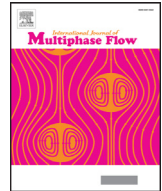




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# An analysis of the convergence of stochastic Lagrangian/Eulerian spray simulations

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## ABSTRACT

This work derives how the convergence of stochastic Lagrangian/Eulerian simulations depends on the number of computational parcels, particularly for the case of spray modeling. A new, simple, formula is derived that can be used for managing the numerical error in two or three dimensional computational studies. For example, keeping the number of parcels per cell constant as the mesh is refined yields an order one-half convergence rate in transient spray simulations. First order convergence would require a doubling of the number of parcels per cell when the cell size is halved. Second order convergence would require increasing the number of parcels per cell by a factor of eight. The results show that controlling statistical error requires dramatically larger numbers of parcels than have typically been used, which explains why convergence has been so elusive.

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## 1. Introduction to the problem

The computational fluid dynamics community expects numerical schemes to be consistent, i.e. they should converge to the exact solution as resolution is increased. Without this assurance, the modeler can wander aimlessly, confused by pathological numerical errors. The present work will identify a simple rule that governs convergence and will bring Lagrangian/Eulerian spray simulation closer to modern standards of simulation quality. The mathematical analysis is intended to also benefit other forms of Lagrangian/Eulerian simulations, such as bubbly or particle-laden flow.

The first step is to identify what is and what is not understood. The typical parts of a Lagrangian/Eulerian spray computation can be categorized as follows:

1. Gas phase equations: The gas phase conservation equations, excluding source terms for interaction with the spray, solved in an Eulerian frame of reference.
2. Particle tracking: The governing ordinary differential equations that describe the evolution of the tracked particles, solved in a Lagrangian frame of reference.
3. Gas to liquid coupling: The interpolation of gas phase quantities to the location of the spray parcels.

4. Liquid to gas coupling: The agglomeration of the scattered point particle effects into source terms in the continuous phase equations.

The first item is well understood. The second category includes the models that describe the evolution of droplets as they move in the Lagrangian reference frame. Are et al. (2005) provided analysis for the basic equations of spray motion. Spray breakup has not been analyzed but is expected, for at least basic breakup models, to behave as ordinary differential equations (ODEs) which are well understood. Droplet collision is beyond the scope of this paper and has been studied elsewhere (Schmidt and Rutland, 2000; Abani et al., 2008). Gas to liquid coupling is equivalent to interpolation and was also analyzed by Are et al.

The final item, representing the effect of the liquid phase on the gas phase, has proven to be the most challenging. Here, the numerical methods accumulate information from the liquid phase about mass, momentum, energy, and species contributions to the gas phase. These methods must contend with the fact that parcels are not collocated with gas phase nodes or finite volume cell centers. Further, because of the limited number of parcels used in spray computations, there is a statistical uncertainty in these terms.

Because of this statistical uncertainty, refinement of gas phase solution without adequately refining the Lagrangian solution by increasing the number of computational parcels can actually result in a less accurate answer. Early work by Subramaniam and O'Rourke (1998) concluded that the convergence of spray simulations was conditional on employing a sufficient number of parcels.

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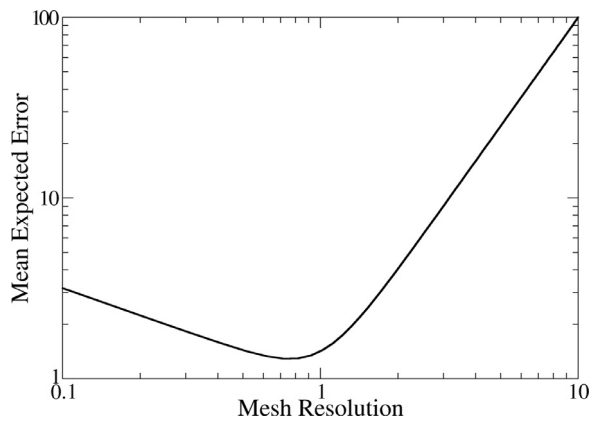


Fig. 1. General behavior of error when the number of parcels is held constant. This situation corresponds to employing Eq. (10) with a value of  $a = 0$ .

Subsequent analysis by Schmidt (2006) saw similar trends. If the number of parcels is held constant while the mesh is refined, the error begins to increase after passing an optimum, as shown in Fig. 1.

There have been several past investigations of liquid to gas coupling. The work of Stalsberg-Zarling et al. (2004) applied Lagrange polynomial interpolation to interphase coupling in order to produce a more stable, less mesh-dependent simulation. The work of Garg et al. (2007) used several problems that admitted analytical solutions in order to empirically study the convergence rate of fairly sophisticated coupling schemes. For completeness, they included statistical factors in their tests by varying the number of parcels per cell. In order to understand the behavior and causes of the error, they modeled deterministic, bias, and statistical contributions using a framework suggested by Dreeben and Pope (1992).

