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Method of moments over orthogonal polynomial bases

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HIGHLIGHTS

- A numerical scheme based on the method of moments and characteristics is derived.
- It is suitable for a wide class of PBEs with size-dependent growth rate.
- It represents an enhancement to an earlier scheme based on Taylor approximation.
- This is accomplished by introducing least square approximation instead.
- The method is generalized to multivariate particulate systems.

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ABSTRACT

A method for the design of approximate models in the form of a system of ordinary differential equations (ODE) for a class of first-order linear partial differential equations of the hyperbolic type with applications to monovariate and multivariate population balance systems is proposed in this work. We develop a closed moment model by utilizing a least square approximation of spatial-dependent factors over an orthogonal polynomial basis. A bounded hollow shaped interval of convergence with respect to the order of the approximate ODE model arises as a consequence of the structural and finite precision computation numerical errors. The proposed modeling scheme is of interest in model-based control and optimization of processes with distributed parameters.

1. Introduction

We propose a generalized method of moments for particulate systems in the property space $\mathbb{R} \ni x$, described by the linear partial differential equations (PDEs) of the form:

$$\frac{\partial f}{\partial t}+\frac{\partial}{\partial x}(G(x,t)f(x,t))=B(t)\delta(x), \tag{1a}$$

as well as its extensions to the corresponding multivariate systems with $x \in \mathbb{R}^n$. In (1a), $f=f(x,t)$, $G=G(x,t)$, $B(t)$, and $\delta(x)$ represent the distribution function, the size-dependent growth-rate, the birth-rate and the Dirac-function, respectively. Our work is based on the factorizing condition specified by

$$G(x,t)=\gamma(x)G_0(t), \tag{1b}$$

where $\gamma(x)$ and $G_0(t)$ represent arbitrary piece-wise continuous positive functions. Note that the time dependency of functions $G_0=G_0(t)$ and $B=B(t)$ in the particulate processes of our interest shall be rather implicit, in that we assume

$$G_0(t):=G_0(u(t),\mu(t)), \quad B(t):=B(u(t),\mu(t)), \tag{2}$$

where $u(t)$ refers to some fixed external variable (e.g. the temperature T) and $\mu(t)$ to the moments of the distribution function. In particulate systems, the equations (2) are coupled to the PDE (1a) by systems of nonlinear ordinary differential equations (ODEs) that describe the evolution of the state variables of the continuous phase amounting to conservation laws.

In the current work, we propose a generalization of our previous results published in Bajcinca et al. (2011) on approximate characterizations of the solutions of the PDE (1a) by means of an ODE (ordinary differential equation) scheme, which was developed on the basis of a proper utilization of the method of characteristics, method of moments, and Taylor approximation of

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the function $x(\lambda)$ about $\lambda = 0$, which represents the solution to the differential equation

$$\frac{\mathrm{d}x}{\gamma(x)} = \mathrm{d}\lambda, \quad x(0) = 0. \tag{3}$$

Our current work is motivated by the fact that the latter approach is limited by the radius of convergence of the underlying Taylor series. While we show that for linear terms of the form $\gamma(x) = 1 + \alpha x$ this is not an issue, in the nonlinear case, e.g., for $\gamma = (1+\alpha x)^z$, $z < 1$, the scheme may suffer from an insufficient radius of convergence, leading to false divergent solutions. To overcome such difficulties, here, we invoke a generalized approximation of the form

$$x^i(\lambda) \approx \sum_{k=0}^{p} b_{ki}\phi_k(\lambda), \quad i = 0, 1, 2, \ldots, \ll p, \tag{4a}$$

instead, where $\phi_0, \phi_1, \ldots, \phi_p$ represent a fixed polynomial basis. This approach leads eventually to a generalized method of moments in the transformed domain $(\lambda, t) \leftarrow (x, t)$, associated with the scaled density function

$$\tilde{f}(\lambda, t) := \gamma(x(\lambda)) f(x(\lambda), t) \tag{4b}$$

and its generalized moments ν_i, defined in accordance with

$$\nu_i(t) = \int_0^\infty \phi_i(\lambda)\tilde{f}(\lambda, t)\,\mathrm{d}\lambda, \quad i = 0, 1, 2, \text{etc.} \tag{4c}$$

Note that the concepts of the eigenmoments, as introduced in Bajcinca et al. (2011), and the standard monomial moments μ_i from Hulburt and Katz (1964), given by

$$\nu_i(t) = \int_0^\infty \lambda^i \tilde{f}(\lambda, t)\,\mathrm{d}\lambda \quad \text{and} \quad \mu_i(t) = \int_0^\infty x^i f(x, t)\,\mathrm{d}x \tag{4d}$$

respectively, are recovered as special cases thereof, corresponding to the basis of the monomials $\phi_i = \lambda^i$ in the former case, and $\phi_i = x^i$ in the latter case (with $\gamma(x) \equiv 1$).

