Weierstraß-Institut
für Angewandte Analysis und Stochastik
Leibniz-Institut im Forschungsverbund Berlin e. V.

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# Cell size error in stochastic particle methods for coagulation equations with advection

Robert I. A. Patterson[1], Wolfgang Wagner[1]

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[1] Weierstrass Institute
Mohrenstrasse 39
10117 Berlin, Germany
E-Mail: robert.patterson@wias-berlin.de
wolfgang.wagner@wias-berlin.de

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Weierstraß-Institut für Angewandte Analysis und Stochastik (WIAS)
Leibniz-Institut im Forschungsverbund Berlin e. V.
Mohrenstraße 39
10117 Berlin
Germany

Fax: +49 30 20372-303
E-Mail: preprint@wias-berlin.de
World Wide Web: http://www.wias-berlin.de/

**Abstract**

The paper studies the approximation error in stochastic particle methods for spatially inhomogeneous population balance equations. The model includes advection, coagulation and inception. Sufficient conditions for second order approximation with respect to the spatial discretization parameter (cell size) are provided. Examples are given, where only first order approximation is observed.

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## 1 Introduction

We consider the population balance equation

$$\frac{\partial}{\partial t} c(t,x,y) + \frac{\partial}{\partial x}\Big(u(x)\, c(t,x,y)\Big) = \tag{1.1}$$
$$\frac{1}{2}\int_0^y dy_1\, K(y-y_1,y_1)\, c(t,x,y-y_1)\, c(t,x,y_1) -$$
$$c(t,x,y)\int_0^\infty dy_1\, K(y,y_1)\, c(t,x,y_1) + I(x,y)\,,$$

where $u$ is the advection velocity, $K$ is the coagulation kernel and $I$ is the inception rate. The solution $c(t,x,y)$ represents the number density of particles with type $y$ that are located at position $x$ at time $t$ . Equation (1.1) is a spatially inhomogeneous extension of Smoluchowski's coagulation equation [vS16]. Such equations are used in various branches of physics and chemical engineering. We refer to the extended introductions in [PWK11, PW12] concerning details about applications and further references.

Stochastic particle methods are common tools for the numerical treatment of population balance equations. These methods are based on the simulation of finite systems of particles that approximate the solution of (1.1). In the case of "direct simulation" methods the evolution of the particle system imitates the basic physical processes. Particles move independently according to the velocity field, new particles are added to the system according to the inception rate, and pairs of particles stick together according to a rate determined by the coagulation kernel. Since the system is finite, the interaction cannot be strictly local so that some spatial smoothing has to be introduced. For example, the position space can be divided into small cells and particles are allowed to coagulated, while they belong to the same cell. Moreover, the nonlinear part of the evolution is usually decoupled from the transport part in order to simplify the numerical implementation. Particles move independently during some time step, then their positions are fixed and coagulation is generated for particles belonging to the same cell. Thus, in addition to the finite number of particles, stochastic particle methods contain both spatial (cell size) and temporal (splitting time step) discretization parameters.

Stochastic particle methods have been studied in connection with various nonlinear kinetic equations. A classical example is the Boltzmann equation from rarefied gas dynamics (cf. [RW05] and references therein). We refer to [EW03] and [Kol10] concerning the infinite-particle-number limit for stochastic particle systems with rather general interactions. The convergence order with respect to the number of particles was studied, in the case of the Boltzmann equation, in [NT89, GM97], [CPW98] (steady state) and, in the case of the Smoluchowski equation, in [CF11]. The approximation error with respect to the splitting time step was studied for the Boltzmann equation in [Ohw98, BO99, Had00, GW00, RGTW06, RW07], for population balance equations from chemical engineering in [CPKW07], and for semiconductor transport equations in [MW05, MWDS10]. The cell size error was studied in connection with the Boltzmann equation in [BI89, AGA98, Had00, RGTW06].

In this paper we consider stochastic particle methods for the numerical treatment of equation (1.1) and study the approximation error with respect to cell size. Sufficient conditions for second order approximation are provided. In addition, examples are given, where only first order approximation is observed. The structure of the paper is as follows. In Section 2 we introduce a class of direct simulation algorithms and the corresponding infinite-particle-number limit equations. Then we formulate and prove the main result of the paper. Examples illustrating the limitations of the result are given in Section 3. Comments are provided in Section 4.

## 2 Main result

In this section we describe a class of direct simulation algorithms and provide the corresponding infinite-particle-number limit equations. The main result concerns the asymptotic behaviour of the solutions of these equations with respect to cell size.

### 2.1 Direct simulation algorithms

Direct simulation algorithms for equation (1.1) are based on stochastic particle systems of the form

$$\Big(x_i(t), y_i(t)\Big), \qquad i = 1, \ldots, N(t)\,, \qquad t \geq 0\,, \tag{2.1}$$

where $t$ denotes time, $N$ is the total number of particles and each particle is characterized by its position $x_i \in \mathcal{X} = [0,1]$ and its type $y_i \in \mathcal{Y} = (0,\infty)$ . The algorithm consists in generating trajectories of the system and calculating averages. The time evolution of the system (2.1) is as follows.

- The initial state of the system is chosen such that the corresponding empirical measure approximates the initial condition of equation (1.1),

$$\lim_{n\to\infty} \frac{1}{n} \sum_{i=1}^{N(0)} \delta_{x_i(0),y_i(0)}(dx,dy) \quad = \quad c(0,x,y)\,dx\,dy\,. \tag{2.2}$$

- Particles move in the velocity field $u$ .
- New particles $(x,y)$ are added to the system, according to the inception rate $I$ .
- The position space is divided into a finite number of disjoint cells,

$$\mathcal{X} = \cup_{l=1}^{L} \mathcal{X}_l\,, \quad \mathcal{X}_l = [x_{l-1}, x_l)\,, \quad x_l = l\,\Delta x\,, \quad l = 0,1,\ldots,L\,. \tag{2.3}$$

  Particles belonging to the same cell stick together, according to the coagulation rate $K$ . They form a new particle

$$(x_i,y_i)\,,\ (x_j,y_j) \quad \Rightarrow \quad (\tilde{x}, y_i + y_j)\,, \tag{2.4}$$

  where the position $\tilde{x}$ is either $x_i$ , with probability $p(y_i,y_j)$ , or $x_j$ , otherwise.

