla p+\nabla\cdot\tau+\rho\mathbf{b}, \tag{8}$$

have since been made [4, 5], all pointing out the need for consistent treatment of this term and the transport of the indicator function f.

In addition, solving equation 8 also naturally improves the momentum conservation properties of the scheme. The hurdle, however, is that the derivation and implementation of such a scheme is not straightforward.

Proposed Methodology

Previous studies have emphasized the need for consistent discretization of the convective term in the momentum transport equation with the interface transport equation. The proposed method extends this idea by focuses on two fundamentals, discrete conservation and numerical stability.

First, the discretization of the convective term is modified to ensure monotonicity preservation while being consistent with the second order Volume-of-Fluid transport described in [1] and second, the pressure projection equation is modified to guarantee momentum conservation. These properties are achieved using the un-split advection procedure developed for HyLEM, and the key components are presented in the following section, along with the viscous and surface tension implementations.

Momentum Prediction

A conservative treatment of the convective in equation 8 is necessary for stable and accurate computations at high density ratios (10 or higher). Updating the momentum however raises the problem of rescaling to obtain the velocity field. In order not to introduce any spurious oscillations in the velocity field, this means advancing the convective terms in the marker and the momentum equations consistently.

A second order three-dimensional method for achieving this was proposed in [2]. The procedure is similar to the interface capturing method described above. The weak form of the momentum is considered over a material control volume $\Omega\left(t\right)$,

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_{\Omega(t)}\rho\mathbf{u}\,d\mathcal{V}=-\int_{\partial\Omega(t)}p\mathbf{n}\,d\mathcal{S}+\int_{\partial\Omega(t)}\tau\cdot\mathbf{n}\,d\mathcal{S}+\int_{\Omega(t)}\rho\mathbf{b}\,d\mathcal{V}, \tag{9}$$

where $\partial\Omega\left(t\right)$ denotes the boundary.

Considering only the convective term, it was shown [2] that solving,

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\int_{\Omega(t)}\rho\mathbf{u}\,d\mathcal{V}}{\int_{\Omega(t)}d\mathcal{V}}\right)=0. \tag{10}$$

guarantees momentum and velocity boundedness, and that $\forall i\in[\![1,3]\!]$ it was discretely equivalent to solving,

$$\frac{\delta\left(\rho u_i\right)}{\delta t}+\frac{\delta\left(\rho u_i v_j\right)}{\partial x_j}=\rho u_i\frac{\delta v_j}{\delta x_j}, \tag{11}$$

where $\mathbf{v}$ is an effective convective velocity resulting from the mesh deformation step.

The right-hand side of equation 11 was found to introduce a third-order conservation error of very small amplitude. It is however essential for the code stability for high density ratio computations.

Pressure Correction

The grid presented in [2] uses a staggered arrangement of the conserved variables. From the velocity predictor $\mathbf{u}^*$ and the density field defined over each of the momentum control volumes, a Ghost Fluid [6] type projection is used to enforce the divergence free condition. This requires the inversion of the following discrete linear equation,

$$\begin{cases} u_j^{n+1}=u_j^*-\dfrac{\Delta t}{\rho^{(j)}}\dfrac{\delta p}{\delta x_j}, \\ \dfrac{\delta}{\delta x_j}\left(\dfrac{1}{\rho^{(j)}}\dfrac{\delta p}{\delta x_j}\right)=(\Delta t)^{-1}\dfrac{\delta u_j^*}{\delta x_j}, \end{cases} \tag{12}$$

where $\rho^{(j)}$ is the density field defined over the u_j control volume and used for the momentum rescaling. This allows for the pressure correction step not to introduce any momentum conservation errors.

In order for the pressure jump to balance the surface tension forces, it is directly included in equation 12 [11]. This was found to dramatically reduce the spurious currents known to pollute computations of capillary flows.

Viscous Effects

The one-fluid formulation used in the proposed work assumes the velocity gradients to be continuous across the interface. This assumption, combined with a harmonic averaging of the viscosity [10], was found to lead to satisfactory results, even for viscosity dominated flows.

Analysis

The strength of the proposed work is the conservation and stability properties combined with second order interface representation. This points are presented in more details in the following sections.

