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Convergence analysis of sectional methods for solving aggregation population balance equations: The fixed pivot technique

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ABSTRACT

In this paper, we introduce the convergence analysis of the fixed pivot technique given by S. Kumar and Ramkrishna (1996) [28] for the nonlinear aggregation population balance equations which are of substantial interest in many areas of science: colloid chemistry, aerosol physics, astrophysics, polymer science, oil recovery dynamics, and mathematical biology. In particular, we investigate the convergence for five different types of uniform and non-uniform meshes which turns out that the fixed pivot technique is second order convergent on a uniform and non-uniform smooth meshes. Moreover, it yields first order convergence on a locally uniform mesh. Finally, the analysis exhibits that the method does not converge on an oscillatory and non-uniform random meshes. Mathematical results of the convergence analysis are also demonstrated numerically.

1. Introduction

The continuous aggregation population balance equation (PBE) or Smoluchowski coagulation equation describes the kinetics of particle growth in which particles can aggregate via binary interaction to form larger particles. This model arises in many fields of science and engineering: kinetics of phase transformations in binary alloys such as segregation of binary alloys, aggregation of red blood cells in biology, fluidized bed granulation processes, aerosol physics, i.e the evolution of a system of solid or liquid particles suspended in a gas, formation of planets in astrophysics, polymer science and many more. The nonlinear continuous aggregation population balance equation is given by

$$\frac{\partial f(t,x)}{\partial t} = \frac{1}{2}\int_0^x K(x-y,y)f(t,x-y)f(t,y)dy - \int_0^\infty K(x,y)f(t,x)f(t,y)dy, \tag{1.1}$$

with

$$f(x,0) = f^{\text{in}}(x) \geq 0, \quad x \in]0,\infty[$$

where the variables $x > 0$ and $t \geq 0$ denote the size of the particles and time respectively. The number density of particles of size x at time t is denoted by $f(x,t) \geq 0$. The aggregation kernel $K(x,y) \geq 0$ represents the rate at which particles of size x coalesce with those of size y. It will be assumed throughout that $K(x,y) = K(y,x)$ for all $x, y > 0$, i.e. symmetric and $K(x,y) = 0$ for either $x = 0$ or $y = 0$.

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Mathematical results on existence and uniqueness of solutions to Eq. (1.1) can be found in [1–10] for different classes of aggregation kernels. The pure aggregation PBE (1.1) can be solved analytically only for some specific examples of aggregation kernels, see [11–13]. In general we need to solve them numerically. To apply a numerical method, first we need to consider the following truncated form of the problem (1.1) by taking a finite computational domain.

$$\frac{\partial n(t,x)}{\partial t} = \frac{1}{2}\int_0^x K(x-y,y)n(t,x-y)n(t,y)dy - \int_0^{x_{\max}} K(x,y)n(t,x)n(t,y)dy, \tag{1.2}$$

with

$$n(x,0) = n^{\text{in}}(x) \geq 0, \quad x \in \Omega :=]0, x_{\max}],$$

where $n(t,x)$ represents the solution to the truncated Eq. (1.2). The existence and uniqueness of non-negative solutions for the truncated PBE (1.2) has been shown in [14,15,2,10]. In [2–4,10], it is proven that the sequence of solutions to the truncated problems converge weakly to the solution of the original problem in a weighted L^1 space as $x_{\max} \to \infty$ for certain classes of kernels.

Many numerical methods have been proposed to solve the truncated aggregation PBE (1.2): finite element methods [16–18], finite volume methods [19–21], stochastic methods [22–24], moment methods [25] and sectional methods [26–29]. By implementing most of these methods, we may have a quite satisfactory results for the number density but not for moments. However, the moment methods give opposite results. To have a satisfactory information for the number density distribution as well as some selected moments, the sectional methods have become more useful nowadays. Several authors have proposed sectional methods for aggregation PBE: S. Kumar and Ramkrishna [28,29], J. Kumar et al. [26,27] and Vanni [30]. The fixed pivot technique given by S. Kumar and Ramkrishna is the most extensively used sectional method. This technique also efficiently works for a multi-dimensional size variable [31].

Recently J. Kumar and Warnecke [32] have published the numerical analysis of the fixed pivot technique for breakage PBEs. This case was simpler due to the linearity of that equation. However the convergence analysis of the technique was still open for aggregation PBEs (1.2). This was a challenging task due to the non-linearity of the equation. So the purpose of this work is to demonstrate the missing convergence analysis of the fixed pivot technique for aggregation PBEs in the literature.

Let us now briefly outline the contents of this paper. Along with the general idea of sectional methods, a concise review of the mathematical formulation of the fixed pivot technique is given in the following section. A theorem from Hundsdorfer and Verwer [33] used in further analysis and the main result for the convergence of the fixed pivot technique are also stated in Section 2. To show the convergence of the scheme for solving aggregation PBEs (1.2), the consistency and Lipschitz conditions are discussed in Sections 3 and 4, respectively. Numerical simulations are performed in Section 5. And, Section 6 states some conclusions.

2. The sectional methods

The mathematical formulation of sectional methods is reviewed from [32, Section 2]. These methods calculate the total number of particles in finite number of cells. First of all, the continuous interval $\Omega :=]0, x_{\max}]$ is divided into a finite number of cells defining size classes $\Lambda_i :=]x_{i-1/2}, x_{i+1/2}]$, $i = 1, \ldots, I$. Set

$$x_{1/2} = 0, \qquad x_{I+1/2} = x_{\max}, \qquad \Delta x_{\min} \leq \Delta x_i = x_{i+1/2} - x_{i-1/2} \leq \Delta x.$$

For the purpose of later analysis we assume quasi uniformity of the grids, i.e.

$$\frac{\Delta x}{\Delta x_{\min}} \leq C, \tag{2.1}$$

where C is a positive constant. The center point of each cell $x_i = (x_{i-1/2} + x_{i+1/2})/2$, $i = 1, \ldots, I$ is called pivot or grid point. The integration of the truncated PBE (1.2) over each cell gives a *semi-discrete* system in $\mathbb{R}^I$

$$\frac{d\mathbf{N}}{dt} = \mathbf{B} - \mathbf{D}, \quad \text{with } \mathbf{N}(0) = \mathbf{N}^{\text{in}}, \tag{2.2}$$

where $\mathbf{N}^{\text{in}}, \mathbf{N}, \mathbf{B}, \mathbf{D} \in \mathbb{R}^I$. The ith components of vectors $\mathbf{N}$, $\mathbf{N}^{\text{in}}$, $\mathbf{B}$, and $\mathbf{D}$ are respectively, defined as

$$N_i(t) = \int_{x_{i-1/2}}^{x_{i+1/2}} n(t,x)dx, \quad \text{with } N_i^{\text{in}} = \int_{x_{i-1/2}}^{x_{i+1/2}} n^{\text{in}}(x)dx, \tag{2.3}$$

$$B_i = \frac{1}{2}\int_{x_{i-1/2}}^{x_{i+1/2}} \int_0^x K(x-y,y)n(t,x-y)n(t,y)dydx \tag{2.4}$$

and

$$D_i = \int_{x_{i-1/2}}^{x_{i+1/2}} \int_0^{x_{I+1/2}} K(x,y)n(t,y)n(t,x)dydx. \tag{2.5}$$