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# Conditional quadrature method of moments for kinetic equations

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ABSTRACT

Kinetic equations arise in a wide variety of physical systems and efficient numerical methods are needed for their solution. Moment methods are an important class of approximate models derived from kinetic equations, but require closure to truncate the moment set. In quadrature-based moment methods (QBMM), closure is achieved by inverting a finite set of moments to reconstruct a point distribution from which all unclosed moments (e.g. spatial fluxes) can be related to the finite moment set. In this work, a novel moment-inversion algorithm, based on 1-D adaptive quadrature of conditional velocity moments, is introduced and shown to always yield realizable distribution functions (i.e. non-negative quadrature weights). This conditional quadrature method of moments (CQMOM) can be used to compute exact *N*-point quadratures for multi-valued solutions (also known as the multivariate truncated moment problem), and provides optimal approximations of continuous distributions. In order to control numerical errors arising in volume averaging and spatial transport, an adaptive 1-D quadrature algorithm is formulated for use with CQMOM. The use of adaptive CQMOM in the context of QBMM for the solution of kinetic equations is illustrated by applying it to problems involving particle trajectory crossing (i.e. collisionless systems), elastic and inelastic particle–particle collisions, and external forces (i.e. fluid drag).



## 1. Introduction

The kinetic equation for the velocity distribution function is used in many applications [2,8–10,12,16,21,34,35,37,40–42,44,45,60,66,67,70,72,76], and thus there have been many computational methods developed to find numerical solutions. At present, there are two classes of methods that can be used to find accurate solutions to the kinetic equation: (i) direct solvers that discretize velocity phase space [2,7,36,55,59,60] and (ii) Lagrangian methods [4]. However, the computational cost of using either of these methods in many applications is prohibitive. In most applications we are not interested in knowing the exact form of the velocity distribution function, rather knowledge of its lower-order moments is sufficient [70]. Moreover, for systems with strong two-way coupling, the statistical noise inherent in Lagrangian methods makes coupling problematic [61,62]. For these reasons, there is considerable motivation to develop *predictive* moment closures whose accuracy can be improved in a rational manner [41,52,71,72]. Quadrature-based moment methods (QBMM) [17,19,26,28,31,48,56] fall into this category because, in principle, the accuracy of these closures can be improved by increasing the number of quadrature nodes [38,58]. Nevertheless, a key technical challenge with QBMM is the development of efficient moment-inversion algorithms for three-dimensional velocity moments [28] that can be extended to reconstruct the velocity distribution function using higher-order moments, a problem that is closely related to the classical problem of moments [20,22–25,68,69].

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Because the weights are non-negative and the velocity abscissas are located in velocity phase space, QBMM provide a *realizable*, Galilean invariant discretization of velocity phase space that is consistent with the underlying moments [20]. Moreover, if integer moments up to order $\gamma$ are used in the moment-inversion algorithm, the quadrature-based estimation of the moment of order $\gamma + 1$ is optimal in the sense that it is closest to the true value and has the smallest possible error [38,75]. Compared to direct solvers, QBMM discretization of velocity phase space is very sparse (equal to the number of quadrature nodes). An important open question is thus to determine the range of accuracy that can be achieved using QBMM in comparison to direct solvers. Generally, in order to improve the accuracy for finite Knudsen numbers, the number of quadrature nodes (and hence the number of transported velocity moments) must be increased. In [28] the moment-inversion algorithm was limited to 8-node quadrature and 14 velocity moments up to third order. In [29] the problem of finding a moment-inversion algorithm for higher-order velocity moments was addressed. The proposed algorithm computes an $n^3$-node quadrature using $(n^2 + 3)n$ velocity moments, where $n$ is the number of quadrature nodes in each direction. However, because the quadrature weights are found by solving a linear system, for $n \geqslant 3$ non-negative weights are not guaranteed unless the order of the quadrature is reduced to $n = 2$ [28]. For example, in granular systems with sufficiently inelastic collisions [63] some of the weights are negative, thereby limiting the range of applicability of the moment-inversion algorithm to nearly elastic systems. Therefore, in order to expand the range of applicability of QMBB, one of the principal objectives of the present work is to develop a higher-order quadrature with strictly non-negative weights.

