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Modeling and Simulation Challenges in Eulerian-Lagrangian Computations of Multiphase Flows

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Abstract. The present work addresses the numerical methods required for particle-gas and particle-particle interactions in Eulerian-Lagrangian simulations of multiphase flow. Local volume fraction as seen by each particle is the quantity of foremost importance in modeling and evaluating such interactions. We consider a general multiphase flow with a distribution of particles inside a fluid flow discretized on an Eulerian grid. Particle volume fraction is needed both as a Lagrangian quantity associated with each particle and also as an Eulerian quantity associated with the flow. In Grid-Based (GB) methods, the volume fraction is first obtained within each cell as an Eulerian quantity and then interpolated to each particle. In Particle-Based (PB) methods, the particle volume fraction is obtained at each particle and then projected onto the Eulerian grid. Traditionally, GB methods are used in multiphase flow, but sub-grid resolution can be obtained through use of PB methods. By evaluating the total error and its components we compare the performance of GB and PB methods. The standard von Neumann error analysis technique has been adapted for rigorous evaluation of rate of convergence. The methods presented can be extended to obtain accurate field representations of other Lagrangian quantities.

INTRODUCTION

Eulerian-Lagrangian point-particle approach has become an important methodology in the simulation of canonical and complex multiphase flows (Squires and Eaton 1990, Elghobashi and Truesdell 1993, Balachandar and Eaton 2010). 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.

The focus of the present work is to consider numerical methods that are used in the computation of particle volume fraction, which is often required in modeling particle-particle interaction and evaluate their accuracy (rate of convergence). Here we consider a general multiphase flow with a distribution of Lagrangian particles inside a fluid flow discretized on a grid. We address numerical methods for the evaluation of particle volume fraction. We immediately note that 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. 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 we can use interpolation or projection techniques discussed above to obtain the other representation.

We will address two classes of methods for the evaluation of particle volume fraction. 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

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fraction will first be obtained at each particle as a Lagrangian quantity, which then can be projected onto the Eulerian grid.

The discussion to be presented below will focus only on volume fraction evaluation. But the PB methods to be presented and discussed can be extended to obtain field representations of other Lagrangian quantities such as particle velocity, temperature, etc. The resulting field representation will be at a scale dictated by the number and distribution of the Lagrangian particles, rather than the Eulerian grid, thus permitting sub-grid resolution at scales smaller than the Eulerian grid.

METHODOLOGY

Volume Fraction Evaluation for Lagrangian Particles

In order to evaluate the accuracy of the GB and PB methods and compare them, we consider the local particle volume fraction calculated using a finite number of Lagrangian particles within a computational domain. By prescribing a sinusoidal spatial variation in volume fraction and randomly distributing the finite number of Lagrangian particles according to this spatially varying volume fraction we can directly assess the accuracy in each GB and PB method proposed.

Each random distribution of particles will be termed a *realization* and for each realization numerical approximation to the local volume fraction will be obtain using the GB or PB methods. For the GB methods, we first calculate the local particle volume fraction at each grid cell which then is interpolated to each Lagrangian particle. The error of each method is assessed by comparing the exact volume fraction with the calculated volume fraction at each particle location. The GB and PB methods considered are outlined below.

Grid-Based Methods for Particle Volume Fraction Evaluation

In general, particle volume fraction as calculated from GB methods involves summing or weighting the contribution of the Lagrangian particles within a given cell (zeroth order, GB0) or between cell centers (first order, GB1), and so on. The volume fraction value for the Eulerian cell is taken to be stored at the cell center.

In the zeroth order method, the particles contribute directly to the Eulerian grid cell within which they reside. If a particle resides within the cell i, the weight of that particle on cell i is 1; 0 otherwise. In the first order method, the particles contribute to the two cells whose centers enclose the particle. The first order weight function distributes the particle's influence between the two cells, where the total influence of a single particle must sum to unity. For both methods, we can simply sum the weights of all particles over all cells to find the total number of particles per cell. The volume fraction of each Eulerian grid cell is calculated as the average initial volume fraction multiplied by the ratio of the total number of particles per cell to the average number of particles per cell.

