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A semi-Lagrangian transport method for kinetic problems with application to dense-to-dilute polydisperse reacting spray flows

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ABSTRACT

For sprays, as described by a kinetic disperse phase model strongly coupled to the Navier–Stokes equations, the resolution strategy is constrained by accuracy objectives, robustness needs, and the computing architecture. In order to leverage the good properties of the Eulerian formalism, we introduce a deterministic particle-based numerical method to solve transport in physical space, which is simple to adapt to the many types of closures and moment systems. The method is inspired by the semi-Lagrangian schemes, developed for Gas Dynamics. We show how semi-Lagrangian formulations are relevant for a disperse phase far from equilibrium and where the particle–particle coupling barely influences the transport; i.e., when particle pressure is negligible. The particle behavior is indeed close to free streaming. The new method uses the assumption of parcel transport and avoids to compute fluxes and their limiters, which makes it robust. It is a deterministic resolution method so that it does not require efforts on statistical convergence, noise control, or post-processing. All couplings are done among data under the form of Eulerian fields, which allows one to use efficient algorithms and to anticipate the computational load. This makes the method both accurate and efficient in the context of parallel computing. After a complete verification of the new transport method on various academic test cases, we demonstrate the overall strategy's ability to solve a strongly-coupled liquid jet with fine spatial resolution and we apply it to the case of high-fidelity Large Eddy Simulation of a dense spray flow. A fuel spray is simulated after atomization at Diesel engine combustion chamber conditions. The large, parallel, strongly coupled computation proves the efficiency of the method for dense, polydisperse, reacting spray flows.

1. Introduction

Kinetic equations describe systems of particles in a statistical way and as point particles. They can be used to model problems with a large number of particles. Such problems are ubiquitous in physics and mechanical engineering; e.g., plasmas, rarefied gases, stellar clouds, neutron beams, spray clouds, particle suspensions, and granular gases. Kinetic equations are intrinsically related to fluid descriptions [45,6], but are generally used to account for systems that are far from equilibrium. They can be strongly coupled to other systems. For instance the Vlasov equation for charged particles [69] and the

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Williams–Boltzmann equation for polydisperse drops [95] are coupled to Maxwell and Navier–Stokes systems respectively and this coupling can be two-way. Such couplings actually constrain the choice of the resolution method, which is therefore case-dependent.

We are particularly interested in predicting spray injection, atomization, and combustion for mechanical engineering problems. In piston engines, adjusting the injection sequence is considered a viable way to improve efficiency while reducing pollutants. However, the injection process is multiphysics and multiscale: it involves the formation, transport, and evaporation of fuel drops that are 10^3 smaller than the combustion chamber length. Despite the increase in computational power, the representation of all these scales, together with the physics of compressibility, turbulence, entrainment, atomization, spray transport, phase change, mixing, and turbulent combustion, still involves many challenges. The multiscale nature of the disperse phase can be partially mitigated by a kinetic description, provided that the numerical strategy is accurate simultaneously on the transport in physical space, on the evolution of the numerous degrees of freedom of the drop phase space, and on the strong couplings to the compressible, turbulent, and reacting gas phase. In particular the near-nozzle region, which hosts the onset of turbulent and atomizing phenomena that are crucial to the physics of spray penetration and mixing, is characterized by high mass loadings and volume fractions of liquid. This situation is hereafter referred to as a dense spray, that connects to the dilute spray where the stoichiometry allows combustion. It requires one to capture the strong, two-way coupling [4,39] interactions in terms of mass, momentum, and heat transfers between the liquid and the gas. And for high volume fractions, the flow dynamics may also depend on particle–particle interactions (collisions, coalescence, and break-up), a situation sometimes referred to as four-way coupling [4]. Hence a comprehensive simulation strategy for direct fuel injection requires an accurate transport scheme for the kinetic description of sprays that can efficiently render strong coupling, including in the near nozzle region.