The parameter $n$ in (2.2) is also used for scaling the intensities of inception and coagulation. It is related to the number of physical particles represented by one numerical particle. In order to increase numerical efficiency, time splitting of transport and coagulation is used. During the transport step, particles are not allowed to interact. During the coagulation step, particles do not move.

Convergence of the system (2.1) holds in the sense that

$$\lim_{n\to\infty} \frac{1}{n} \sum_{i=1}^{N(t)} \varphi(x_i(t), y_i(t)) \quad = \quad \int_{\mathcal{X}\times\mathcal{Y}} \varphi(x,y)\, \hat{c}(t,x,y)\, dx\, dy\,,$$

for appropriate functions $\varphi$. The function $\hat{c}$ solves the “infinite-particle-number limit equation”

$$\begin{aligned}
&\frac{\partial}{\partial t}\,\hat{c}(t,x,y) + \frac{\partial}{\partial x}\Big(u(x)\,\hat{c}(t,x,y)\Big) = \\
&\quad \int_0^y dy_1\, K(y-y_1,y_1) \frac{p(y-y_1,y_1)+1-p(y_1,y-y_1)}{2} \times \\
&\quad \hat{c}(t,x,y-y_1) \left[\int_{\mathcal{X}} dx_1\, h(x,x_1)\,\hat{c}(t,x_1,y_1)\right] - \\
&\quad \hat{c}(t,x,y) \int_0^\infty dy_1\, K(y,y_1) \left[\int_{\mathcal{X}} dx_1\, h(x,x_1)\,\hat{c}(t,x_1,y_1)\right] + I(x,y)\,,
\end{aligned} \tag{2.5}$$

where

$$h(x,x_1) \quad = \quad \frac{1}{\Delta x} \sum_{l=1}^{L} 1_{\mathcal{X}_l}(x)\, 1_{\mathcal{X}_l}(x_1) \tag{2.6}$$

is determined by the cell structure (2.3). The function $p$ represents the probability for choosing the position of the new particle in a coagulation event (cf. (2.4)). The choices

$$p(y_1,y_2) = \alpha\,, \qquad \text{where} \quad \alpha \in [0,1]\,, \tag{2.7}$$

and

$$p(y_1,y_2) = \frac{y_1}{y_1+y_2}\,, \qquad y_1,y_2 \in \mathcal{Y}\,, \tag{2.8}$$

correspond to the direct simulation algorithms DSA1 and DSA2 in [PW12].

## 2.2 Cell size error

Equation (2.5) takes the form (1.1), when $h$ is replaced by Dirac’s delta-function $\delta$. The function $h$ delocalizes the spatial interaction between particles in the stochastic algorithm. The purpose of the paper is to provide a rigorous result concerning the transition $h \to \delta$. More precisely, we study the order of the approximation error with respect to the cell size $\Delta x$ (cf. (2.3)). Sufficient conditions for second order convergence are given. We consider the norm

$$\|f\| \quad = \quad \sup_{x\in\mathcal{X}} \int_{\mathcal{Y}} |f(x,y)|\, dy \tag{2.9}$$

on the space of measurable functions on $\mathcal{X}\times\mathcal{Y} = [0,1]\times(0,\infty)$, which are bounded with respect to $x$ and integrable with respect to $y$.

**Theorem 2.1** *Let $c_\infty$ and $\hat{c}_\infty$ be steady state solutions of equations (1.1) and (2.5), respectively, with finite norms (2.9) and such that*

$$c_\infty(0,y) = \hat{c}_\infty(0,y) \qquad \forall\, y \in \mathcal{Y}\,. \tag{2.10}$$

*Assume*

- *the advection velocity $u$ satisfies*

$$\inf_{x\in\mathcal{X}} u(x) > 0 \tag{2.11}$$

  *and is twice differentiable so that*

$$\sup_{x\in\mathcal{X}} |u'(x)| < \infty \qquad \text{and} \qquad \sup_{x\in\mathcal{X}} |u''(x)| < \infty\,; \tag{2.12}$$

- *the inception rate $I$ is non-negative and twice differentiable with respect to $x$ so that*

$$\|I\| < \infty\,, \qquad \|I'\| < \infty \qquad \text{and} \qquad \|I''\| < \infty\,; \tag{2.13}$$

- *the coagulation kernel $K$ is non-negative, symmetric and satisfies*

$$K(y,y_1) \;\; \leq \;\; C_K \qquad \forall\, y, y_1 \in \mathcal{Y}\,, \tag{2.14}$$

  *for some $C_K \in (0,\infty)$ .*

*Then*

$$\limsup_{\Delta x\to 0} \frac{\|c_\infty - \hat{c}_\infty\|}{\Delta x^2} \;\; < \;\; \infty\,. \tag{2.15}$$

## 2.3 Proof of Theorem 2.1

Let $f, g$ be functions on $\mathcal{X} \times \mathcal{Y}$ with finite norms (2.9). Denote

$$B(f,g) \;\; = \;\; B_1(f,g) - B_2(f,g)\,, \tag{2.16}$$

where

$$B_1(f,g)(x,y) \;\; = \;\; \int_0^y dy_1\, \hat{K}(y-y_1,y_1)\, f(x,y-y_1)\, g(x,y_1)\,, \tag{2.17}$$

with

$$\hat{K}(y,y_1) \;\; = \;\; K(y,y_1)\, \frac{p(y,y_1)+1-p(y_1,y)}{2}\,, \tag{2.18}$$

and

$$B_2(f,g)(x,y) \;\; = \;\; f(x,y) \int_0^\infty dy_1\, K(y,y_1)\, g(x,y_1)\,. \tag{2.19}$$

Using symmetry of $K$, one obtains

$$\frac{1}{2}\int_0^y dy_1\, K(y-y_1,y_1)\, f(x,y-y_1)\, f(x,y_1) = \int_0^y dy_1\, K(y-y_1,y_1) \times \frac{p(y-y_1,y_1)+1-p(y_1,y-y_1)}{2}\, f(x,y-y_1)\, f(x,y_1)\,. \tag{2.20}$$