Particle-Based Methods for Particle Volume Fraction Evaluation

In general, PB methods of calculating local particle volume fraction are independent of the underlying Eulerian grid. For each particle the local volume fraction value depends only on the number and location of its neighboring particles. We introduce a method where the neighboring particles exert a weighted influence, termed the "Gaussian method". For the Gaussian method, the equation for the local volume fraction of each particle is calculated using the Gaussian distribution, where the mean is the distance of the neighboring particle and the variance is the width of the Gaussian averaging. Small values of Gaussian averaging (variance) yield a more narrow Gaussian and only the location of a few neighboring particles will contribute to local volume fraction evaluation.

Definition of Errors

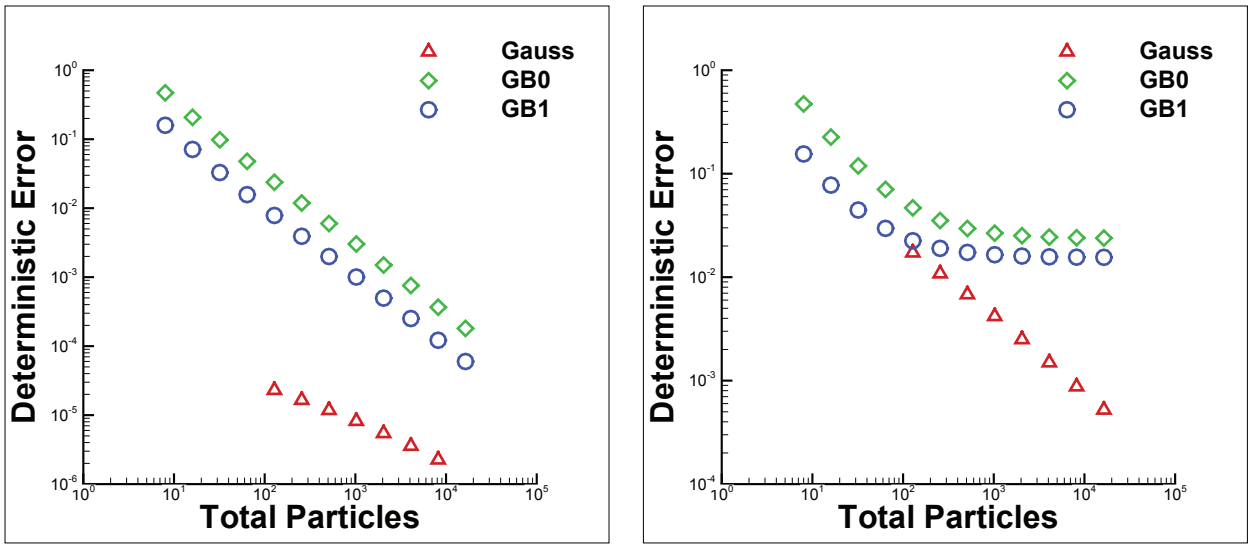
In each realization, for a given random distribution of particles, the above defined GB and PB methods are used to numerically evaluate the local particle volume fraction. The resulting numerical approximation of the local volume fraction at the j^{th} particle can be directly compared to the exact local volume fraction to obtain an error estimate. We can calculate the mean squared error for a single realization. We observe that each particle has an error

in the computed local volume fraction. We repeat the realization many times to construct an ensemble of realizations. For the ensemble of realizations, the average mean squared error is calculated.

Following Xu and Pope (1999) and Garg et al (2007) we separate the overall error into stochastic and deterministic components. The error depends on both the number of grid cells and the number of particles per grid cell. The deterministic error separates into two components: bias and discretization errors. The bias error represents the error of using a finite number of Lagrangian particles versus an infinite number of particles. The discretization error is the difference in representing the continuous spatial variation in volume fraction with a finite number of Eulerian grid cells. The mean square error of the ensemble is a superposition of the deterministic and stochastic error components, where the stochastic error is the difference between an individual realization and the ensemble average error.

