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Towards efficient tracking of inertial particles with high-order multidomain methods

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Abstract

This paper develops an efficient particle tracking algorithm to be used in fluid simulations approximated by a high-order multidomain discretization of the Navier–Stokes equations. We discuss how to locate a particle's host subdomain, how to interpolate the flow field to its location, and how to integrate its motion in time. A search algorithm for the nearest subdomain and quadrature point, tuned to a typical quadrilateral isoparametric spectral subdomain, takes advantage of the inverse of the linear blending equation. We show that to compute particle-laden flows, a sixth-order Lagrangian polynomial that uses points solely within a subdomain is sufficiently accurate to interpolate the carrier phase variables to the particle position. Time integration of particles with a lower-order Adams–Bashforth scheme, rather than the fourth-order Runge–Kutta scheme often used for the integration of the carrier phase, increases computational efficiency while maintaining engineering accuracy. We verify the tracking algorithm with numerical tests on a steady channel flow and an unsteady backward-facing step flow.

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1. Introduction

The tracking of particles along their path in time (Lagrangian formulation) in a continuous field (Eulerian formulation) finds application in several areas of fluid dynamics, such as flow visualization and multi-phase flows. In the so-called mixed Eulerian–Lagrangian formulation, the continuous field, typically called the carrier phase, is solved through constitutive equations on a fixed mesh. Particles are tracked individually.

The tracking algorithm consists of three stages per particle: the search for the computational cell in which a particle is located, the interpolation of the carrier phase variables to the particle location, and finally, pushing the particle forward with a time integration method. The particles are assumed not to affect the carrier phase. The numerical method and the type of mesh used to solve the carrier phase determines the algorithm needed for each stage of the tracking.

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The first stage, locating the host cell, is most simply performed on a Cartesian mesh: the host cell of the particle may be found by a comparison of the particle coordinate to the mesh coordinate. In complex geometries, searching is more involved, so several methods have been proposed for this in the past. The localization scheme of Seldner and Westermann [17] lays a fine equidistant mesh over a boundary-fitted grid. The particle is then localized in the Cartesian mesh. A relationship between the equidistant mesh and the boundary-fitted grid is used to obtain the addresses of the particles with respect to the grid. In Westermann [18], the location of the particle with respect to a cell is found by comparing the area of the triangles that subdivide the original element to the area of the original element. For curvilinear elements, Allievi and Bernejo [1] devised an iterative method to invert the bijective method that determines the particle coordinate in mapped space. Comparing the mapped particle coordinate to the isoparametric map of the element readily determines the host cell. Patankar and Karki [15] advance the particle in mapped space rather than in physical space. This eliminates the need for a search algorithm, at the additional cost of the interpolation of the metric terms to the particle position.

To compute the field variables at the particle location, linear interpolation is usually used when the carrier phase is computed with a low-order method. For higher-order methods, such as spectral methods, linear interpolation is inaccurate but interpolation on the order of the scheme is computationally expensive. Yeung and Pope [19] showed that linear interpolation is inaccurate. They suggested a third-order Taylor expansion interpolation scheme or a cubic spline scheme. In a comparison of several interpolation schemes, Balachandar and Maxey [2] concluded that the choice of the interpolation scheme depends on the physical problem at hand. If one is only interested in individual particle dispersion statistics, it is sufficient to settle for a less accurate but computationally faster scheme such as a low-order Lagrange interpolant. For experiments such as the simulation of particle coagulation, where close interaction of particles plays a crucial role, the choice of the interpolation scheme is determined more by the need for accuracy. Kontomaris et al. [11] concluded that a Lagrange polynomial of order six suffices to extract particle dispersion statistics in simulations of a turbulent channel flow computed with a Fourier–Chebyshev spectral method.

The time integration stage in the mixed Eulerian–Lagrangian methods has been less studied. In general, the time schemes for the Eulerian and Lagrangian integrations are chosen to be the same [14]. Kontomaris et al. [11], however, note that in the computation of turbulent flow the time-step size on the Eulerian method is too stringent for the Lagrangian method. A larger time step for the Lagrangian tracking is shown to give sufficiently accurate single-particle statistics.

In this paper, we tailor the three particle tracking stages to multidomain spectral methods. Although we will focus on the staggered-grid Chebyshev method developed in Kopriva [12], the findings are generally applicable to high-order spectral methods such as discontinuous Galerkin methods or spectral *hp* element methods. To the best of the authors' knowledge, no studies exist on tracking algorithms for this type of numerical methodology.

Our study is part of a larger work [7–9] in which the multidomain staggered-grid spectral method is developed to simulate turbulent multi-phase compressible flows. Thus, we focus in this paper on tracking particles that move under the influence of a Stokes drag force in a compressible fluid. We will concentrate on flow situations such as turbulent flows that have a large range of scales.

Spectral multidomain methods distinguish themselves from other numerical methods, like finite volume, finite element or finite difference methods, by combining high accuracy (exponential convergence) with an ease to handle complex geometries through the use of multiple non-overlapping isoparametric subdomains. As a result, we cannot use tracking algorithms that are developed for other methods. Most notably, the high-order interpolation, intrinsic to the method weighs heavily on the computational time. We concentrate on minimizing this time, and compare various less expensive interpolation schemes to the expensive spectral interpolation. We also look at interpolation schemes with no overlap between subdomains. These would be effective for a parallel version of the code. In our choice for the search algorithm, the high computational cost of interpolation eliminates the mapping method of Patankar and Karki [15], since that requires interpolation of the metric terms (four in 2D and nine in 3D).

We will introduce a search algorithm for straight-sided subdomains that is competitive with the method in Westermann [18]. Our method takes advantage of the inverse of the isoparametric linear blending formula. In addition, we discuss the advantages of using a second-order Adams–Bashforth (AB) time scheme to track the particles in place of the fourth-order Runge–Kutta (RK) scheme that is used to integrate the carrier phase in time. We also discuss how some physical dependencies influence the accuracy of the time integration scheme.

This paper is organized as follows. The governing equations and a short introduction to the multidomain staggered-grid spectral method set the stage. Next, the search algorithm is presented. An investigation into interpolation schemes