In principle, an optimal moment-inversion algorithm could be based on the iterative solution of $(1 + d)n^3$ nonlinear equations for the same number of velocity moments. However, the nonlinear system is poorly conditioned and convergence is never guaranteed. Another opinion is to solve directly the transport equations for the quadrature weights and abscissas using the direct quadrature method of moments (DQMOM) [26,27,56] and a set of so-called 'optimal moments' [30]. Indeed, in some sense, the weights and abscissas can be considered as the 'primitive variables', and the moments as the 'conserved variables'. Therefore, since conservation errors seriously degrade the accuracy of the flow solver, QBMM are usually preferred to DQMOM for solving kinetic equations. Other challenges to using DQMOM for hyperbolic systems are that the abscissas need not be continuous in space [31], and that the number of abscissas can change due to particle trajectory crossings leading to multi-valued solutions [1,6,19,39,46,47,53,54,77]. Thus, in summary, our goal is to develop a moment-inversion algorithm for QBMM that (i) ensures realizable weights for any set of realizable moments, (ii) avoids iterative solution of the moment constraints, and (iii) utilizes the maximum number of the $(1 + d)n^3$ optimal moments. Ideally, the moment-inversion algorithm would also generate exact quadratures for systems defined by an $N$-point distribution[1] (i.e. the truncated $K$-moment problem in several variables [18]). The algorithm presented in Section 3, based on conditional moments, achieves all of these goals.

Another difficulty with existing moment-inversion algorithms [28,29,48] is that they, in fact, define an infinite number of different quadratures, one for each angle of the rotation matrix used to diagonalize the velocity covariance matrix. Moreover, none of these quadratures is guaranteed to reproduce an $N$-point distribution, resulting in a quadrature error that depends on the rotation angle. For continuous distributions, the principal inconvenience of using the existing moment-inversion algorithms is the number of moments that must be transported for higher-order quadrature due to the rotation [29] (i.e. many more than are actually controlled by the moment-inversion algorithm). The conditional moment-inversion algorithm proposed in this work also has multiple quadratures (i.e. one for each permutation of the conditioning variables), but because all permutations exactly reproduce an $N$-point distribution, we show that they can be treated as multiple *non-random* samples of the distribution function without introducing a quadrature error. Furthermore, the set of transported moments used in this work is fixed (i.e. the optimal moment set used in DQMOM) and much smaller than the moment sets used in the high-order moment-inversion algorithms derived in [29].

The remainder of this work is organized as follows. In Section 2 we provide a brief overview of the kinetic equation and the corresponding moment equations, as well as a short discussion of QBMM. Readers interested in more details can consult our earlier works [19,28,29,32,62]. In Section 3 a detailed derivation of the conditional moment-inversion algorithm is provided, along with sample codes in Appendices A and B to illustrate the numerical implementation of the theory. In Section 4 we describe how the new moment-inversion algorithm, combined with finite-volume methods, can be used to solve the moment transport equations, while ensuring that the moment set is always realizable. In Appendix C we discuss two types of quadrature errors associated with finite-volume methods. Example applications of kinetic equations solved using QBMM and the proposed moment-inversion algorithm are provided in Section 5. Finally, conclusions are drawn in Section 6.

## 2. Moment methods for kinetic equations

QBMM and the moment-inversion algorithm introduced in Section 3 should be applicable to any closed kinetic equation.[2] For clarity, in this work we will consider the kinetic equation for fluid-particle flows with terms for free transport, acceleration forces, and particle–particle collisions. Note that most moment methods are designed to work for systems near equilibrium where the collisions are dominant [41,52,70,71] (i.e. small Knudsen numbers). In contrast, QBMM can be applied for arbitrary

[1] An $N$-point distribution is composed of $N$ delta functions located at distinct points in $d$-dimensional phase space.

[2] A *closed* kinetic equation contains only the one-particle distribution function. Terms involving multi-particle physics (e.g. collisions) must therefore be modeled in terms of the one-particle distribution function in order to close the kinetic equation.