RESULTS

We can directly compare the GB and PB methods using the deterministic error and total number of particles. For the domain that is minimally divided, Fig. 1a and 1b show the deterministic error comparison. For constant volume fraction, the GB and PB methods show the error decreases with increasing number of particles and the PB method has significantly less deterministic error. When a sinusoidal volume fraction is considered, the bias error component is initially reduced by the increase in number of particles but the discretization error dominates beyond 100 particles per wave. The PB methods clearly out-perform the GB methods for the sinusoidal volume fraction; there is no dependence on the grid scale, allowing a continual reduction in deterministic error.



a) (b)

FIGURE 1. Deterministic error for (a) constant volume fraction and (b) sinusoidal volume fraction.

We can also directly compare the GB and PB methods using the stochastic error. For the same minimally divided domain, Fig. 2a and 2b show the stochastic error comparison. The stochastic errors are very small, particularly when compared to the deterministic error, suggesting the statistical deviation of individual realizations from the ensemble average is quite small. When estimating the constant volume fraction, the PB method has very little statistical error, and all methods show error decreasing with increasing number of particles. The GB and PB methods show similar stochastic error when estimating a sinusoidal volume fraction.

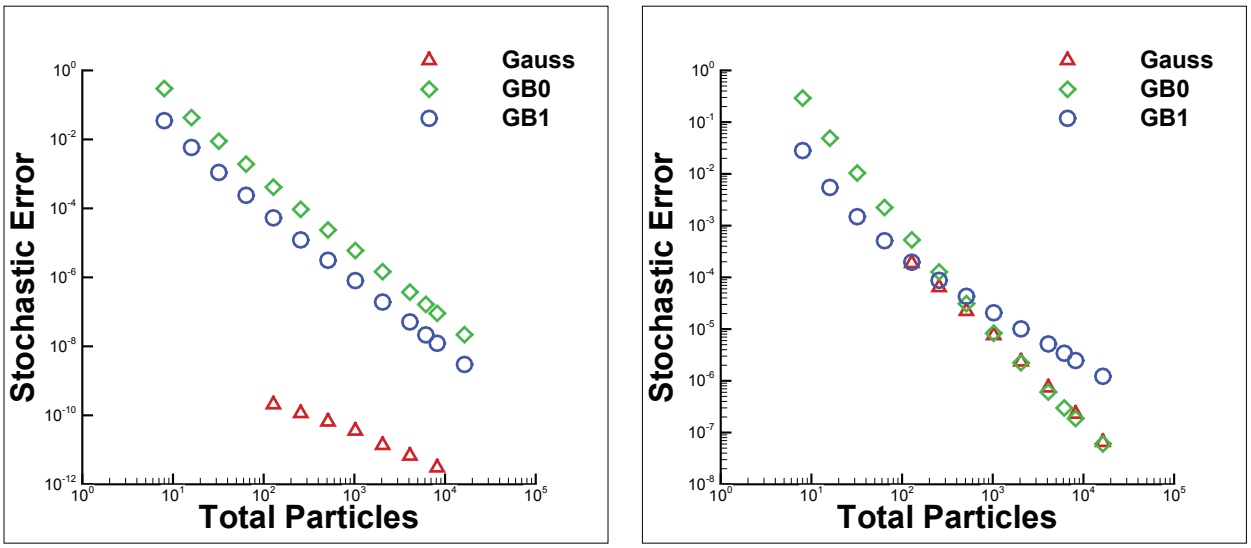


FIGURE 2. Stochastic error for (a) constant volume fraction and (b) sinusoidal volume fraction.

CONCLUSIONS

The GB methods are dependent on the grid scale, making their ability to accurately estimate the volume fraction impaired by the number of grid cells considered per wave. For a minimally divided domain, the discretization error can saturate the deterministic error, resulting in constant error as additional particles are added. However, PB methods show a continual decrease in deterministic error as the numbers of particles are increased.

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. PB methods are independent of the grid scale and can therefore be used to reveal sub-grid resolution.

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