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Fast evaluation of univariate aggregation integrals on equidistant grids

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ABSTRACT

A variety of production processes in chemistry and biotechnology are concerned with particles dispersed in an environmental phase. The particle distribution is mathematically described by the solution of population balance equations of integro-differential type. We are concerned with the aggregation process: it invokes an integral term that is usually numerically expensive to evaluate and often dominates the total simulation cost. We will expose the algorithmic details of an efficient approach based on a separable approximation of the aggregation kernel and a subsequent fast Fourier transformation. This approach reduces the originally quadratic complexity to an almost optimal complexity $\mathcal{O}(n \log n)$ in the dimension of the approximation space. We include numerical tests illustrating its application to representative aggregation kernels from the literature. While originally developed in the context of a discretization with piecewise constant functions, we illustrate how these ideas can be applied in the setting of the popular sectional methods.

1. Introduction

A variety of production processes in chemistry and biotechnology are concerned with particles dispersed in an environmental phase. Examples are the crystallization and precipitation of pharmaceutical materials, the synthesis of polymers, the formulation of emulsions, the generation of nanoparticles by flame pyrolysis, the growth of living cell populations in fermentation processes, and the separation of fermentation broths by flocculation and sedimentation. In all these processes, the dispersed phase consists of a population of particles which can be characterized by property coordinates x, e.g. the particle size, the particle area, or the chemical composition, to mention only a few. The state of the whole particle population is quantified by a number density function $f(x, t)$ which describes the property distribution of the particles at given time t Ramkrishna (2000). Due to growth, birth and death phenomena the density function f varies dynamically with time. Neglecting spatial variations, the dynamic evolution of f is governed by a population balance equation (PBE) which is a partial integro-differential equation of the general form

$$\frac{\partial f(x,t)}{\partial t} + \nabla_x \cdot (G f(x,t)) = Q(f) = Q_{\text{nuc}}(f) + Q_{\text{break}}(f) + Q_{\text{agg}}(f), t \in [0,T]. \quad (1)$$

The second term of the left-hand side of (1) represents the growth of particles at the rate G. On the right-hand side, Q summarizes the birth and death terms of particles due to nucleation Q_{nuc}, breakage Q_{break} and aggregation Q_{agg}. Nucleation, i.e. the birth of new particles in the continuous phase, is a local effect in the property space, while breakage and aggregation are long range effects, i.e. they describe the interaction of (mother and daughter) particles belonging to different parts of the property space. Neglecting breakage at this point, the aggregation term can be expressed by the following source (birth) and sink (death) integrals:

$$Q_{\text{agg}}(f) = Q_{\text{source}}(f) - Q_{\text{sink}}(f) \quad (2)$$

with

$$Q_{\text{source}}(f)(x,t) = \frac{1}{2}\int_0^x \kappa(x-y,y) f(x-y,t) f(y,t)\, dy, \quad (3)$$

$$Q_{\text{sink}}(f)(x,t) = f(x,t)\int_0^{1-x} \kappa(x,y) f(y,t)\, dy. \quad (4)$$

where $\kappa(x, y)$ stands for the kernel function describing the rate constant of aggregation in dependence on the properties of two

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aggregating particles, x and y. The source integral (3) is quadratic with respect to f and is of convolution type. It describes the effect that new particles are generated by the combination of smaller ones, while the sink integral (4) quantifies the effect that particles are consumed by aggregation with others. Note that we assume here that all particles have (non-dimensionalized) properties in the interval $(0, 1]$. Consequently, a particle of size x can only aggregate with particles up to the maximum size $(1-x)$.

Only for special expressions of the kernel function, in particular for $k(x, y) = \text{const}$., analytical solutions of PBEs with aggregation terms can be obtained, for example by application of Laplace transformation. Thus, several groups have elaborated numerical schemes for the evaluation of univariate aggregation integrals, i.e. aggregation of particles characterized by one single property coordinate x. The particle size (or mass/volume) was usually considered as particle property.

One of the most popular numerical techniques, often denoted as the sectional method, was introduced in Kumar and Ramkrishna (1996a), Kumar and Ramkrishna (1996b). It is based on fixed or moving pivotal points (or simply pivots) which concentrate the particles in different intervals along x at a finite number of representative points. Later, in Kumar et al. (2006), an improved sectional method was established which assigns the particles within the cells more precisely and thereby achieves higher accuracy and better convergence. The same authors compared the cell averaging technique also to the finite volume scheme developed in Filbert and Laurencot (2004). It was concluded that the best choice of the numerical technique depends on the priorities set by the applications, Kumar et al. (2009).

