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Evaluation of methods for calculating volume fraction in Eulerian–Lagrangian multiphase flow simulations

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ABSTRACT

The present work addresses numerical methods required to compute particle volume fraction or number density. Local volume fraction of the lth particle, α_l, is the quantity of foremost importance in calculating the gas-mediated particle–particle interaction effect in multiphase flows. A general multiphase flow with a distribution of Lagrangian particles inside a fluid flow discretized on an Eulerian grid is considered. Particle volume fraction is needed both as a Lagrangian quantity associated with each particle and also as an Eulerian quantity associated with the grid cell for Eulerian–Lagrangian simulations. In Grid-Based (GB) methods the particle volume fraction is first obtained within each grid cell as an Eulerian quantity and then the local particle volume fraction associated with any Lagrangian particle can be obtained from interpolation. The second class of methods presented are Particle-Based (PB) methods, where particle volume fraction will first be obtained at each particle as a Lagrangian quantity, which then can be projected onto the Eulerian grid. Traditionally, the GB methods are used in multiphase flow, but sub-grid resolution can be obtained through use of the PB methods. By evaluating the total error, and its discretization, bias and statistical error components, the performance of the different PB methods is compared against several common GB methods of calculating volume fraction. The standard von Neumann error analysis technique has been adapted for evaluation of rate of convergence of the different methods. The discussion and error analysis presented focus on the volume fraction calculation, but the methods can be extended to obtain field representations of other Lagrangian quantities, such as particle velocity and temperature.

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1. Introduction

The Eulerian–Lagrangian point-particle approach has become an important methodology in the simulation of canonical and complex multiphase flows [1–3]. In this approach the continuous carrier phase is solved in the Eulerian frame of reference, typically using a fixed Eulerian grid, while the time evolution of the dispersed phase (can be particles, droplets or bubbles) is considered in the Lagrangian frame by tracking every individual particle's position, velocity and other properties.[1]

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[1] Henceforth the term "particles" will apply equally well to droplets and bubbles.

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There are four key components to a general Eulerian–Lagrangian point-particle simulation: 1) Fluid–fluid interaction represented by the continuous phase Navier–Stokes equation, whose solution on an Eulerian grid is the subject matter of standard CFD. 2) Fluid-to-particle forward coupling which accounts for the effect of the continuous phase on the dispersed phase. 3) Particle-to-fluid coupling which accounts for the back effect of particles on the fluid. 4) Particle–particle coupling which accounts for the interaction between the particles, either through direct collisions or as mediated by the continuous phase [4–8]. In one-way coupled simulations only the first two interactions are modeled and in two-way coupled simulations particle-to-fluid back coupling is also included. When particle–particle interactions are important, the multiphase flow problem is considered to be four-way coupled [9,10].

Fluid-to-particle coupling requires *interpolation* of the Eulerian continuous phase properties to the location of the Lagrangian particles, which in general will not coincide with the Eulerian grid points. A number of interpolation schemes, such as linear interpolation, fourth and sixth order Lagrange interpolation, and Hermite interpolation, have been proposed and their accuracies analyzed [11,12].

Particle-to-fluid coupling involves *projection* of the Lagrangian quantities, such as particle drag force and heat transfer, back to the continuous phase momentum and energy equations as source terms. This projection is from the position of the Lagrangian particles to the Eulerian grid points. Due to conservation of momentum and energy, the projection operation must satisfy partition of unity – in other words, the total feedback of momentum and energy from each particle to the surrounding Eulerian grid must be equal and opposite to those of the particle. The following three projection schemes have been widely considered in the past: 1) particle-in-cell (PIC) method pioneered by Evans et al. [13] and Harlow [14], 2) projection on neighboring node method [1,2] and 3) projection onto identical stencil method advanced by Sundaram and Collins [15]. The accuracy and relative performance of the different projection methods have been considered by Boivin et al. [16] and Narayanan et al. [17].

Of particular significance is the work of Garg et al. [18] who presented a rigorous analysis of the different projection operations in conjunction with different interpolation operations and separated the error into deterministic (discretization and bias errors) and stochastic (statistical error) components. They demonstrated it is important for numerical convergence to maintain the number of Lagrangian points per grid cell while performing a grid refinement study.

The focus of the present work is to extend the above investigations and consider an aspect of fluid-mediated particle–particle interaction (i.e., the effect of neighboring particles on quantities such as particle drag force). Different methods that are used in the computation of particle volume fraction will be considered and their accuracy evaluated. Local particle volume fraction around the lth particle, α_l, and the volume fraction at the ith grid cell are the quantities of foremost importance. These information are often required in the modeling fluid-mediated particle–particle interaction and back coupling of momentum to the carrier fluid. Local volume fraction can be defined in different ways. Particle volume fraction is traditionally defined as the fractional volume occupied by the particles inside a reference volume, whose size is chosen to be much smaller than the scale of volume fraction variation. In this definition local volume fraction around any particle depends on the distribution of a cloud of particles around it within the reference volume. On the other hand, given the location of all the particles within the flow domain, one can consider Voronoi tessellation of the entire domain and define the volume of the Voronoi element around each particle to be the volume of space associated with that particle [19]. Then the local particle volume fraction of a particle can be defined as the ratio of the particle volume to the volume of space associated with it. In this later definition, local particle volume fraction depends only on the location of the nearest neighbors. Irrespective of the precise definition, it is clear that particle volume fraction is fundamental information that depends on inter-particle distances.

Here a general multiphase flow with a distribution of Lagrangian particles inside a fluid flow discretized on an Eulerian grid is considered. Numerical methods for the evaluation of particle volume fraction are addressed. In Eulerian–Lagrangian simulations particle volume fraction is needed both as a Lagrangian quantity associated with each particle and also as an Eulerian quantity associated with the grid cell. For instance, correlations have been proposed to account for the effect of volume fraction on the drag force on a particle. Thus, in the evaluation of drag force, local particle volume fraction is needed as a Lagrangian quantity. On the other hand, in the continuous phase governing equations in order to account for the spatial variation of the fluid volume fraction, it is also necessary to represent particle volume fraction as an Eulerian quantity (note by definition the sum of the local particle and fluid volume fraction is unity). Clearly it is sufficient to first obtain particle volume fraction either in the Lagrangian frame for each particle or in the Eulerian frame as a field variable. Once one of these two representations is known interpolation or projection techniques can be used to obtain the other representation.

Two classes of methods for the evaluation of particle volume fraction are addressed. The first will be termed *Grid-Based* (GB) methods, where particle volume fraction will first be obtained within each grid cell as an Eulerian quantity, from which local particle volume fraction associated with any Lagrangian particle can be obtained from interpolation. The second class of methods will be termed *Particle-Based* (PB) methods, where particle volume fraction will first be obtained at each particle as a Lagrangian quantity, which can then be projected onto the Eulerian grid.

The traditional approach to particle volume fraction evaluation has been using GB methods. For instance, the lowest order GB method to calculate particle volume fraction is to count all particles within a grid cell and add their volume contributions to obtain the local particle volume fraction within that cell. At the next level, each particle contributes part of its volume to the particle volume fraction of the grid cells surrounding it, according to its location with respect to the surrounding grid cell centers. By construction, the GB methods can represent particle volume fraction variation only on the grid scale – any volume fraction variation on scales smaller than the grid is erased in the grid-scale averaging process.