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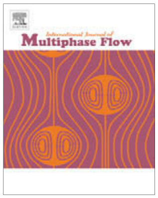

Review

Spectral-based simulations of particle-laden turbulent flows

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ABSTRACT

In this paper, we discuss the application of spectral-based methods to simulation of particle-laden turbulent flows. The primary focus of the article is on the past and ongoing works by the authors. The particles are tracked in Lagrangian framework, while direct numerical simulation (DNS) or large-eddy simulation (LES) is used to describe the carrier-phase flow field. Two different spectral methods are considered, namely Fourier pseudo-spectral method and Chebyshev multidomain spectral method. The pseudo-spectral method is used for the simulation of homogeneous turbulence. DNS of both incompressible and compressible flows with one- and two-way couplings are reported. For LES of particle-laden flows, two new models, developed by the authors, account for the effect of sub-grid fluctuations on the dispersed phase. The Chebyshev multidomain method is employed for the works on inhomogeneous flows. A number of canonical flows are discussed, including flow past a square cylinder, channel flow and flow over backward-facing step. Ongoing research on particle-laden LES of inhomogeneous flows is briefly reported.

1. Introduction

Computational analysis of particle-laden turbulent flows has been applied to problems ranging from fundamental physics (Crowe et al., 1998) to industrial applications (Tsuji, 1982; Gidaspow, 1994). The predominant approach for computation of turbulent flows laden with many particles has been the Eulerian–Lagrangian (EL) method where each particle is traced in its Lagrangian frame, i.e. the frame moving with the particle. The treatment of particles as volumeless mathematical points in EL economizes the tracing of many particles. This treatment is often referred to as the "point-particle" approach to distinguish it from finite-size particle approach where the finite sizes or better said volumes of particles are accounted for in the simulation of carrier phase. The point-particle EL has been the basis for most simulations of particle-laden turbulent flows. With a point-particle assumption, simulation of large number of particles, typical of any realistic industrial flow is feasible.

Despite significant advances in EL methods (Maxey and Patel, 1997; Prosperetti and Oguz, 2001; Takagi et al., 2003), the point-particle EL method is and will be, in our opinion, for quite some time the only feasible method that computes industrial scale particle-laden engineering flows with reasonable accuracy. Nevertheless, it should be understood that point-particle EL has its limitations. This model omits flow details around particles that are typically taken spherical. Particle wake effects on the carrier flow cannot be modeled. For the influence of the particle on the carrier flow to be accurate, the particle size must be smaller than the smallest turbulent flow scale, i.e. the Kolmogorov scale. This limits the physical representation of real flows with particle sizes larger than the Kolmogorov scale. Furthermore, the point-particle EL method should also be considered a statistical approach, that is suited to model the averaged influence of many particles on the flow and vice versa, rather the influence of individual particles. Despite these limitations, many flows can be modeled by EL.

The authors of this paper have in the last decade made efforts to develop and use EL type methods for analysis of realistic particle-laden turbulent flows through the point-particle approach. We have done so in a structured manner starting from a one-way coupled simulation in isotropic turbulence up to currently two-way coupled large-eddy simulation (LES) in complex geometries. We have been particularly motivated to simulate droplet-laden flows in liquid-fuel or spray combustors. In this paper, we will review our efforts in the development of a computational tool based on spectral carrier phase solvers for simulation of realistic particle-laden flows. To enable computation of realistic flows, we have firstly focused on the development of point-particle EL methods that enable computation of particle-laden flow in complex geometry and secondly we have focused on the modeling of small scales of the

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flow to reduce the required degrees of freedom in a simulation, thus increasing the computational efficiency and allowing for larger scale simulations of realistic flows.

This article primarily reviews the work conducted by the authors. We will discuss, where relevant, the works of others but do not claim a comprehensive review on point-particle EL literature. In particular, we will review the development of point-particle EL based on high-order spectral methods for computation of the carrier flow with direct numerical simulation (DNS) and LES in complex geometry and the development of LES subgrid models that account for the effect of the subgrid scales on the particle motion. We will give a brief background on these two topics in the two sub-sections below, before we review our works in more detail in the remainder of the paper. In Section 2, we describe the governing equations for the carrier and dispersed phases. In Section 3, we report our works on DNS and LES of particle-laden homogeneous turbulence using Fourier spectral methods. In Section 4, we discuss particle-laden inhomogeneous flows, where a spectral multidomain method is used for simulation of the carrier phase. Again, both DNS and LES treatments of the carrier phase are considered. Finally, we draw general conclusions on the use of spectral-based methods for simulation of particle-laden turbulent flows and discuss future directions.