As the main alternative to the sectional approach, various quadrature methods of moments (QMOM) were developed. A systematic comparison of these quadrature methods can be found in Grosch et al. (2007). Marchisio et al. (2003) were among the first who applied the QMOM approach for the numerical solution of aggregration-breakage processes. The QMOM overcomes the problem of the standard method of moments which is applicable to size-independent aggregation and breakage kernels only. It is able to track with very small error all the moments involved in the quadrature approximation, thereby solving the problem of most of the sectional methods, which are able to preserve only two moments of the particle size distribution (PSD). But the main disadvantage of using the QMOM is that the PSD is not directly accessible.

Hence, it is desirable to develop a numerical technique which directly yields the PSD, in particular the aggregation integral terms, at high precision and low computational costs. For this purpose, Hackbusch (2006) has introduced an approach which combines a separable approximation of the kernel function $\kappa(x, y)$ with the fast Fourier transform for the arising convolution integrals. This approach drastically reduces the evaluation cost of the most challenging integral term (3) in each time step to $\mathcal{O}(n \log n)$ if the interval is divided into n subintervals. The aim of the present contribution is to expose the algorithmic details of the technique of Hackbusch (2006) for equidistant grids and to illustrate its application to several aggregation kernels taken from the literature.

The remainder of this paper is organized as follows: In Section 2, we present the separable kernel approximation. Section 3 reviews the fast evaluation of the aggregation source integral through multiple use of fast Fourier transformations and presents it explicitly in algorithmic form. While originally developed for a discretization with piecewise constant functions, it is shown how the same approach can be applied in the setting of sectional methods, leading to highly efficient algorithms. In Section 4, we provide numerical results illustrating the performance of the proposed algorithms for different kernel functions. The entire work is focused on the univariate aggregation problem. Subsequent investigations will be concerned with the bivariate case.

2. Kernel functions and separable approximations

The aggregation source and sink integrals (3), (4) include a kernel function $\kappa(x, y)$ which specifies the rate constant at which particles of mass x and y aggregate. In this paper, we will consider the following representative aggregation kernels taken from the literature Aldous (1999), Bramley et al. (1996) and illustrated for $(x, y) \in [0, 1]^2$ in Fig. 1:

Kernel	Comment
$\kappa_B(x, y) := (x^{1/3} + y^{1/3}) \cdot (x^{-1/3} + y^{-1/3})$	Brownian motion (continuum)
$\kappa_S(x, y) := (x^{1/3} + y^{1/3})^{7/3}$	shear (non-linear velocity profile)
$\kappa_G(x, y) := (x^{1/3} + y^{1/3})^2 \cdot \lvert x^{2/3} - y^{2/3} \rvert$	inertia and gravitational settling
$\kappa_K(x, y) := (x^{1/3} + y^{1/3})^2 \cdot (xy)^{1/2}(x + y)^{-3/2}$	based on kinetic theory

The efficient evaluation of the aggregation source and sink integrals will be based on a separable approximation of the kernel. A function $\kappa(x, y)$ is called separable with separation rank k if it can be expressed in the form

$$\kappa(x, y) = \sum_{\nu=1}^{k} \alpha_\nu(x)\beta_\nu(y)$$

where α_ν and β_ν are some suitable functions, which in our context need to be integrable. The length k of the sum is called the separation rank.

Among the four aggregation kernels presented above, only the Brownian motion kernel κ_B is separable. It has separation rank 3 in view of

$$\kappa_B(x, y) = 2 + x^{1/3}y^{-1/3} + x^{-1/3}y^{1/3}.$$

The shear kernel κ_S and kinetic kernel κ_K are not separable because of the rational (non-integer) exponents of sums of functions in x and y, and the gravitational kernel is not separable because of the factor involving the absolute value of sums of functions in x and y. For these remaining three kernel functions, one may approximate $\kappa(x, y)$ either by a global separable rank-k approximation

$$\kappa(x, y) \approx \sum_{\nu=1}^{k} \alpha_\nu(x)\beta_\nu(y), \tag{5}$$

or, if necessary, locally by

$$\kappa(x, y) \approx \sum_{\nu=1}^{k_{ij}} \alpha_\nu^{ij}(x)\beta_\nu^{ij}(y) \qquad \text{for } (x, y) \in I_i \times I_j \tag{6}$$

with subintervals $I_i, I_j \subset [0, 1]$. The global approach (5) will turn out to be suitable for the shear kernel κ_S as well as for the kinetic kernel κ_K. The gravitational kernel, however, requires locally different separable approximations (6).

We will provide details on the construction of separable approximations for the three kernels of interest in Section 4 on numerical results. In general, there exist several analytic approaches in the literature to derive such separable approximations, including (Chebyshev) interpolation, sinc approximation Hackbusch (2009b) or approximation by exponential sums. Alternatively, a separable approximation could also be computed on the discrete side. This approach would require the computation of a low rank (global approach) or a blockwise low rank (local approach) approximation to the discrete kernel matrix $K = (\kappa_{ij}) \in \mathbb{R}^{n \times n}$ where $\kappa_{ij} := \kappa(i/n, j/n)$.