Conservation Error

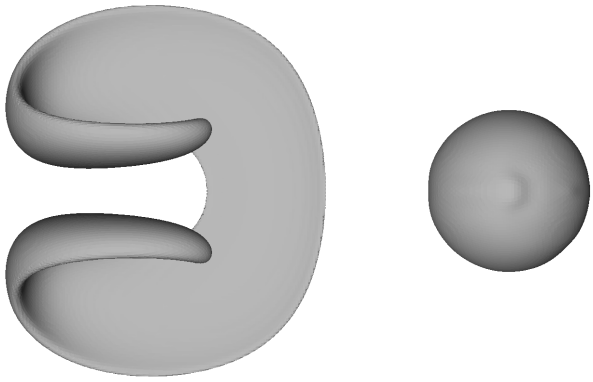
In a discrete sense, equations 4 and 10 are not conservative. They are retained however for they guarantee that the updated values (mass fraction, momentum and velocity) remain bounded. Hence, the mass and momentum error is solely due to an error term of the form,

$$f\frac{\delta v_j}{\delta x_j}\text{ and }\rho u_i\frac{\delta v_j}{\delta x_j}, \tag{13}$$

in the marker and i^{th}-momentum equations respectively. For incompressible non-vaporizing flows, the volume fraction transport equation 2 can analytically be rewritten as,

$$\underline{\Omega}\left(t\right)\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\int_{\Omega(t)}f\left(\mathbf{x},t\right)\,d\mathcal{V}}{\underline{\Omega}\left(t\right)}\right)+\frac{\int_{\Omega(t)}f\left(\mathbf{x},t\right)\,d\mathcal{V}}{\underline{\Omega}\left(t\right)}\frac{\mathrm{d}\underline{\Omega}\left(t\right)}{\mathrm{d}t}=0, \tag{14}$$

where $\underline{\Omega}\left(t\right)$ denotes the volume of $\Omega\left(t\right)$. Analytically, both time derivatives in 14 are zero. Numerically, however, HyLEM only guarantees the rate of change of cell-averaged volume fraction to be zero. The second term, which depends on the mesh deformation, is guaranteed to be zero only for linear solenoidal velocity fields [1].



(a) $t = T/2$ (b) $t = T$

Figure 1: Sphere deformation (192^3 mesh).

Using the divergence theorem, in the absence of evaporation,

$$\frac{\mathrm{d}\underline{\Omega}\,(t)}{\mathrm{d}t} = \int_{\partial\Omega(t)} \mathbf{u}\cdot\mathbf{n}\,d\mathcal{S} = \int_{\Omega(t)} \nabla\cdot\mathbf{u}\,d\mathcal{V}. \tag{15}$$

Because the effective convective velocity $\mathbf{v}$ does not necessarily match the projected velocity $\mathbf{u}$, exact mass and momentum conservation are only guaranteed for linear velocities.

The amplitude of the conservation error however, remains very low, and as shown in the example section, it is third order. The same analysis also holds for the momentum advection equation.

Stability

Provided that the projected mesh at time $n+1$ does not suffer from any singularities (overlapping cells and/or gaps between adjacent cells), it can be shown [2] that the updated volume fraction and momentum values are a convex combination of the old values in the adjacent cells. The resulting weights are only function of the geometry. Boundedness is therefore guaranteed for these two quantities.

The consistency between volume and momentum advection becomes obvious after momentum rescaling. It was indeed shown [2] that this requirement leads to the updated velocity values to also be convex combinations of the old values. As opposed to the volume fraction and momentum values, the weights were however function of both the geometry and the two fluid densities.

Results

This section focuses on results assessing the properties of the proposed framework. It includes a set of standard test case, which are generally used to validate interface transport schemes. Such a case is also used to illustrate the robustness of the momentum discretization at extremely high density ratio. Finally, in order to illustrate the capabilities of the proposed framework, preliminary results from a turbulent round jet computation are provided.

Sphere in deformation field

While numerous interface capturing methods have been developed, a lot of them are limited to two dimensions or/and very tedious to implement for three dimensional computations. This test shows the ability of the proposed framework to perform accurate three-dimensional computations in complex topologies.

An initially spherical interface is transported in a discretely solenoidal swirling field, which after a maximum stretching (as pictured on Fig. 1a) is reversed until the initial shape is restored (Fig. 1b).

As far as the conservation errors are concerned, as seen from Fig. 2, the single-step advection schemes (Backward and Forward Euler) show a third order convergence rate of the relative mass error, while two-step combination (Trapezoidal rule) systematically reduces the error by orders of magnitude.

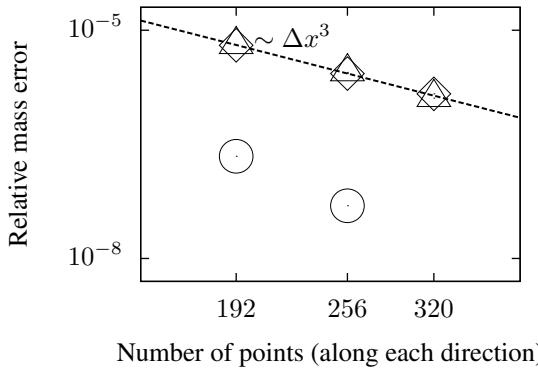


Figure 2: Relative mass error for sphere deformation test case (backward: triangles, forward: diamonds, trapedoidal: circles).

High density drop advection

In order to illustrate the impact of the proposed new solver, this test case, first proposed in [5], simulates the advection of a high density drop of diameter D in a $5D \times 5D$ periodic domain in a initially quiescent gas. In the limit of the density ratio tending to infinity, the drop should behave like a hard sphere.

