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Realizable second-order finite-volume schemes for the advection of moment sets of the particle size distribution

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ABSTRACT

The accurate description and robust simulation at relatively low cost of a size polydisperse population of fine particles in a carrier fluid is still a major challenge for many applications. For this purpose, moment methods, derived from a population balance equation, represent a very interesting strategy. However, one of the major issues of such methods is the realizability: the numerical schemes have to ensure that the moment sets stay realizable, *i.e.* that an underlying distribution exists. This issue is all the more crucial that some moment vectors can be at the boundary of the moment space for practical applications, corresponding to a population of particles with only one or a few sizes. It is then investigated here for the advection operator, for which it is particularly significant. Then second order realizable kinetic finite volume schemes are designed, with two strategies for the fluxes evaluation based on the work of Kah et al. [1] and of Vikas et al. [2], which are here completely revisited, extended to take into account the boundary of the moment space and any number of moments, analyzed and compared in a Cartesian mesh context. For a potential easiest generalization to unstructured meshes, simplified but still realizable versions of these schemes are also developed. The high accuracy of all the schemes is then numerically checked on 1D and 2D test cases, with Cartesian meshes, and their robustness is shown, even when some moment vectors are at the boundary of the moment space.

1. Introduction

Populations of non-inertial particles in a carrier fluid are encountered in several kinds of applications (see [3] and references therein): soot in combustion applications, nanoparticles synthesis, microbubbles in biology processes, aerosol technology, ... Its evolution can be described by a population balance equation (PBE) [3–6], which is a transport equation for the number density function (NDF) of the particles. This NDF depends on time, spatial location and one or several internal coordinates, which can for example describe the size of the particles. The PBE includes usually the spatial transport terms, describing for example advection and diffusion, and some localized source terms describing, at each spatial location, phenomena such as nucleation, aggregation, coagulation, breakup, growth or oxidation/dissolution. It is coupled with the equations, usually Navier–Stokes equations, describing the carrier fluid [7].

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In this work, only one internal variable is considered, describing the size of the particles, assuming for example that they are spherical. In order to be able to describe the size polydispersion of the particles at a reasonable cost, the use of moment methods seems to be an interesting strategy (see for example [8,9,4]): only a finite set of moments of the NDF are then transported. It can also be hybridized with a discretization along the internal coordinate [10–14]. However, two major issues arise for moment methods. The first one is the closure of the moment equations essentially due to the source terms in the PBE. Several strategies were used: some of them provide a functional dependence of the unknown moments using the transported moment set, such as the interpolative closure (MOMIC) [15]. For the other ones, a NDF, or its corresponding measure, is reconstructed from the moment set, allowing evaluation of all the unclosed terms. This reconstruction can be for example the entropy maximization [16–18], a sum of Dirac delta function (quadrature method of moment, QMOM) [8] or a superposition of kernel density functions (kernel density element method, KDEM [19] or extended quadrature method of moment EQMOM [20–22]). The second major issue of moment methods is the realizability. Indeed, since the set of variables are the moments of a non-negative NDF (or, more rigorously, a positive measure) on $\mathbb{R}_+$ or a sub-interval of $\mathbb{R}_+$, it belongs to a space strictly included in $\mathbb{R}_+^N$, where N is the number of moments [23–25]. This space is called the moment space. The numerical methods have to ensure that the variables stay in this moment space, *i.e.* that the moments stay realizable. This issue is not always considered, thus leading to unphysical results (*e.g.* invalid moment sets). Indeed, the classical schemes for high-order transport in physical space can lead to invalid moment sets [26,2,27], as well as for the source terms [13,12], even if the closure itself ensures the realizability at the continuous level. This happens all the more easily when some moment sets are at the boundary of the moment space, thus corresponding to a sum of a few weighted Dirac delta functions, as obtained through nucleation. To circumvent this issue, some authors resort to moment correction algorithms [28,26] based on a necessary but eventually not sufficient condition for realizability in order to obtain a valid moment set. The cost of the method then increases and the correction spoils the overall accuracy.

It is then very important to develop realizable schemes, *i.e.* schemes directly preserving the realizability of the moment set. Moreover, an operator splitting strategy, solving separately the spatial transport of both phases and the source terms was shown to be efficient and well adapted to industrial-oriented codes [29]. This allows us to deal separately with the spatial transport and the source terms. Concerning the source terms, realizable schemes were already developed for moment methods where the closure is based on a reconstruction of the NDF [13,4,12]. A realizable scheme was also provided for the diffusion operator in the case of QMOM [27,4]. In this work, only advection then is considered. In practice, this operator, at least when using first order explicit finite volume methods, is usually much less costly than the potentially complex source term operator, composed of one ODEs system for each considered moment vector. So, it will be very interesting to minimize the number of degree of freedom by using a high order scheme for advection, as soon as its cost is not prohibitive.

A Lagrangian type of scheme has been developed [30]. The advection of the moments is then obtained through the advection of some numerical particles for which a moment vector is affected. The resulting scheme is then naturally realizable. However, it suffers from the same drawbacks as usual Lagrangian methods: the need of interpolation of the carrier phase properties, the non-easy coupling with this phase and the complexity in term of parallelization for high performance computing. Moreover, it could need a large number of numerical particles to converge, for which the eventually costly source terms operator has to be solved. That is why only Eulerian schemes are studied here. On the one hand, a second-order realizable kinetic finite volume method has been developed in a structured mesh context [1], when the support of the NDF is compact. It was recently applied in a context of a mesh refinement [31]. It is based on a kinetic evaluation of the fluxes thanks to the use of the analytical solution at the kinetic level and on a MUSCL type of reconstruction on the canonical moments, which define a one to one relation between the interior of the moment space and the interior of an hypercube. However, it was only applied for inertial particles and for a four moments method, the algebra being otherwise difficult. On the other hand, a pseudo–second-order realizable finite volume method [2] has been developed in structured and unstructured mesh contexts. Fluxes computation is then based on a reconstruction of the moments at the cell interfaces; it is obtained thanks to the Gauss quadrature of the moments, just reconstructing the weights. However, it was reduced to an even number of moments and suffers from some accuracy reduction when the quadrature points evolve strongly. In this work, the last two schemes are completely revisited, generalizing them to any number of moments and allowing them to deal with the boundary of the moment space without loosing the realizability, which is an hard task. They are also analyzed, especially looking for conditions to obtain the second order of accuracy, and they are compared. This is done for NDF of support included in $[0, +\infty)$, the case of a compact support being discussed in the appendix. Kinetic schemes are thus derived in a structured mesh context, first with a reconstruction on variables defining a one to one relation between the interior of the moment space and $(0, +\infty)^N$, where N is the number of moments in the set. Algorithms are then adapted to the case of the support included in $[0, +\infty)$ and generalized to any number of moments. The weight reconstruction is also considered, for an even or an odd number of moments, in a different way compared to [2], thus not being dependent of abscissas differences between the cells. Simplified schemes are then derived with the two kinds of reconstructions, the first one being modified for this case. It will be generalizable to unstructured meshes in a cell-centered context.

The paper is then organized as follows. In Section 2, the moment equations for the pure advection case are given, as well as the realizability constraints. Then, in Section 3, realizable finite volume kinetic schemes are provided and their orders of accuracy discussed. Some simplified versions of these schemes are also given in Section 4, as well as the new constraint on the CFL to guarantee the realizability. Finally some verifications are given, considering systems with high numbers of moments, first for 1D configurations with steady or unsteady and compressible carrier phase velocity fields in Section 5 and for the 2D configuration of the Taylor–Green vortices in Section 6.