According to (2.20), equation (1.1) can be written as

$$\frac{\partial}{\partial t}\, c(t,x,y) + \frac{\partial}{\partial x}\Big(u(x)\, c(t,x,y)\Big) = I(x,y) + B(c(t),c(t))(x,y)\,. \tag{2.21}$$

Equation (2.5) takes the form

$$\frac{\partial}{\partial t}\, \hat{c}(t,x,y) + \frac{\partial}{\partial x}\Big(u(x)\, \hat{c}(t,x,y)\Big) = I(x,y) + B(\hat{c}(t),H\hat{c}(t))(x,y)\,, \tag{2.22}$$

where (cf. (2.6))

$$(Hf)(x,y) = \int_{\mathcal{X}} h(x,x_1)\, f(x_1,y)\, dx_1\,. \tag{2.23}$$

First we derive some auxiliary estimates. Assumption (2.14) implies

$$\begin{aligned} \|B_1(f,g)(x,.)\|_1 &\le C_K\, \|f(x,.)\|_1\, \|g(x,.)\|_1\,, \\ \|B_2(f,g)(x,.)\|_1 &\le C_K\, \|f(x,.)\|_1\, \|g(x,.)\|_1 \end{aligned} \tag{2.24}$$

and

$$\begin{aligned} &\|B(f,g)(x,.) - B(f_1,g_1)(x,.)\|_1 \le \\ &\qquad \|B(f,g)(x,.) - B(f,g_1)(x,.)\|_1 + \|B(f,g_1)(x,.) - B(f_1,g_1)(x,.)\|_1 \\ &\le\; 2\, C_K\Big(\|g(x,.)-g_1(x,.)\|_1\, \|f(x,.)\|_1 + \|f(x,.)-f_1(x,.)\|_1\, \|g_1(x,.)\|_1\Big), \end{aligned} \tag{2.25}$$

where $\|.\|_1$ denotes the $L_1$-norm of integrable functions on $\mathcal{Y}$ . It follows from (2.24) and (2.25) that (cf. (2.9))

$$\|B(f,g)\| \;\le\; C_K\, \|f\|\, \|g\| \tag{2.26}$$

and

$$\|B(f,g) - B(f_1,g_1)\| \;\le\; 2\, C_K\Big(\|g-g_1\|\, \|f\| + \|f-f_1\|\, \|g_1\|\Big). \tag{2.27}$$

Moreover, one obtains (cf. (2.23))

$$\|Hf\| \;\le\; \|f\|\,. \tag{2.28}$$

In the following, we will write $c, \hat{c}$ instead of $c_\infty, \hat{c}_\infty$ . We use the notation $O(\Delta x^k)$ for any expression $F(\Delta x)$ such that (cf. (2.9))

$$\limsup_{\Delta x \to 0} \frac{\|F(\Delta x)\|}{\Delta x^k} < \infty \,.$$

**Step 1.** The steady state form of equation (2.21) is

$$\frac{\partial}{\partial x}\Big(u(x)\, c(x,y)\Big) = I(x,y) + B(c,c)(x,y)\,. \tag{2.29}$$

One obtains

$$\frac{\partial^2}{\partial x^2}\Big(u(x)\, c(x,y)\Big) = I'(x,y) + B(c',c)(x,y) + B(c,c')(x,y) \tag{2.30}$$

and

$$\begin{aligned} &\frac{\partial^3}{\partial x^3}\Big(u(x)\, c(x,y)\Big) = \\ &\qquad I''(x,y) + B(c'',c)(x,y) + 2\,B(c',c')(x,y) + B(c,c'')(x,y)\,. \end{aligned} \tag{2.31}$$

It follows from the smoothness assumptions (2.12), (2.13) and property (2.26) that the norm of the expressions (2.29)-(2.31) is finite. Thus, one obtains

$$\begin{aligned} u(x)\, c(x,y) &= (uc)(x_{l-1},y) + \\ &\quad (uc)'(x_{l-1},y)\,(x-x_{l-1}) + (uc)''(x_{l-1},y)\,\frac{(x-x_{l-1})^2}{2} + O(\Delta x^3) \\ &= O(\Delta x^3) + (uc)(x_{l-1},y) + \Big[I(x_{l-1},y) + B(c,c)(x_{l-1},y)\Big](x-x_{l-1}) + \\ &\quad \Big[I'(x_{l-1},y) + B(c',c)(x_{l-1},y) + B(c,c')(x_{l-1},y)\Big]\frac{(x-x_{l-1})^2}{2}\,, \end{aligned} \tag{2.32}$$

for any $x \in [x_{l-1}, x_l]$ .

**Step 2.** The steady state form of equation (2.22) is

$$\frac{\partial}{\partial x}\Big(u(x)\, \hat{c}(x,y)\Big) = I(x,y) + B(\hat{c}, H\hat{c})(x,y)\,. \tag{2.33}$$

Note that $h$ is constant in the cell $\mathcal{X}_l$ (cf. (2.6)). Thus, one obtains

$$\frac{\partial^2}{\partial x^2}\Big(u(x)\, \hat{c}(x,y)\Big) = I'(x,y) + B(\hat{c}', H\hat{c})(x,y) \tag{2.34}$$

and

$$\frac{\partial^3}{\partial x^3}\Big(u(x)\, \hat{c}(x,y)\Big) = I''(x,y) + B(\hat{c}'', H\hat{c})(x,y)\,. \tag{2.35}$$