The work of Garg et al. judged the efficacy of these liquid to gas coupling schemes based on empirical tests. In later work, Garg et al. (2009) developed a parcel number density control system to moderate statistical error and, with the help of a sophisticated liquid-to-gas source estimation scheme, produced convergence of a fully-coupled Lagrangian/Eulerian calculation. Their success strongly supports the notion that the distribution of sources from the Lagrangian phase to the Eulerian is the crux of controlling overall error.

In contrast, the work of Are et al. excluded considerations of statistical error in both their analytical and empirical tests. The analysis took the limit of an infinite number of parcels, while the empirical tests used arbitrary, large numbers of parcels. They succeeded in showing theoretically, for each of the elements listed above, how to achieve second order accuracy. They then combined these elements into a full Lagrangian/Eulerian simulation and demonstrated second order convergence. Later, Schmidt (2006) studied how second order and higher accuracy schemes converge considering both spatial and statistical error. However, Schmidt only considered liquid-to-gas coupling and only for fixed numbers of parcels per cell.

The outstanding question that has never been answered is: "In a Lagrangian/Eulerian simulation, how fast must the number of parcels increase in order to observe convergence during mesh refinement?" Without knowing the answer, one cannot reliably demonstrate spray calculation convergence. The present work derives a recipe that answers this question and performs demonstrations in order to empirically confirm the predictions.

This effort will add to the body of literature that has empirically studied convergence, such as Senecal et al. (2012). These studies have proceeded without analysis to provide guidance. Senecal et al. is an example where the authors successfully achieved convergence by a combination of careful numerical methods and em-

ploying a substantial number of computational parcels. In a subsequent section of this paper, their approach will be compared to the rule which we derive.

## 2. Analysis of a single time step

Our analysis examines the calculation of particle to gas source terms as a function of location in a  $d$  dimensional space. The magnitude of the sources in this analysis is determined by the gas-to-particle coupling, reducing the particle-to-gas coupling to a determination of how the sources are to be distributed on the gas phase mesh. Consequentially, the distribution of sources can be represented by a density function  $f(\vec{x})$  which is estimated from  $n$  non-uniformly spaced parcels (See Pai and Subramaniam, 2009 for an investigation of discrete particle representations of smooth distribution functions). For each continuous phase cell, the contributions of the local parcel sample is summed using a kernel with compact support.

Our approach will be to construct an estimate of the combined error due to statistical and spatial contributions. This estimate will be dependent on both the number of parcels and the level of spatial resolution. We will then assert that the number of parcels must be tied to the cell size by a simple power law relation, which then results in an error estimate that is only a function of cell size. Finally, we will calculate the convergence rate of this error.

The analysis begins with our representation of the kernel used to connect parcel contributions to the source term. As reviewed by Garg et al. (2007) and Schmidt (2006) there are several approaches that can achieve varying degrees of spatial accuracy or reduced statistical error. The simplest and most common approach in Lagrangian/Eulerian spray simulations is the nearest-node kernel. This treatment, in a finite volume context, is simply: if a parcel resides in a cell, then all of the contributions from the parcel go the gas phase equation for that cell.

The nearest node kernel can be represented as a function  $K$  that depends on the dimensionless distance  $y$  from the center of the cell in a  $d$ -dimensional Cartesian space, where  $m$  is the index of a dimension.

$$K_m(y) = 1 \quad |y| \leq \frac{1}{2} \quad (1)$$

The present work will consider the simplified case where the kernel is the same in each dimension and the mesh spacing  $\Delta x_m$  is uniform and constant in each dimension, and so the subscript  $m$  is dropped. The argument of the kernel,  $y$ , is defined for the  $j_{th}$  parcel below, where  $\vec{x}$  is the location of the nearest cell center. Similarly,  $\vec{x}_j$  is the location of the parcel. The symbol  $\hat{m}$  represents a unit vector in the  $m$  direction.

$$y = \frac{(\vec{x} - \vec{x}_j) \cdot \hat{m}}{\Delta x} \quad (2)$$

The numerical estimate of the source term distribution function,  $f_n(\vec{x})$ , is the result of applying the kernel in all dimensions to all parcels. Here,  $n$  represents the number of parcels in the entire domain.

$$f_n(\vec{x}) = \frac{1}{n \Delta x^d} \sum_{j=1}^n \prod_{m=1}^d K_m \left( \frac{(\vec{x} - \vec{x}_j) \cdot \hat{m}}{\Delta x} \right) \quad (3)$$

The mean square error,  $E^2$ , is defined as the square of the difference between the true source distribution function,  $f$ , and the expected numerical value,  $f_n$ , produced by Eq. (3). Here, we can build on prior efforts to understand the related problem of finding the optimal kernel for estimating density functions. Epanechnikov (1969) calculated the mean square error for a  $d$  dimensional space and a general kernel.

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