For a density ratio of one billion, Fig. 3a shows the interface topology after 5% of a flow through time (FTT) using a solver based on the non-conservative form of the Navier-Stokes equations. The computation then essentially stalls, for the velocity values rapidly tend to infinity. Note that the density ratio used here is extreme, but a similar behavior is witnessed for density ratios close to those encountered in geothermal sciences (molten rocks) or other industrial applications (molten alloys, molten glass, ...).

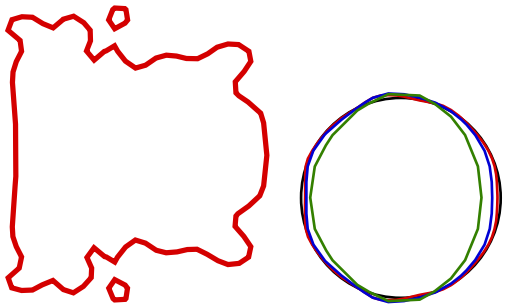


Figure 3: High density ratio (10^9) drop (32×32: green, 64×64: blue, 128×128: red): non-conservative scheme at time $t/T = 0.05$ and conservative scheme at time $t/T = 1.0$.

The momentum conservative formulation on the other hand remains stable at all time. For the coarsest mesh shown in Fig. 3b, where the drop spreads approximately 6 points, the shape is close to a sphere, and then converges to the sphere when the mesh is refined.

The absence of oscillations in the momentum conservative implementation is a direct consequence of the consistency between volume fraction and momentum advection, along with the pressure projection.

Turbulent round jet in diesel-type configuration

In order to validate the proposed method for complex interface topology, a spatially evolving round jet is computed. The objective here is not to study the underlying atomization process, but rather to provide a realistic interface topology to illustrate the applicability of the proposed framework to realistic computations.

The interface is shown at $t = 15U_{\text{bulk}}/D$ in Fig. 5, along with a cloud of droplets in a dilute region of the flow. It can be seen that three to four points are enough to resolve a droplet. In addition, a ligament is also represented, with a curvature radius locally comparable to the grid spacing.

In order to evaluate the performances of the proposed method, the configuration shown in Fig. 5 is used as

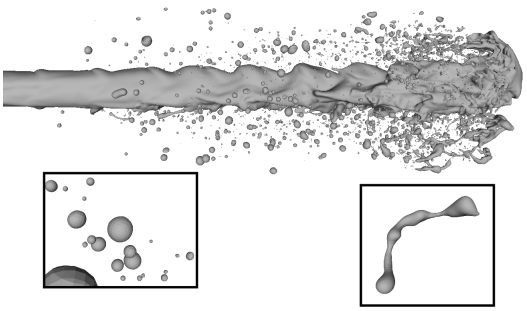


Figure 4: Interface representation.

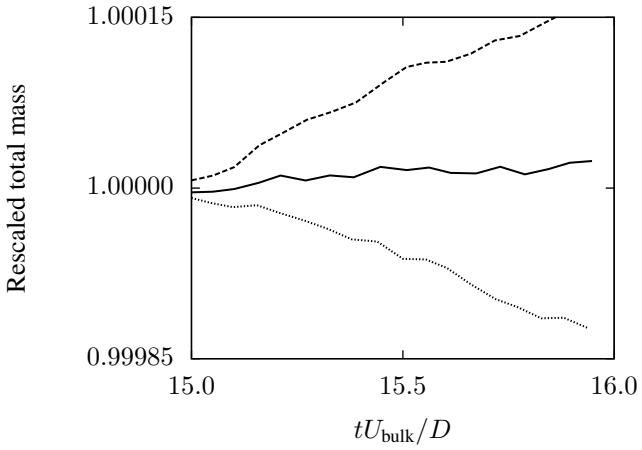


Figure 5: Relative mass error in diesel jet (backward: dashed line, forward: dotted line, trapedoidal: solid line).

initial condition, and the flow is advanced for one characteristic time scale U_{bulk}/D. The relative mass errors are shown in Fig. 6.

As expected, the errors for the Forward and Backward schemes are negatively correlated. The error levels are relatively low (of the order of 0.015%), and the combination of both is seen to reduce the mass loss by an order of magnitude (of the order of 0.002% after one characteristic time scale).

Conclusion and Future Work

In this work, a robust and accurate solver for arbitrary density ratio two-phase flows was developed, which does not require any numerical dissipation to remain stable. The proposed strategy was shown to have excellent mass and momentum conservation properties, and to accurately capture viscous and surface tension effects. The proposed framework proved in addition to be a good candidate for efficient use of high-performance computing and is therefore suited for more realistic computations.

Before such flows can be computed however, grid requirements still need to be evaluated. Future work therefore will involve grid convergence studies on semi-realistic flows involving complex topologies, before applications to primary atomization simulations of diesel jets are carried.

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