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Analytical integration of 0th, 2nd, and 4th order polynomial filtering functions on unstructured grid for dispersed phase fraction computation in an Euler–Lagrange approach

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ABSTRACT

This paper presents an analytical approach to evaluate the volume integrals emerging during dispersed phase fraction computation in Lagrangian–Eulerian methods. It studies a zeroth, second, and fourth order polynomial filtering function in test cases featuring structured and unstructured grids. The analytical integration is enabled in three steps. First, the divergence theorem is applied to transform the volume integral into surface integrals over the volumes' boundaries. Secondly, the surfaces are projected alongside the first divergence direction. Lastly, the divergence theorem is applied for the second time to transform the surface integrals into line integrals. We propose a generic strategy and simplifications to derive an analytical description of the complex geometrical entities such as non-planar surfaces. This strategy enables a closed solution to the line integrals for polynomial filtering functions. Furthermore, this paper shows that the proposed approach is suitable to handle unstructured grids. A sine wave and Gaussian filtering function is tested and the fourth order polynomial is found to be a good surrogate for the sine wave filtering function as no expensive trigonometric evaluations are necessary.

1. Introduction

An Euler–Lagrange approach consists of a continuous description of the carrier fluid flow using an Eulerian reference frame and an interpenetrating disperse phase in Lagrangian formulation. The disperse phase is a collection of particles which are tracked using Newton's law. Such a setup can be applied for the investigation of multiphase flows, e.g. bubbly flows or particulate flows. The reader is referred to the recent review paper Subramaniam (2013) for details. The disperse phase is unresolved in an Euler–Lagrange framework, cf. (van der Hoef et al., 2008), and thus it is necessary to model the influence of the particles onto the continuous phase as the exact interface between the phases. This paper focuses on the dispersed phase volume computation to account for the volume displaced by the disperse phase in the continuous phase. As the particle is treated point-like, a filtering function is applied at each particle position to smear the volume of the corresponding dispersion onto the fluid domain. The fluid field is subdivided into non-overlapping control volumes which might be a cell or an element in a finite volume or finite element representation of the carrier fluid field. Finally, the volume occupied by the disperse phase V_d within a control volume V can be used to compute the fluid fraction

$$\epsilon = 1 - \frac{V_d}{V}$$

which is the fill level of remaining fluid in the control volume. The fluid fraction is necessary in e.g. the volume-averaged Navier–Stokes equations (Anderson and Jackson, 1967). The dispersed phase volume computation requires the evaluation of a volume integral over each fluid cell over the filtering functions of submerged particles. The solution of these volume integrals using an analytical integration is the key aspect considered in this paper.

Several options for filtering functions can be found in literature depending on the desired accuracy and the computational effort to be invested. The most trivial approach, known as *center of volume* or *point approximate method*, assumes that the particle's volume is not distributed across several fluid cells. The corresponding filtering function is a Dirac delta at the particle center. Thus, the volume is assigned to the cell in which the center of the particle resides. This leads to jumps in the dispersed phase fraction when a particle passes cell boundaries which leads to artificial pressure

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waves and detrimental pulsatile fluid flow profiles. A common assumption in Euler–Lagrange approaches are spherical shapes of the particles under consideration. Also, the support of the filtering function is assumed spherical and hence the volume integral during dispersed phase volume computation includes spherical domains. Dependent on the discretization of the continuous phase, Freireich et al. (2010) presents an exact method to compute the dispersed phase volume when a Cartesian grid for the fluid is used and Wu et al. (2009) gives the equations to compute the dispersed phase volume on an unstructured fluid grid. In the latter, tetrahedral, hexahedral, and wedge elements are considered. Although both methods lead to an exact analytical solution, the former is restricted to Cartesian grids which might not be appropriate in case of flow in complex domains and the latter contains expensive trigonometric calculations. Boyce et al. (2014) states that the proposed look-up table in Wu et al. (2009) only circumvents the expensive calculations, nevertheless finding the position of the particle relative to the element boundaries remains very costly.

In case the assumption of spherical particles might not hold, Tomiyama et al. (1997) proposes to use an approximation with cubic shape for the possibly complex particle contour in order to ease computation. Hence, the filtering function has a cubic support. This approximation can also be plugged in when sphericity is prevailing which then leads to a filtering function with cubic support that circumscribes the sphere. According to Khawaja et al. (2012) this can lead to errors up to 20% compared to a spherical support of the filtering function and therefore a correction is proposed to reduce the error significantly. In Kitagawa et al. (2001), a cubic support for the filtering function is applied and different filtering functions, namely a (clipped and enhanced) Gaussian function and a sine wave function, are spanned in the cube. The different filtering functions are compared with respect to velocity fluctuations when the dispersed phase passes across cells of the underlying fluid. A clear relationship between the choice of the filtering function and velocity fluctuations is reported with an improvement when the filtering function is smoother, i.e. the value and its first derivative of the filtering function are zero at the boundary of the filtering function. Unfortunately, there is no hint in Kitagawa et al. (2001) how the arising volume integrals are evaluated.