These ideas are completed by involving an orthogonal polynomial basis $\{\phi_k\}_{k=0}^{\infty}$, as a convenient and numerically efficient approach to solving the problem (4a) in the least square sense. To this end, we focus on the evaluation of the method by utilizing the orthonormal family of the discrete Gram polynomials. In addition, we carry out a number of steps towards further improvement of the numerical efficiency and robustness of the scheme, for instance, by employing the three-term recurrence characterization of sequences of orthogonal polynomials.

As already mentioned, the proposed method relies on a combination of the method of characteristics (see, e.g. Sarra, 2003), method of moments (Hulburt and Katz, 1964) and special approximation techniques. Numerous related methods and numerical schemes that are able to deal with the class of processes involving advection and nucleation, cf. (1a), as well as with additional physical phenomena in population balance systems such as aggregation and breakage, are spread across the engineering and applied mathematics literature. Such schemes include those based on the method of characteristics (Kumar and Ramkrishna, 1997; Févotte and Févotte, 2010), the quadrature method of moments (QMOM) (McGraw, 1997; Qamar et al., 2010; Grosch et al., 2007; Aamir et al., 2009; Marchisio and Fox, 2005), method of weighted residuals or orthogonal collocation (Singh and Ramkrishna, 1977; Rawlings et al., 1992; Chiu and Christofides, 1999), the Monte Carlo simulation (Smith and Matsoukas, 1998), the finite difference schemes/discrete population balances (Kumar and Ramkrishna, 1996), the high-resolution finite volume methods (HRFV) (Koren, 1993; Gunawan et al., 2004; Qamar et al., 2006), etc. An early work which is related to our approach in terms of the expansion technique by means of orthogonal polynomials is Wang et al. (1987), whereby a direct expansion of the distribution function is involved, leading to a differing scheme.

In contrast to most of these contributions, our main concern refers to the design of explicit ODE models of the form

$$\dot{\mathbf{x}} = \mathbf{a}(\mathbf{x}, u(t)), \quad \mathbf{y} = \mathbf{b}\mathbf{x}, \tag{5}$$

with $u \in \mathbb{R}$, $\mathbf{x} \in \mathbb{R}^{p+1}$ and $\mathbf{y} \in \mathbb{R}^q$. Hereby, the vector $\mathbf{x}$ collects the moments, as defined by (4c), u refers to a fixed external variable, and $\mathbf{y}$ to some observables, such as the standard monomial moments (4d) (right) or a function thereof; $\mathbf{a}$ represent a real vector field and $\mathbf{b}$ is a real matrix. In the case of monovariate crystallization processes we show that this leads to a bilinear affine model (cf. Section 7.1). The computational benefits of our scheme result from its lean finite dimensional ODE structure of a model corresponding to a system which is inherently infinite dimensional. Thus, our approach amounts to derivation of reduced-order models and it is tailored to address different control and optimization tasks for the process models described by the PDE (1a) by means of standard ODE tools and techniques. For instance, it is well suited for the applications in the context of trajectory planning and optimal control in batch crystallization (Miller and Rawlings, 1994; Bajcinca, 2013), real-time feedback model predictive control (Shi et al., 2005, 2006), particle shape manipulation in multivariate crystallization (Patience and Rawlings, 2001; Lovette et al., 2008), and dynamic inversion in preferential crystallization of enantiomers, where a coupling of two or more PDEs (1a) arises (Hofmann and Raisch, 2012, 2013), just to name a few. The limitations of our scheme result from the structural assumptions on the PDE (1a), e.g., related to the factorizing condition (1b). For instance, our scheme does not apply to the size-dependent growth rate models such as those based on the LSW-theory (Iggland and Mazzotti, 2012) without a further ado. On the other hand, the proposed method of moments shall not address additive filtering terms and aggregation/breakage kernels in the PDE (1a). Several approaches mainly motivated by the idea of the Gaussian quadrature (see, e.g. Qamar et al., 2006; Aamir et al., 2009) have been developed to address such phenomena, but have to dispense with a pure ODE structure. We provide a thorough comparison of our scheme to the popular and widely used QMOM and HRFV on a series of case-studies. On this basis, we demonstrate numerically the advantages of our ODE scheme in terms of accuracy, efficiency and robustness for the underlying class of systems (1a). It turns out that a trade-off between the structurally induced errors and numerical least-square round-offs, both due to (4a), has to be made. Our investigations reveal thereby the existence of a hollow shaped p-interval of convergence, which is lower bounded by a sufficiently large number of the polynomials in approximating $x^i(\lambda)$ in (4a) and upper bounded by the related numerical round-off errors that may lead to diverging solutions.

The remainder of the paper is organized as follows. In Section 2, we review the analytical steps in solving (1a) based on the method of characteristics. In Section 3, we review briefly our related previous work based on Taylor expansion and give an insight into the corresponding convergence issues. The generalizing ideas are presented in Section 4, while the least square application and related numerical techniques are discussed in Sections 5 and 6, respectively. The usability of our approach is illustrated on univariate and bivariate batch crystallization processes with size-dependent growth rate kinetics in Section 7. Additionally, we provide a numerical comparison to QMOM and HRFV schemes in terms of accuracy using various numerical scenarios. The utilized nomenclature is given in Table 1.