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Algorithms for the Haar wavelet based fast evaluation of aggregation integrals in population balance equations

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ABSTRACT

In several production processes, the distribution of particles dispersed in an environmental phase may be mathematically described by the solution of population balance equations. We are concerned with the development of efficient numerical techniques for the aggregation process: It invokes an integral term that is usually numerically expensive to evaluate and often dominates the total simulation cost.

We describe an approach on locally refined nested grids to evaluate both the source and the sink terms in almost linear complexity (instead of quadratic complexity resulting from a direct approach). The key is to switch from a nodal to a wavelet basis representation of the density function. We illustrate the numerical performance of this approach, both in comparison to a discretization of piecewise constant functions on a uniform grid as well as to the fixed pivot method on a geometric grid.

1. Introduction

Several production processes in chemistry and biotechnology are concerned with particles dispersed in an environmental phase. In such 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 entire particle population is quantified by a number density function $f(x,t)$ which describes the property distribution of the particles at a given time t [19]. Due to growth, birth and death phenomena, the density function f varies dynamically with time. In this paper, we will focus on the numerical treatment of the source (birth) and sink (death) terms of particle aggregation. Neglecting spatial variations as well as terms modeling particle nucleation, growth or breakage, the dynamic evolution of f is governed by a population balance equation (PBE) which is a partial integro-differential equation of the form

$$\begin{aligned}\frac{\partial f(x,t)}{\partial t} &= Q_{\text{agg}}(f)(x,t)\\ &:= Q_{\text{source}}(f)(x,t) - Q_{\text{sink}}(f)(x,t), \qquad x \in (0,1],\ t \in [0,T],\end{aligned} \tag{1}$$

with aggregation source and sink terms

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

$$Q_{\text{sink}}(f)(x,t) = f(x,t) \int_0^{1-x} \kappa(x,y) f(y,t)\, dy. \tag{3}$$

Here, $\kappa(x,y)$ stands for the kernel function describing the rate of aggregation in dependence on the properties of two aggregating particles, x and y (here assumed to be time-independent). The source integral (2) 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 (3) quantifies the effect that particles are consumed by aggregation with others. In a previous study, the calculation of the aggregation integral took around 85% of the overall computational time of a population balance simulation [2]. Note that we assume here that all particles have (non-dimensionalized) properties x in the interval $(0,1]$. Consequently, a particle of size x can only aggregate with particles up to the maximum size $(1-x)$. In this paper, the particle mass is considered as particle property.

In [9], an algorithm for the efficient evaluation of the (source) aggregation integral has been developed both for uniform as well as for locally refined nested grids. The approach requires a separable approximation of the kernel function and employs multiple applications of (inverse) fast Fourier transformations for the evaluation of convolution sums on equidistant grids. In the case of a locally refined nested grid, a transformation to a wavelet basis is introduced which allows for the recursive application of the efficient FFT-based techniques for equidistant grids on equidistant portions of the graded grid corresponding to (grid) levels of refinement.

In [17], this algorithm has been illustrated numerically on equidistant grids for several representative kernel functions from the literature. In particular, the computation of the sink term has been included and the fast evaluation techniques have been extended to the fixed pivot technique on equidistant grids.

Toward the goal of (further) reducing the computational complexity, graded meshes have been proposed which are finer for small compared to large particle sizes. The motivation for using such a grid is given in situations with larger quantities of small particles compared to large ones, suggesting finer partitions for the small particles. The particular structure of the suggested nested grading results from the observation that the aggregation of particles of similar sizes leads to new particles of approximately twice the size.

The geometric grid, defined through gridpoints $x_{i+1} = 2^s x_i$ with an initial gridpoint $x_0 > 0$ and a suitable $s \in (0,1]$, is a popular example of a graded mesh which can be used in connection with the fixed pivot technique, however, leading to a computational complexity that is quadratic in the number of grid points. A different type of graded grid, a so-called *locally refined nested grid*, permits an evaluation algorithm of almost optimal complexity. Locally refined nested grids are similar to the above mentioned geometrically graded grids in the sense that intervals close to the origin are smaller than those further away. However, they differ since they are of a nested nature, i.e., the finer mesh results from the local refinement of (certain intervals of) a coarser one. An example of such a grid is shown in Fig. 1 (bottom).

The novel contributions of this current paper consist of the development and numerical illustration of an algorithm that permits the evaluation of the aggregation source and sink terms on a locally refined nested grid in almost optimal complexity. In particular, this paper presents

- the development of an efficient implementation of the (almost) optimal complexity evaluation technique for the source term of the aggregation integral whose theoretical foundation has been established in [9]. We propose suitable data structures (e.g., (10), (11)), expose connections between different parts of the algorithm that can be exploited for its efficient implementation (Lemma 1) and provide explicit algorithmic representations (chapters 2, 3),
- the development of a novel efficient evaluation algorithm for the aggregation sink term on graded grids, exploiting properties of wavelet bases (in chapter 4),
- a numerical illustration of the constants involved in the complexity estimates (in chapter 6), i.e., to show in practice how the contruction of a graded grid affects the computational time and in particular when the computational overhead of basis transformations required in a graded grid pays off compared to an equidistant grid. In addition to a comparison with the aggregation term evaluation on an equidistant grid, we also include numerical tests for the popular fixed pivot technique on geometrically graded grids.

The remainder of this paper is organized as follows: In section 2, we define locally refined nested meshes, associate function spaces and bases for these spaces. In sections 3 and 4, we discuss the efficient evaluation of the source and sink terms of the aggregation, respectively, for the grids and function spaces of the preceding section. Section 5 reviews the fixed pivot technique which is used for comparison in the numerical results provided in section 6. The paper finishes with conclusions and an outlook to future work.