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# A globally Eulerian locally Lagrangian particle concentration scheme

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ABSTRACT

For gas flows, a Lagrangian Concentration Differential Equation (LCDE) was solved along a particle path using Eulerian derivatives for the particle velocity divergence field. This equation is solved by a Globally Eulerian Locally Lagrangian (GELL) discretization technique which avoids the computationally intensive Jacobian calculations of the Full Lagrangian method, the steady-state assumption of the area method, and the computational inefficiency of the box-counting methods. The LCDE–GELL method was compared to such methods using a high-order temporal integration technique and evaluated for two fundamental flowfields: flow past a corner and past a cylinder. In the dilute limit, the particle concentration fields were predicted for various particle inertias (characterized by a range of Stokes numbers) including the zero-mass (tracer) limit for which an exact particle concentration solution exists. Both the weighted-average and ensemble-average methods required far more parcels to achieve the same accuracy demonstrated by the LCDE–GELL method. It is recommended that future work investigates the LCDE approach for three-dimensional, complex flows with particle–particle interaction to investigate its robustness.



## 1. Introduction

A natural approach when simulating particle interactions with a gas is to use Lagrangian particle trajectories. These particle path-lines are defined based on the center of mass of the particle (or the center of mass for a cloud of particles) in which Ordinary Differential Equations are used to update particle position, velocity, mass, temperature, etc. The Lagrangian approach provides high accuracy with respect to a particle path, including particle–wall and particle–particle reflections. As a result, most numerical methods used to predict describe particle mass flux and concentration for aerodynamic and turbulent flows employ Lagrangian methods for the particle field [1–5]. The conventional Lagrangian approach has been successfully employed in modeling many engineering processes [6,7]. However, use of these Lagrangian trajectories to determine local particle concentration or other Eulerian cell quantities generally requires statistical sampling based on the summation of several instantaneous particle locations. This "bin-averaging" uses weighted and un-weighted summation based on a computational cell or the vicinity of a computational node, and employs an area average for 2D flows (Fig. 1) or a volume average for 3D flows. The averaging can lead to uncertainty and/or inaccuracy unless a very large number of trajectories are employed [8–10]. The numerical errors of particle concentration predictions obtained from Lagrangian trajectories can also lead to significant errors of the gas flow when two-way coupling is important [11].

This averaging problem can be avoided with Eulerian dispersed-phase representations. Such a technique is described by reference [12] for dilute gas flows. This approach employs partial differential equations (PDEs) for the particle characteristics (e.g. velocity and concentration) at discrete cell nodes or cell volumes on an Eulerian grid. These fields are integrated in time based on discrete spatial and temporal gradients and assumptions of continuity. While an Eulerian particle field representation can consistently describe two-way coupling between the particle concentration and the gas flow properties, it cannot accurately incorporate particle reflection off surfaces, history force effects (which require a Lagrangian acceleration), or stochastic turbulent diffusion [12,13]. Furthermore, Eulerian methods have difficulty with regions with trajectory crossing and concentration discontinuities due to numerical diffusion as in reference [14] and become computationally expensive if a broad particle size distribution is to be incorporated.

As such, it is desirable to develop a method that can incorporate the trajectory accuracy and robustness of the Lagrangian approach and the concentration accuracy of the Eulerian approach. There are two Lagrangian methods which have made significant headway toward this goal. The method of reference [15] employs a discrete Lagrangian approach which avoids bin-averaging but gives numerical difficulties when the particle divergence is infinity (due to trajectory crossing). The Full Lagrangian method of reference [16] was further developed by reference [8] and [17] to avoid the numerical difficulties of infinite divergence, whereby a Jacobian tensor is used to provide the particle

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velocity divergence. This method dramatically reduces the number of particles needed by orders of magnitude compared to a conventional Lagrangian bin method, while avoiding the numerical diffusion of a conventional Eulerian method. However, this approach assumes linear drag and can be computationally expensive, as it requires a set of eight ODEs for a 2D flow and eighteen for a 3D flow.

The approach developed in this study seeks to use key elements of the Full Lagrangian approach while preserving the simplicity of conventional Lagrangian approaches, e.g. allowing for generalized surface forces and trajectory ODE's which do not require linearization. This is accomplished by using Eulerian spatial derivatives to estimate the particle velocity divergence coupled with discretization of the Lagrangian Concentration Differential Equation. The technique is also compared to conventional Lagrangian bin techniques for two fundamental flows in terms of particle concentration, in the dilute limit. To the authors' knowledge, this is the first such hybrid Lagrangian–Eulerian method for particle concentration and the first to provide detailed quantitative comparisons of weighted and un-weighted bin methods with the area–ratio method in terms of prediction fidelity of particle concentration.