It follows from the smoothness assumptions (2.12), (2.13) and properties (2.26), (2.28) that the norm of the expressions (2.33)-(2.35) is finite. Moreover, the norm of the functions $\hat{c}'$ and $\hat{c}''$ is finite (cf. (2.11)). Note that

$$\begin{aligned} (H\hat{c})(x,y) &= \frac{1}{\Delta x}\int_{x_{l-1}}^{x_l} \hat{c}(\tilde{x},y)\, d\tilde{x} \\ &= \hat{c}(x_{l-1},y) + \hat{c}'(x_{l-1},y)\,\frac{\Delta x}{2} + O(\Delta x^2)\,, \end{aligned} \tag{2.36}$$

for any $x \in [x_{l-1}, x_l]$ . Thus, one obtains

$$
\begin{aligned}
u(x)\,\hat{c}(x,y) \;&=\; (u\hat{c})(x_{l-1},y) + \Big[I(x_{l-1},y) + B(\hat{c},H\hat{c})(x_{l-1},y)\Big](x-x_{l-1}) + \\
&\quad \Big[I'(x_{l-1},y) + B(\hat{c}',H\hat{c})(x_{l-1},y)\Big]\frac{(x-x_{l-1})^2}{2} + O(\Delta x^3) \\
&=\; (u\hat{c})(x_{l-1},y) + \Big[I(x_{l-1},y) + B(\hat{c},\hat{c})(x_{l-1},y)\Big](x-x_{l-1}) + \\
&\quad B(\hat{c},\hat{c}')(x_{l-1},y)\,\frac{(x-x_{l-1})\,\Delta x}{2} + \\
&\quad \Big[I'(x_{l-1},y) + B(\hat{c}',\hat{c})(x_{l-1},y)\Big]\frac{(x-x_{l-1})^2}{2} + O(\Delta x^3)\,.
\end{aligned}
\tag{2.37}
$$

**Step 3.** Let $x \in [x_{l-1}, x_l]$ . It follows from (2.32) and (2.37) that

$$
\begin{aligned}
&(uc)(x,y) - (u\hat{c})(x,y) = (uc)(x_{l-1},y) - (u\hat{c})(x_{l-1},y) + O(\Delta x^3) + \\
&\quad \Big[B(c,c)(x_{l-1},y) - B(\hat{c},\hat{c})(x_{l-1},y)\Big](x-x_{l-1}) + \\
&\quad \Big[B(c',c)(x_{l-1},y) - B(\hat{c}',\hat{c})(x_{l-1},y)\Big]\frac{(x-x_{l-1})^2}{2} + \\
&\quad B(c,c')(x_{l-1},y)\,\frac{(x-x_{l-1})^2}{2} - B(\hat{c},\hat{c}')(x_{l-1},y)\,\frac{(x-x_{l-1})\,\Delta x}{2} \\
&= (uc)(x_{l-1},y) - (u\hat{c})(x_{l-1},y) + O(\Delta x^3) + \\
&\quad \frac{1}{u(x_{l-1})^2}\Big[B(uc,uc)(x_{l-1},y) - B(u\hat{c},u\hat{c})(x_{l-1},y)\Big](x-x_{l-1}) + \\
&\quad \frac{1}{u(x_{l-1})^2}\Big[B(uc',uc)(x_{l-1},y) - B(u\hat{c}',u\hat{c})(x_{l-1},y) + \\
&\quad B(uc,uc')(x_{l-1},y) - B(u\hat{c},u\hat{c}')(x_{l-1},y)\Big]\frac{(x-x_{l-1})^2}{2} + \\
&\quad B(\hat{c},\hat{c}')(x_{l-1},y)\,\frac{(x-x_{l-1})\,(x-x_l)}{2}\,.
\end{aligned}
\tag{2.38}
$$

Using (2.25) one obtains from (2.38) that

$$
\begin{aligned}
&\|(uc)(x) - (u\hat{c})(x)\|_1 \le R(x,\Delta x) + \|(uc)(x_{l-1}) - (u\hat{c})(x_{l-1})\|_1 + \\
&\quad \frac{2\,C_K}{u(x_{l-1})^2}\,\|(uc)(x_{l-1}) - (u\hat{c})(x_{l-1})\|_1 \times \\
&\quad \Big(\|(uc)(x_{l-1})\|_1 + \|(u\hat{c})(x_{l-1})\|_1\Big)\Delta x + \frac{2\,C_K}{u(x_{l-1})^2} \times \\
&\quad \Big\{\|(uc')(x_{l-1}) - (u\hat{c}')(x_{l-1})\|_1\Big(\|(uc)(x_{l-1})\|_1 + \|(u\hat{c})(x_{l-1})\|_1\Big) + \\
&\quad \|(uc)(x_{l-1}) - (u\hat{c})(x_{l-1})\|_1\Big(\|(uc')(x_{l-1})\|_1 + \|(u\hat{c}')(x_{l-1})\|_1\Big)\Big\}\,\frac{\Delta x^2}{2}\,,
\end{aligned}
\tag{2.39}
$$

where

$$
R(x,\Delta x) = \begin{cases} O(\Delta x^2)\,, & \text{if} \quad x < x_l\,, \\ O(\Delta x^3)\,, & \text{if} \quad x = x_l\,. \end{cases}
\tag{2.40}
$$

**Step 4.** Since (cf. (2.29))

$$u(x)\,\frac{\partial}{\partial x}\,c(x,y) = -u'(x)\,c(x,y) + I(x,y) + B(c,c)(x,y)$$

and (cf. (2.33))

$$u(x)\,\frac{\partial}{\partial x}\,\hat{c}(x,y) = -u'(x)\,\hat{c}(x,y) + I(x,y) + B(\hat{c},H\hat{c})(x,y)\,,$$

it follows that (cf. (2.24), (2.28))

$$\begin{aligned} &\|(uc')(x_{l-1})\|_1 + \|(u\hat{c}')(x_{l-1})\|_1 \leq \\ &\quad |u'(x_{l-1})|\,(\|c(x_{l-1})\|_1 + \|\hat{c}(x_{l-1})\|_1) + \\ &\quad 2\,\|I(x_{l-1})\|_1 + 2\,C_K\left(\|c(x_{l-1})\|_1^2 + \|\hat{c}(x_{l-1})\|_1^2\right). \end{aligned} \tag{2.41}$$