1.1. High-order spectral methods

The consensus in the community is that high-order methods are required for simulation of turbulent flows that are characterized by a large range of scales. High-order methods have been the norm for these simulations because of their low diffusion and dispersion errors. Both errors affect accuracy of a simulation and both are significantly smaller in high-order schemes than in low-order schemes. High-order schemes require far fewer grid points to resolve the smallest scales than low-order methods do (Jacobs et al., 2004b). This reduced resolution requirement is typically referred to as *high-order resolution*. When we refer to dispersion errors, we mean the misrepresentation of waves (e.g. phase errors) by a numerical scheme when marching in time (Karniadakis and Sherwin, 2005). The turbulent spectrum in wave space is directly affected by these errors. When dispersion errors are small, long time integration in turbulent flow simulations is accurate. Dispersion errors are closely connected to the spatial discretization. Fourier spectral methods are well known to have zero dispersion errors. General higher order methods have virtually no dispersion and hence are characterized *long-time accurate*.

For DNS of homogeneous particle-laden turbulence, it is natural to use the Fourier spectral method (Canuto et al., 1987). In the Fourier spectral method, the dependent variables are approximated in a hexahedral domain by truncated discrete Fourier series that ideally represent the homogeneous flow variables and inherently deal with periodic boundary conditions. Typically, the Fourier series approximations are substituted into the partial differential equation and are consequently weighted by a test function according to the generic method of weighted residuals. This approach yields an ordinary differential equation system that is easily updated with a temporal integration. Fourier spectral methods rely on the Fourier transformations of the flow variables from physical space to spectral space. The transformations may be performed in a computationally efficient manner using Fast Fourier Transform (FFT). Within the broad class of Fourier spectral methods, we have exclusively used the pseudo-spectral method for our homogeneous particle-laden turbulent flow simulations. In the pseudo-spectral method, the non-linear terms are treated in physical space. Treatment in physical space is particularly useful for the particle tracing and determination of coupling source terms between the carrier and particle phases that are also carried out in physical space.

A major drawback of the spectral method described above is that the approximation of the equations based on Fourier series dictates a simple geometry, which in practice means a cube (in 3D) or a rectangle (in 2D). Another restriction is that parallelization of Fourier-spectral methods can only be performed on the FFT routines limiting the general parallelization efficiency. It is clear that a scheme other than the traditional Fourier spectral method has to be considered for large-scale flow simulation in complex geometries. Several low-order alternatives are of course available, such as finite volume, finite element and finite difference methods, but as mentioned above they are not as suitable for DNS of turbulent flows as high-order methods. Essentially, two suitable high-order schemes have come forth, including “compact finite difference (FD) schemes with spectral-like resolution” developed by Lele (1992), and spectral/*hp* element (SE) type schemes introduced by Patera (1984).

Finite difference (FD) is relatively easy to implement and program on structured grids. The application of boundary conditions in high-order FD, however, is complicated by the overlapping nature of the stencil. The use of high-order FD (Zhang et al., 2006) requires large multi-block structured grid that is not trivial to implement. First, generation of grids of high-quality, essential to preserve the favorable characteristics of the method, with multiblock meshing is labor intensive and not always consistent when establishing grid convergence. Second, parallel codes are not optimal, since the overlap in FD stencil leads to a relatively large amount of data that needs to be exchanged between blocks on different processors. This reduces the applicability and efficiency of FD codes.

In SE, the computational domain is divided into elements that are non-overlapping, providing a flexible meshing, easy boundary condition implementation, and highly parallel method. In each element the solution values are approximated by orthogonal (mostly Chebyshev or Legendre) polynomials that are also typically used in single domain spectral simulations of turbulent flows (Moin and Kim, 1982; Ounis et al., 1991; Pedinotti et al., 1992; Chen et al., 1995; Rouson et al., 1997; Narayan et al., 2003) SE is exponentially convergent with increasing the degree of the polynomial approximation without widening the discretization stencil and the overlap like in FD. Therefore, in addition to mesh flexibility, SE achieves high-order resolution. The grid convergence study is also simple and consistent and does not require changing the grid's topology.

Within the broad class of spectral element methods, one should distinguish between *continuous* and *discontinuous* SE. Both methods converge exponentially and are characterized by the high-order resolution and long-time accuracy discussed above, but establishes connectivity between elements differently. In the *continuous* SE (Karniadakis and Sherwin, 1999; Deville et al., 2002) connectivity between the elements is established by *global* assembly of local mass and stiffness matrices into one large matrix–vector formulation similar to finite element methods. This assembly is rather expensive and not very convenient for parallel implementation. In *discontinuous* spectral element methods (Hesthaven and Warburton, 2008) connectivity between elements is achieved by forcing the convective and diffusive fluxes to be continuous at the local element boundary only, while the solution is allowed to be discontinuous over element boundaries. When a computation is underresolved (i.e. too few grid points are used to resolve the Kolmogorov scale) this discontinuity is clearly visible in visualizations of the solution, but much less so when the solution is resolved. In other methods like continuous spectral element and even more so in FD, visualizations are much smoother. Smoothness in the solution, however, should not be confused with accuracy, a wrongful perception by many that are not familiar with the discontinuous formulation. In FD an underresolved computation is usually smooth, but clearly inaccurate. The discontinuous method is