Our work is based on the ideas of Rathod and Govinda Rao (1995) and Dasgupta (2003) in which the volume integral in the dispersed phase volume computation is transformed into a surface integral and in a second step into a parametric line integral via applying divergence theorem twice. Rathod and Govinda Rao (1995) performs symbolic integration of the integrand and Dasgupta (2003) applies Gaussian quadrature to evaluate the resulting line integrals. As our approach aims on solving a priori known filtering functions it is possible to perform the integration and implement the resulting equation in order to circumvent the need of repeated symbolic integration during the simulation. Three different filtering functions, namely a constant, quadratic, and a quartic polynomial will be compared. The constant polynomial filtering function is well-known but also its drawbacks are well-known. The fourth order polynomial was proposed in Deen et al. (2004) but it is investigated here in detail for the first time also considering unstructured grids. To the best of our knowledge, the quadratic polynomial filtering function has not been used thus far in the literature. As we rely on analytical integration, the usual spurious oscillations do not appear. We apply our approach using the polynomial filtering functions to the test case proposed in Kitagawa et al. (2001) in which a single filtering function is moved through a Cartesian domain. Furthermore, we modify this test case to show that our approach is also able to handle unstructured grids.

This paper is structured as follows. In Section 2, we present the polynomial filtering functions and describe the procedure to derive the line integrals via applying *divergence theorem* twice onto the volume integral in order to compute the dispersed phase fraction. The analytical solution of the line integrals is given and exemplarily, the solution for the zeroth order polynomial filtering function is calculated. We proceed in Section 3 with the computational approach to obtain the geometry of the integration lines via geometric intersection calculations between the fluid grid and the domain covering the filtering function. Section 4 presents numerical examples. We conclude the findings of this work with Section 5.

2. Dispersed phase fraction evaluation: from volume integration to line integration

In an Euler–Lagrange approach, it is necessary to account for the displaced volume of the disperse phase in the continuous fluid phase. The disperse phase in the Lagrangian frame is modeled with point-like particles interacting with the fluid in Eulerian description. As the volume of a point is zero, the concept of dispersed phase fraction is used in the fluid to account for the volume of the disperse phase. The dispersed phase volume is subtracted from the fluid domain, leaving the volume purely occupied with fluid. We compute the liquid phase volume fraction in a discretized cell Ω_j as

$$\epsilon_{l,j} = 1 - \frac{\sum_{k=1}^{k_P} V_{P,k} \int_{\Omega_j} \psi_i(x,y,z) d\Omega}{\int_{\Omega_j} 1 d\Omega}, \tag{1}$$

where k_P is the number of particles whose filtering cubes lie partially or fully in cell Ω_j and $V_{P,k}$ is the volume of particle k. Therein, $\psi_i(x, y, z)$ and i denote the filtering function and its order, respectively. The challenge in computing (1) lies in evaluating the volume integral in the nominator on the right-hand side accurately and efficiently. Once this is accomplished, then the computation of the denominator in (1) follows analogously. The proposed methodology in this paper allows to integrate

$$\int_{\Omega_j} \psi_i(x,y,z) d\Omega \tag{2}$$

analytically using polynomial filtering functions and an appropriate description of the underlying geometry. The underlying cells Ω_j of the grid are assumed to be convex.

Remark 1. The dispersed phase in this work may consist of solid, fluid, or gas particles.

2.1. Analytical integration with the divergence theorem

The following sections outline the mathematical foundations of the proposed method to gain an analytic solution of (2). The conceptual idea is to formulate the three-dimensional volume integral as a collection of one-dimensional line integrals over the volumes' boundaries. We follow three steps to achieve this objective, cf. (Sudhakar et al., 2014; Sudhakar and Wall, 2013):

(i) first, we formulate the volume integral as surface integrals over the volumes' bounding surfaces with the divergence theorem (Arens et al., 2015; Morse and Feshbach, 1953),
(ii) then, we project the surfaces alongside the divergence directions in i), and
(iii) finally, we evaluate the surface integrals with line integrals along the edges of the surfaces by applying the divergence theorem again.