Moreover, one obtains

$$u(x_{l-1})\,c'(x_{l-1},y) = -u'(x_{l-1})\,c(x_{l-1},y) + I(x_{l-1},y) + B(c,c)(x_{l-1},y)$$

and (cf. (2.36))

$$\begin{aligned} &u(x_{l-1})\,\hat{c}'(x_{l-1},y) = \\ &\quad -u'(x_{l-1})\,\hat{c}(x_{l-1},y) + I(x_{l-1},y) + B(\hat{c},\hat{c})(x_{l-1},y) + O(\Delta x) \end{aligned}$$

so that

$$\begin{aligned} (uc')(x_{l-1},y) - (u\hat{c}')(x_{l-1},y) = -\frac{u'(x_{l-1})}{u(x_{l-1})}\Big[(uc)(x_{l-1},y) - (u\hat{c})(x_{l-1},y)\Big] + \\ \frac{1}{u(x_{l-1})^2}\Big[B(uc,uc)(x_{l-1},y) - B(u\hat{c},u\hat{c})(x_{l-1},y)\Big] + O(\Delta x) \end{aligned}$$

and (cf. (2.24))

$$\begin{aligned} &\|(uc')(x_{l-1}) - (u\hat{c}')(x_{l-1})\|_1 \leq \\ &\quad O(\Delta x) + \left|\frac{u'(x_{l-1})}{u(x_{l-1})}\right|\,\|(uc)(x_{l-1}) - (u\hat{c})(x_{l-1})\|_1 + \frac{2\,C_K}{u(x_{l-1})^2}\times \\ &\quad \|(uc)(x_{l-1}) - (u\hat{c})(x_{l-1})\|_1\Big(\|(uc)(x_{l-1})\|_1 + \|(u\hat{c})(x_{l-1})\|_1\Big) \\ &= \|(uc)(x_{l-1}) - (u\hat{c})(x_{l-1})\|_1\times \\ &\quad \left(\left|\frac{u'(x_{l-1})}{u(x_{l-1})}\right| + \frac{2\,C_K}{|u(x_{l-1})|}\Big(\|c(x_{l-1})\|_1 + \|\hat{c}(x_{l-1})\|_1\Big)\right) + O(\Delta x)\,. \end{aligned} \tag{2.42}$$

**Step 5.** It follows from (2.39), (2.41) and (2.42) that

$$\begin{aligned} &\|(uc)(x) - (u\hat{c})(x)\|_1 \leq \|(uc)(x_{l-1}) - (u\hat{c})(x_{l-1})\|_1 + \\ &\quad \|(uc)(x_{l-1}) - (u\hat{c})(x_{l-1})\|_1\,\frac{2\,C_K}{|u(x_{l-1})|}\Big(\|c(x_{l-1})\|_1 + \|(\hat{c}(x_{l-1})\|_1\Big)\Delta x + \end{aligned}$$

$$\|(uc)(x_{l-1}) - (u\hat{c})(x_{l-1})\|_1 \, \frac{2\,C_K}{u(x_{l-1})^2} \times$$
$$\Big\{ \Big[ |u'(x_{l-1})| + 2\,C_K \Big( \|c(x_{l-1})\|_1 + \|\hat{c}(x_{l-1})\|_1 \Big) \Big] \Big( \|c(x_{l-1})\|_1 + \|\hat{c}(x_{l-1})\|_1 \Big) +$$
$$|u'(x_{l-1})| \Big( \|c(x_{l-1})\|_1 + \|\hat{c}(x_{l-1})\|_1 \Big) + 2\,\|I(x_{l-1})\|_1 +$$
$$2\,C_K \Big( \|c(x_{l-1})\|_1^2 + \|\hat{c}(x_{l-1})\|_1^2 \Big) \Big\} \, \frac{\Delta x^2}{2} + R(x, \Delta x)$$

and

$$\|(uc)(x) - (u\hat{c})(x)\|_1 \le \\ \|(uc)(x_{l-1}) - (u\hat{c})(x_{l-1})\|_1 \, (1 + C\,\Delta x) + R(x, \Delta x)\,, \tag{2.43}$$

for any $x \in [x_{l-1}, x_l]$ , where

$$C = \frac{2\,C_K}{\inf_{x \in \mathcal{X}} u(x)} \Big( \|c\| + \|\hat{c}\| \Big) + \\ \frac{C_K}{(\inf_{x \in \mathcal{X}} u(x))^2} \Big\{ \Big[ \|u'\|_\infty + 2\,C_K \Big( \|c\| + \|\hat{c}\| \Big) \Big] \Big( \|c\| + \|\hat{c}\| \Big) + \\ \|u'\|_\infty \Big( \|c\| + \|\hat{c}\| \Big) + 2\,\|I\| + 2\,C_K \Big( \|c\|^2 + \|\hat{c}\|^2 \Big) \Big\}$$

and $\|.\|_\infty$ denotes the $\sup$-norm of bounded functions on $\mathcal{X}$ .

**Step 6.** According to (2.40), (2.43) and assumption (2.10), one obtains (cf. (2.3))

$$\|(uc)(x_l) - (u\hat{c})(x_l)\|_1 \le (1 + C\,\Delta x)^l \, \|(uc)(x_0) - (u\hat{c})(x_0)\|_1 + \\ \Big[ 1 + (1 + C\,\Delta x) + \ldots + (1 + C\,\Delta x)^{l-1} \Big] O(\Delta x^3) \\ = \frac{(1 + C\,\Delta x)^l - 1}{(1 + C\,\Delta x) - 1} \, O(\Delta x^3) \le \frac{(1 + C\,\Delta x)^L}{C} \, O(\Delta x^2) = O(\Delta x^2)$$

and

$$\|(uc)(x) - (u\hat{c})(x)\|_1 = O(\Delta x^2)\,. \tag{2.44}$$

Finally, (2.15) is a consequence of (2.9), (2.11) and (2.44).

# 3 Examples

In this section we provide examples, where the second order convergence (2.15) of Theorem 2.1 does not hold. More precisely, the following properties are obtained.

- In Example 3.4 (Section 3.1) there is $u = 0$ and

$$\liminf_{\Delta x \to 0} \frac{\|c_\infty - \hat{c}_\infty\|}{\Delta x} \quad > \quad 0\,. \tag{3.1}$$

  Thus, assumption (2.11) of Theorem 2.1 is essential.

- In Example 3.5 (Section 3.2) there is $\Delta t > 0$ and $u = 1$, but

$$\liminf_{\Delta x \to 0} \frac{\|c_\infty^{\Delta t} - \hat{c}_\infty^{\Delta t}\|}{\Delta x} \quad > \quad 0\,, \tag{3.2}$$

  where $c_\infty^{\Delta t}$ and $\hat{c}_\infty^{\Delta t}$ are steady state solutions of splitted versions of equations (1.1) and (2.5), respectively. This is consistent with the observation for $u = 0$, since the splitting step with coagulation has no transport.