## 2. Theoretical and numerical background

### 2.1. Lagrangian particle trajectory ODEs

The overall particle translational equation of motion equates the rate of change of the particle's linear momentum to the net sum of the forces acting on the particle of a given mass. This mass ($m_p$) can be expressed in terms of the particle volume ($\forall_p$) and density ($\rho_p$), or in terms of the particle diameter (d):

$$m_p = \forall_p \rho_p = \frac{\pi d^3 \rho_p}{6} \tag{1}$$

If one assumes negligible contact interactions (i.e. particles are small enough such that particle–particle collisions are not significant), the Lagrangian equation for particle velocity ($\mathbf{v}$) is given by

$$m_p(d\mathbf{v}/dt) = m_p\mathbf{g} + \mathbf{F}_{surf} \tag{2}$$

The left-hand side (LHS) includes the temporal derivative of the particle velocity along the particle path while the right-hand side (RHS) includes the body force based on gravity ($\mathbf{g}$) and fluid dynamic surface forces ($\mathbf{F}_{surf}$). Similarly, a Lagrangian ordinary differential equation (ODE) can be written for particle position ($\mathbf{x}_p$) as

$$d\mathbf{x}_p/dt = \mathbf{v} \tag{3}$$

The dominant contribution of the surface force is typically the drag component that is non-zero in the presence of finite viscosity of the surrounding fluid ($\mu_f$). For a spherical solid particle surrounded by a uniform continuum flow of constant density, this force can be represented by the Stokes drag as:

$$\mathbf{F}_D = -3\pi d f \mu_f \mathbf{w} \tag{4}$$

This uses the particle relative velocity ($\mathbf{w}$) based on the "unhindered" continuous-fluid velocity ($u_{@p}$), extrapolated to the particle centroid ($\mathbf{x}_p$)

$$\mathbf{w}(t) \equiv \mathbf{v}(t) - \mathbf{u}_{@p}(t) \tag{5}$$

The "unhindered" velocity neglects local flow disturbances caused by the particle itself, i.e. it is the velocity of the fluid that would occur at the centroid if the particle was not present. Temporal response to the drag force can be used to define a particle response time as

$$\tau_p \equiv \frac{m_p|\mathbf{w}|}{F_D} \tag{6}$$

The Stokes number (St) that relates particle response time to the continuous-phase flow time-scale ($\tau_f$) is defined as

$$St \equiv \frac{\tau_p}{\tau_f} \tag{7}$$

As with Eq. (6), the right-hand side expression assumes linear drag. In addition, a high density ratio between the particles and the surrounding gas coupled with negligible particle spin and weak flow vorticity renders the other surface force components to be generally negligible compared to the drag [18] so that the other surface force can be approximated simply as

$$\mathbf{F}_{surf} \approx \mathbf{F}_D \tag{8}$$

Note that while these assumptions are helpful to focus on this study's fundamental characterization and comparison of several methods, the present method can be extended to non-linear drag expressions and additional force terms [19].

### 2.2. Lagrangian numerical methods for particle trajectories

The momentum and position ODE's (Eqs. (2) and (3)) may be integrated in time for a discrete time increment ($\Delta t$) assuming constant $\tau_p$ and $\mathbf{u}_{@p}$ using a generalized high-order method proposed by reference [20], which accounts for time variations in the fluid velocity seen by the particle (along its path):

$$\begin{aligned}\mathbf{v}_p^{n+1} = {} & \mathbf{v}_p^n e^{-\Delta t/\tau_p^n} + \mathbf{u}_{@p}^n\left(1-e^{-\Delta t/\tau_p^n}\right) + \mathbf{A}\left\{\Delta t - \tau_p^n\left(1-e^{-\Delta t/\tau_p^n}\right)\right\} \\ & + \mathbf{B}\left\{\Delta t^2 - 2\tau_p^n\Delta t + 2\left(\tau_p^n\right)^2\left(1-e^{-\Delta t/\tau_p^n}\right)\right\}\end{aligned} \tag{9a}$$

$$\begin{aligned}\mathbf{x}_p^{n+1} = {} & \mathbf{x}_p^n - \tau_p^n\left(\mathbf{u}_{@p}^n - \mathbf{v}_p^n\right)\left(1-e^{-\Delta t/\tau_p^n}\right) + \mathbf{u}_{@p}^n\Delta t \\ & + \mathbf{A}\left\{\frac{\Delta t^2}{2} - \tau_p^n\Delta t + \left(\tau_p^n\right)^2\left(1-e^{-\Delta t/\tau_p^n}\right)\right\} \\ & + \mathbf{B}\left\{\frac{\Delta t^3}{3} - \tau_p^n\Delta t^2 + 2\left(\tau_p^n\right)^2\Delta t - 2\left(\tau_p^n\right)^3\left(1-e^{-\Delta t/\tau_p^n}\right)\right\}\end{aligned} \tag{9b}$$

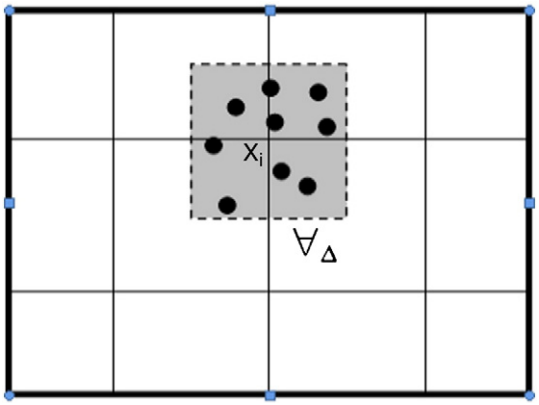


**Fig. 1.** Schematic of a two-dimensional Eulerian continuous-phase grid with particles (black dots) in a discrete computational volume ($\forall_\Delta$), i.e. a control volume, associated with a node $\mathbf{x}_i$.