A widespread technique to solve kinetic equations is the stochastic Lagrangian approach. The qualification of stochastic is sometimes omitted but it is worth stressing the differences compared to deterministic Lagrangian approaches. The latter treatment would only be possible if the number of particles were sufficiently low and their initial and boundary conditions (IC/BC) sufficiently well known. On the contrary, the stochastic Lagrangian approach is insensitive to the physical number of particles and deals with IC/BC through modeled distributions. In most applications, the Lagrangian treatment of particles is in fact the result of a Monte-Carlo technique [40], so that it is referred to as Direct Simulation Monte-Carlo or DSMC by Bird [11]. DSMC computations therefore use parcels, which are misleadingly thought as being (bundles of) the physical particles. Still, many of the DSMC closures resemble the microscopic laws for a single particle, which makes DSMC a convenient choice together with its ease in describing high degrees of freedom of the underlying kinetic approach. It is an accurate way to describe the convection of particle clouds with multiple spatial scales and strong density gradients. Lagrangian methods have been widely applied to the simulation of sprays stemming from fuel injection [40,75,1,2] and to particle-laden flows [28,57,66,67]. Lagrangian methods are also applied to the simulation of charged particles in plasmas, the reader being referred to Birdsall and Langdon's monograph [12]. In the case of particle-laden flows, DSMC is considered as a reference method to solve the transport operator and is used to validate velocity closures [29,72,91]. It is also a well established approach in mechanical engineering problems such as gas turbines [87,60], solar concentrators [96], and chemical engineering risers [17]. For internal combustion engines with direct fuel injection, DSMC descriptions of the spray have allowed Reynolds Average Navier–Stokes (RANS) simulations with multiple physical phenomena like a moving piston [90] or a detailed turbulent-chemistry interaction model [77] as well as Large Eddy Simulations (LES) [58,93]. But stochastic Lagrangian simulations are difficult to converge leading to statistical noise and to spurious correlation patterns. For example in solid rocket boosters (SRB), the effect of aluminum oxide drop coalescence on polydispersity is sought in a space and time resolved fashion. But the dynamics of the aluminum oxide spray size distribution is rich enough for coalescence terms to require many DSMC samples to be present at a given location, typically more than 200 [57]. So that Lagrangian methods provide very noisy SRB results, even when coarse meshes are used in order to involve more samples in the local averages [37]. In general, the number of parcels with respect to physical space (particle size phase space) has a similar effect as the discretization of the physical (phase) space for Eulerian approaches. The uniformity of the parcels in spanning these spaces drives the accuracy of DSMC. But the uniformity strongly varies with time. The initial Monte-Carlo sampling may also influence the level of uniformity at each time in a way that depends on the flow. Therefore the evolution of sampling, which governs the accuracy of DSMC, is difficult to predict. Thus, efficiently converging DSMC simulations requires in fact knowledge of the conditionings and correlations stemming from the physics that is sought. Also, stochastic Lagrangian codes are more difficult to parallelize when two-way coupled to a phase described with the Eulerian formalism [50]. The coupling of two phases, one being described by a Lagrangian approach and the other one by an Eulerian approach, is sometimes referred to as the particle-in-cell method [24]. First, balancing the load among processors in the context of domain decomposition is made difficult. Stochastic Lagrangian parcels can indeed accumulate in some physical locations, whereas the Eulerian phase always has an even load by construction of the domains. Second, enforcing strong coupling between two phases which space discretizations do not match each other imposes a complex treatment [62,78]; e.g., a computationally extensive coupling between all the physical locations of the domain or an iterative procedure, resulting in a trade-off between accuracy and parallel efficiency.

As an alternative, one can consider Eulerian methods to solve kinetic equations; e.g., if any strong coupling exists (collisions, exchanges with another phase). The dynamics of charged particles in a plasma has been described on fixed grids using a Eulerian set of equations by many authors [20,47,46,18]. However, Eulerian methods require the reduction of the phase space size to be tractable. For instance, the peculiar dynamics of Water-Bag models for plasmas stems from such

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