- If $\Delta t > 0$ and $u$ is not constant, then even a weaker distance defined by cell averages (cf. (2.23), (2.28)) does not provide second order convergence, i.e.,

$$\|H c_\infty^{\Delta t} - H \hat{c}_\infty^{\Delta t}\| \quad \sim \quad \Delta x\,. \tag{3.3}$$

  This will be illustrated by a numerical experiment in Section 3.3.

We consider a constant coagulation kernel $K$ and the functionals

$$m_0(t,x) = \int_{\mathcal{Y}} c(t,x,y)\,dy\,, \qquad \hat{m}_0(t,x) = \int_{\mathcal{Y}} \hat{c}(t,x,y)\,dy\,, \tag{3.4}$$

which represent the number density. Equation (1.1) implies

$$\frac{\partial}{\partial t} m_0(t,x) + \frac{\partial}{\partial x}\left(u(x)\, m_0(t,x)\right) = I_0(x) - \frac{K}{2} m_0(t,x)^2\,. \tag{3.5}$$

We also consider a constant function $p$ (cf. (2.7)). In this case, equation (2.5) implies

$$\frac{\partial}{\partial t} \hat{m}_0(t,x) + \frac{\partial}{\partial x}\left(u(x)\, \hat{m}_0(t,x)\right) = I_0(x) - \frac{K}{2} \hat{m}_0(t,x)\,(H\hat{m}_0)(t,x)\,, \tag{3.6}$$

where

$$I_0(x) \quad = \quad \int_{\mathcal{Y}} I(x,y)\,dy \tag{3.7}$$

and $H$ is defined in (2.23). The following remarks will be used later in the construction of the examples mentioned above.

**Remark 3.1** *Assume that $u$ and $I_0$ do not depend on $x$. If $u > 0$ and $K > 0$, then the stationary version of equation (3.5),*

$$u \frac{d}{dx} m_{0,\infty}(x) = I_0 - \frac{K}{2} m_0(x)^2\,,$$

*has the solution*

$$m_{0,\infty}(x) \quad = \quad \sqrt{\frac{2I_0}{K}}\, \tanh\left(\sqrt{\frac{K\,I_0}{2}}\;\frac{x}{u}\right), \tag{3.8}$$

*with boundary condition* $m_{0,\infty}(0) = 0$ *. Note* $\tanh x = (e^x - e^{-x})/(e^x + e^{-x}) \sim x$ *as* $x \to 0$ *. If* $K \to 0$ *, then the steady state (3.8) takes the form*

$$m_{0,\infty}(x) \quad = \quad I_0 \, \frac{x}{u} \, , \tag{3.9}$$

*with the same boundary condition. If* $u \to 0$ *, then one obtains*

$$m_{0,\infty}(x) \quad = \quad \sqrt{\frac{2I_0}{K}} \, . \tag{3.10}$$

**Remark 3.2** *The equation*

$$\frac{d}{dt} \, g(t) = a(t) \, g(t) + b(t) \, , \qquad g(0) = g_0 \, ,$$

*has the solution*

$$g(t) = \exp\left( \int_0^t a(s) \, ds \right) \left[ \int_0^t \exp\left( - \int_0^s a(z) \, dz \right) b(s) \, ds + g_0 \right] .$$

**Remark 3.3** *Consider a Markov process* $\xi_x(t)$ *with the semigroup*

$$P(t) f(x) = \mathbb{E} f(\xi_x(t)) \, ,$$

*for any bounded measurable function* $f$ *. Let* $A$ *be the corresponding generator. The adjoint operators are denoted by* $P(t)^*$ *and* $A^*$ *, respectively. Then the equation*

$$\frac{d}{dt} \, g(t) = A g(t) + \gamma(t) \, , \qquad g(0) = g_0 \, ,$$

*has the solution*

$$g(t) = P(t) g_0 + \int_0^t P(t-s) \, \gamma(s) \, ds \, , \tag{3.11}$$

*while the equation*

$$\frac{d}{dt} \, g(t) = A^* g(t) + \gamma(t) \, , \qquad g(0) = g_0 \, ,$$

*has the solution*

$$g(t) = P(t)^* g_0 + \int_0^t P(t-s)^* \, \gamma(s) \, ds \, .$$

*Note that* $\frac{d}{dt} P(t)^* = A^* P(t)^*$ *and* $\frac{d}{dt} P(t) = A \, P(t)$ *are abstract forms of Kolmogorov's forward and backward equation.*

## 3.1 Zero velocity

In preparation for Example 3.4 we consider the general case $u = 0$ . Equation (3.5) takes the form

$$\frac{\partial}{\partial t} m_0(t,x) \;=\; I_0(x) - \frac{K}{2}\, m_0(t,x)^2 \tag{3.12}$$

and has the explicit solution (cf. (3.8))

$$m_0(t,x) \;=\; \sqrt{\frac{2I_0(x)}{K}}\, \tanh\left(\sqrt{\frac{K\, I_0(x)}{2}}\; t\right), \tag{3.13}$$

with initial condition $m_0(0,x) = 0$ . The boundary value $m_0(t,0)$ depends on $I_0$ . Since

$$\lim_{t\to 0} m_0(t,0) \;=\; \sqrt{\frac{2I_0(0)}{K}}\,,$$

there is a discontinuity at $t = 0$ and $x = 0$ , when $I_0(0) > 0$ . The stationary solution of equation (3.12) is

$$m_{0,\infty}(x) \;=\; \sqrt{\frac{2I_0(x)}{K}}\,, \tag{3.14}$$

which generalizes (3.10).

