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Divergence-free condition in transport simulation

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ABSTRACT

In this work, two adaptations of the particle method allowing one to reduce the numerical errors induced by the non-zero divergence of flow fields in the numerical simulations of particle transport are presented. The first adaptation is based on the renormalization method allowing one to use an irregular distribution of particles induced by the non-zero divergence of flow fields. The second adaptation consists in applying a correction on the weight of the particles by using the relation between the divergence of flow fields and the particles' volume evolution. This adaptation may be considered as a relaxation method. The accuracy of both methods is evaluated by simulating the transport of an inert tracer by the flow of a jet in crossflow whose concentration fields were measured experimentally. The comparison between the numerical and experimental results shows clearly that the two adaptations of the particle method correct efficiently the effect of a non-zero divergence velocity field on the computed concentration.

1. Introduction

The numerical simulations of particle transport involves several difficulties, which have been widely addressed, particularly that of the numerical stability. Among the numerous discretization methods proposed to solve this problem, those using Lagrangian coordinates have a particular place since they usually yield new difficulties while naturally solving the stability issue. Using particles requires the computation of their trajectories, which can be readily achieved with a Runge–Kutta high-order scheme. However, the results have been found to be very sensitive to the quality of the velocity field approximation, particularly regarding the satisfaction of the divergence-free condition. Such errors result in the existence within the flow field of sources and sinks which in some cases yield non-physical crossing trajectories [1,2]. Another consequence is the non-uniformity of the particle distribution, which implicitly yields particles with non-constant volume or surface [3,4]. The solution to these problems requires the design of specific solutions, particularly when the Lagrangian coordinates are used to solve the flow equations. There are basically two families of particle methods used for the flow simulation: the SPH method [5,6], and the vortex method [7,8]. In both cases, some methods have been proposed to overcome the non-divergence-free problem. In the last case, the difficulty is even greater for three-dimensional flows because not only the velocity field, but also the vorticity field as well, must be divergence free. In this paper, we consider the rather different and somewhat simpler problem of the transport of inert tracer particles by a given flow field. This flow can result either from a numerical CFD calculation or of an experimental PIV velocity field. In both cases, the divergence is only approximately zero and techniques derived from the previously mentioned works can be applied. These two different ways to solve this problem are described hereafter and tested on a measured 3D velocity field [9,10].

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2. Particle method

2.1. Approximated concentration field

As usual in the particle method, the concentration field $c(\mathbf{x},t)$ is discretized in a set of numerical particles. Each particle $\mathcal{P}_i$ is defined by its location $\mathbf{X}_i(t)$ and its weight $C_i(t)$:

$$\mathbf{X_i}(t) = \int_{\sigma_i} \mathbf{x}(t)\,\mathrm{d}v / \int_{\sigma_i} \mathrm{d}v \quad \text{and} \quad C_i(t) = \int_{\sigma_i} c(\mathbf{x},\mathbf{t})\,\mathrm{d}v \tag{1}$$

where σ_i denotes the support surface or volume of the particle $\mathcal{P}_i$. σ_i is usually constant for an incompressible flow. Thanks to the particle discretization, the concentration field $c(\mathbf{x},t)$ can be estimated by means of a sum of products of weight $C_i(t)$ and Dirac measure $\delta(\mathbf{x})$:

$$c(\mathbf{x},t) = \int_{R^d} c(\mathbf{x}',t)\,\delta(\mathbf{x}'-\mathbf{x}) = \sum_i C_i(t)\,\delta(\mathbf{X}_i(t)-\mathbf{x}) \tag{2}$$

where d is the space dimension. In order to obtain a continuous approximation of the concentration field $c_h(\mathbf{x},t)$, the Dirac measure $\delta(\mathbf{x})$ is approximated by a smooth function $\zeta_\epsilon(\mathbf{x})$ in the previous equation:

$$c_h(\mathbf{x},t) = \sum_i C_i(t)\,\zeta_\epsilon(\mathbf{X}_i(t)-\mathbf{x}) \quad \text{with} \quad \zeta_\epsilon(\mathbf{x}) = (1/\epsilon^d)\zeta(\mathbf{x}/\epsilon) \tag{3}$$

where ϵ is the smoothing parameter proportional to the diameter of the numerical particles. In order to check the consistency of Eq. (3), the smoothing function $\zeta_\epsilon(\mathbf{x})$ has to satisfy momentum conditions:

$$\int_{\mathcal{R}^d} \zeta_\epsilon(\mathbf{x})\,\mathrm{d}\mathbf{x} = 1 \quad \text{and} \quad \int_{\mathcal{R}^d} \mathbf{x}\zeta_\epsilon(\mathbf{x})\,\mathrm{d}\mathbf{x} = 1 \tag{4}$$

As the approximated concentration field $c_h(\mathbf{x},t)$ is a sum of products of $C_i(t)$ and $\zeta_\epsilon(\mathbf{X}_i(t)-\mathbf{x})$, an irregular particle distribution will lead to a shaky approximation of the concentration field $c_h(\mathbf{x},t)$.

2.2. Lagrangian transport equations

In the case of pure advection, the transport equation of an inert tracer can be written as follows:

$$\frac{\partial c(\mathbf{x},t)}{\partial t} + \nabla(\mathbf{u}(\mathbf{x},t)c(\mathbf{x},\mathbf{t})) = 0 \tag{5}$$

where $\mathbf{u}(\mathbf{x},t)$ is the velocity field. In the particle method, this transport equation is written in a Lagrangian framework yielding the discrete approximation:

$$\frac{\mathrm{d}\mathbf{X}_i(t)}{\mathrm{d}t} = \mathbf{u}(\mathbf{X}_i,t) \quad \text{and} \quad \frac{\mathrm{d}C_i(t)}{\mathrm{d}t} = 0 \tag{6}$$

The first equation can be numerically solved by using a 4th-order accurate Runge–Kutta scheme. As the transport equation is an advection equation (Eq. (5)), the weight $C_i(t)$ of a numerical particle $\mathcal{P}_i$ is constant (Eq. (6), right). Thus the particle method is a conservative method in this case.

2.3. Renormalized smoothing function

The discrete form of the first moment condition (Eq. (4), left) reads:

$$\mathbf{1}(\mathbf{x},t) = \sum_i \zeta_\epsilon(\mathbf{X}_i(t)-\mathbf{x}) \tag{7}$$

The previous equation is equal to 1 as long as the particle volumes remain constant. This is not the case of flow fields with a non-zero divergence where an irregular particle distribution can appear. This problem has been addressed by Gingold and Monaghan [5,6], who proposed the renormalization method. This method consists in dividing Eq. (3) (left) by the renormalization coefficient $\mathbf{1}(\mathbf{x},t)$ defined by Eq. (7). As a result, the approximated concentration field $c_h(x,t)$ reads:

$$\frac{c_h(\mathbf{x},t)}{\mathbf{1}(\mathbf{x},t)} = \frac{\sum_i C_i(t)\zeta_\epsilon(\mathbf{X}_i(t)-\mathbf{x})}{\sum_i \zeta_\epsilon(\mathbf{X}_i(t)-\mathbf{x})} \tag{8}$$

The renormalization coefficient $\mathbf{1}(\mathbf{x},t)$ accounts for the actual volume variations of numerical particles. In the paper, the renormalization method will be denoted RSF (Renormalized Smoothing Function).