Equation (3.6) takes the form

$$\frac{\partial}{\partial t} \hat{m}_0(t,x) \;=\; I_0(x) - \frac{K}{2}\, \hat{m}_0(t,x)\,(H\hat{m}_0)(t,x)\,, \tag{3.15}$$

which implies (cf. (2.6), (2.23))

$$\frac{\partial}{\partial t} (H\hat{m}_0)(t,x) = (HI_0)(x) - \frac{K}{2}\, [(H\hat{m}_0)(t,x)]^2$$

so that (cf. (3.13))

$$(H\hat{m}_0)(t,x) \;=\; \sqrt{\frac{2\,(HI_0)(x)}{K}}\, \tanh\left(\sqrt{\frac{K\,(HI_0)(x)}{2}}\; t\right),$$

with initial condition $(H\hat{m}_0)(0,x) = 0$ . According to Remark 3.2, one obtains the solution of (3.15) in the form

$$\hat{m}_0(t,x) \;=\; I_0(x) \int_0^t \exp\left(-\frac{K}{2}\int_s^t (H\hat{m}_0)(z,x)\,dz\right) ds\,.$$

It follows from

$$\int \tanh(\alpha\, s)\, ds = \frac{1}{\alpha}\, \log\cosh(\alpha\, s) + C$$

that

$$\int_s^t (H\hat{m}_0)(z,x)\,dz = \frac{2}{K}\left[\log\cosh\left(\sqrt{\frac{K\,(HI_0)(x)}{2}}\;t\right) - \log\cosh\left(\sqrt{\frac{K\,(HI_0)(x)}{2}}\;s\right)\right]$$

and

$$\begin{aligned}\hat{m}_0(t,x) = \\ & I_0(x)\,\cosh\left(\sqrt{\frac{K\,(HI_0)(x)}{2}}\;t\right)^{-1}\int_0^t \cosh\left(\sqrt{\frac{K\,(HI_0)(x)}{2}}\;s\right)\,ds \\ = \; & I_0(x)\sqrt{\frac{2}{K\,(HI_0)(x)}}\;\tanh\left(\sqrt{\frac{K\,(HI_0)(x)}{2}}\;t\right),\end{aligned} \tag{3.16}$$

with initial condition $\hat{m}_0(0,x) = 0$ . The value at the $x = 0$ boundary satisfies

$$\lim_{t\to 0}\hat{m}_0(t,0) \;=\; I_0(0)\sqrt{\frac{2}{K\,(HI_0)(0)}}\,.$$

The stationary solution of equation (3.15) is

$$\hat{m}_{0,\infty}(x) \;=\; \sqrt{\frac{2}{K}}\,\frac{I_0(x)}{\sqrt{(HI_0)(x)}}\,. \tag{3.17}$$

**Example 3.4** *Let* $K = 2$ *and*

$$I_0(x) = 1 + 2b\,x\,, \qquad x\in[0,1]\,, \quad b\geq 0\,.$$

*Then (cf. (3.13))*

$$m_0(t,\Delta x) \;=\; \sqrt{1+2b\,\Delta x}\;\tanh\left(\sqrt{1+2b\,\Delta x}\;t\right) \tag{3.18}$$

*and (cf. (2.6), (2.23))*

$$(HI_0)(x) = 1 + b\,\Delta x\,, \qquad x\in[0,\Delta x]\,,$$

*so that (cf. (3.16))*

$$\hat{m}_0(t,\Delta x) \;=\; \frac{1+2b\,\Delta x}{\sqrt{1+b\,\Delta x}}\;\tanh\left(\sqrt{1+b\,\Delta x}\;t\right). \tag{3.19}$$

*Since* $(\tanh x)' = 1 - (\tanh x)^2$ *, one obtains*

$$\frac{\partial}{\partial x}\tanh\left(\sqrt{1+2b\,x}\;t\right) = \left[1 - \left(\tanh\left(\sqrt{1+2b\,x}\;t\right)\right)^2\right]\frac{b\,t}{\sqrt{1+2b\,x}}$$

*so that*

$$\tanh\left(\sqrt{1+2b\,\Delta x}\;t\right) = \tanh t + \left[1-(\tanh t)^2\right] b\,t\,\Delta x + O(\Delta x^2)\,. \tag{3.20}$$

*It follows from (3.18), (3.20) and*

$$\sqrt{1+2b\,\Delta x} = 1 + b\,\Delta x + O(\Delta x^2)$$

*that*

$$m_0(t,\Delta x) = \tanh t + \left(\left[1-(\tanh t)^2\right] b\,t + b\,\tanh t\right)\Delta x + O(\Delta x^2)\,. \tag{3.21}$$

*It follows from (3.19), (3.20) (with $2b$ replaced by $b$) and*

$$\frac{1}{\sqrt{1+b\,\Delta x}} = 1 - \frac{b}{2}\,\Delta x + O(\Delta x^2)$$

*that*

$$\begin{aligned}\hat{m}_0(t,\Delta x) = \tanh t + \\ \left(2b\,\tanh t - \frac{b}{2}\,\tanh t + \left[1-(\tanh t)^2\right]\frac{b\,t}{2}\right)\Delta x + O(\Delta x^2)\,.\end{aligned} \tag{3.22}$$

*According to (3.21) and (3.22), one obtains*

$$m_0(t,\Delta x) - \hat{m}_0(t,\Delta x) = \left(-\tanh t + \left[1-(\tanh t)^2\right]\,t\right)\frac{b}{2}\,\Delta x + O(\Delta x^2)$$

*so that*

$$\liminf_{\Delta x\to 0}\frac{\|m_0(t)-\hat{m}_0(t)\|_\infty}{\Delta x} \geq \liminf_{\Delta x\to 0}\frac{|m_0(t,\Delta x)-\hat{m}_0(t,\Delta x)|}{\Delta x} > 0\,, \tag{3.23}$$

*for all $b>0$ and $t>0$ . Recall that $\|.\|_\infty$ denotes the $\sup$-norm. Since (cf. (2.9))*

$$\|m_0(t)-\hat{m}_0(t)\|_\infty \quad\leq\quad \|c(t)-\hat{c}(t)\|\,, \tag{3.24}$$

*(3.23) implies*

$$\liminf_{\Delta x\to 0}\frac{\|c(t)-\hat{c}(t)\|}{\Delta x} \quad>\quad 0\,.$$

*Analogous estimates hold for the steady states (3.14) and (3.17) so that (3.1) follows.*

## 3.2 Time splitting

Time splitting schemes are based on a separation of transport and coagulation. Let $\mathcal{T}_I(t)$ denote the solution operator of equation (1.1) with $K=0$ . Let $\mathcal{K}(t,.)$ and $\hat{\mathcal{K}}(t,.)$ denote the solution operators of equations (1.1) and (2.5), with $u=0$ and $I=0$ . In analogy, we introduce the operators $\mathcal{T}(t)$ , $\mathcal{K}_I(t,.)$ and $\hat{\mathcal{K}}_I(t,.)$ , when inception is attached to coagulation. Let

$$t_j = j\,\Delta t\,,\;\; j=0,1,\ldots\,.$$

Godunov splitting schemes are of the form

$$c^{\Delta t}(t_j) = \mathcal{K}(\Delta t, \mathcal{T}_I(\Delta t)\, c(t_{j-1}))\,, \qquad \hat{c}^{\Delta t}(t_j) = \hat{\mathcal{K}}(\Delta t, \mathcal{T}_I(\Delta t)\, \hat{c}(t_{j-1}))\,, \tag{3.25}$$

while Strang splitting schemes are of the form

$$\begin{aligned} c^{\Delta t}(t_j) &= \mathcal{T}_I(\Delta t/2)\, \mathcal{K}(\Delta t, \mathcal{T}_I(\Delta t/2)\, c^{\Delta t}(t_{j-1})) \\ \hat{c}^{\Delta t}(t_j) &= \mathcal{T}_I(\Delta t/2)\, \hat{\mathcal{K}}(\Delta t, \mathcal{T}_I(\Delta t/2)\, \hat{c}^{\Delta t}(t_{j-1}))\,, \end{aligned} \tag{3.26}$$

where $j \geq 1$ and

$$c^{\Delta t}(0) = \hat{c}^{\Delta t}(0) = c(0)\,. \tag{3.27}$$

Since $K$ and $p$ are assumed to be constant, the functionals (3.4) of the solutions $c^{\Delta t}$ and $\hat{c}^{\Delta t}$ of the splitted equations (1.1) and (2.5) are obtained as solutions of the splitted equations (3.5) and (3.6). We denote the corresponding solution operators also by $\mathcal{K}, \hat{\mathcal{K}}$ and $\mathcal{T}_I$ . We now derive simple representations for these operators.

**Solution operator for coagulation**

Consider the pure coagulation step, i.e., $u = 0$ and $I = 0$ . Equation (3.5) takes the form

$$\frac{\partial}{\partial t}\, m_0(t,x) = -\frac{K}{2}\, m_0(t,x)^2$$

and has the solution

$$m_0(t,x) \quad = \quad \frac{m_0(0,x)}{1 + \frac{K}{2}\, m_0(0,x)\, t}\,.$$

Thus, the solution operator for the coagulation step is

$$\mathcal{K}(t,f)(x) = \frac{f(x)}{1 + \frac{K}{2}\, f(x)\, t} \tag{3.28}$$

Equation (3.6) takes the form

$$\frac{\partial}{\partial t}\, \hat{m}_0(t,x) = -\frac{K}{2}\, \hat{m}_0(t,x)\, (H\hat{m}_0)(t,x)\,, \tag{3.29}$$

which implies

$$\frac{\partial}{\partial t}\, (H\hat{m}_0)(t,x) = -\frac{K}{2}\, [(H\hat{m}_0)(t,x)]^2$$

so that

$$(H\hat{m}_0)(t,x) \quad = \quad \frac{(H\hat{m}_0)(0,x)}{1 + \frac{K}{2}\, (H\hat{m}_0)(0,x)\, t}\,.$$

According to Remark 3.2, one obtains the solution of (3.29) in the form

$$\hat{m}_0(t,x) = \hat{m}_0(0,x)\,\exp\left(-\frac{K}{2}\int_0^t (H\hat{m}_0)(s,x)\,ds\right)$$
$$= \hat{m}_0(0,x)\,\exp\left(-\frac{K}{2}\int_0^t \frac{(H\hat{m}_0)(0,x)}{1+\frac{K}{2}\,(H\hat{m}_0)(0,x)\,s}\,ds\right)$$
$$= \hat{m}_0(0,x)\,\exp\left(-\log\left(1+\frac{K}{2}\,(H\hat{m}_0)(0,x)\,t\right)\right) = \frac{\hat{m}_0(0,x)}{1+\frac{K}{2}\,(H\hat{m}_0)(0,x)\,t}\,.$$

Thus, the solution operator for the coagulation step is

$$\hat{\mathcal{K}}(t,f)(x) = \frac{f(x)}{1+\frac{K}{2}\,(Hf)(x)\,t}\,. \tag{3.30}$$

**Solution operator for transport**

Consider the transport step with inception, i.e., $K = 0$. The first part of the derivation is performed for a multi-dimensional position space. Equation (3.5) takes the form

$$\frac{\partial}{\partial t}\,m_0(t,x) = A^*_x\,m_0(t,x) + I_0(x)\,, \tag{3.31}$$

where

$$(Af)(x) = (u(x),\nabla_x)f(x) \tag{3.32}$$

is the generator of the independent particle evolution and

$$(A^*\varphi)(x) = -(\nabla_x, u(x)\varphi(x))$$

is the adjoint operator. The corresponding semigroup is

$$P(t)\,f(x) = f(X_t(x))\,, \tag{3.33}$$

where

$$\frac{d}{dt}\,X_t(x) = u(X_t(x))\,, \qquad X_0(x) = x\,. \tag{3.34}$$

Assuming that $X_t$ is invertible, one obtains

$$\int \varphi(x)\,(P(t)f(x))\,dx = \int \varphi(x)\,f(X_t(x))\,dx$$
$$= \int \varphi(X_t^{-1}(y))\,f(y)\,|\det(X_t^{-1})'(y)|\,dy$$

so that

$$P(t)^*\varphi(x) = \varphi(X_t^{-1}(x))\,|\det(X_t^{-1})'(x)|\,. \tag{3.35}$$

According to Remark 3.3, it follows from (3.31) and (3.35) that

$$\mathcal{T}_I(t)f(x) = \tag{3.36}$$
$$f(X_t^{-1}(x))\,|\det(X_t^{-1})'(x)| + \int_0^t I_0(X_s^{-1}(x))\,|\det(X_s^{-1})'(x)|\,ds\,.$$

If

$$u(x) = \alpha\,x + \beta \tag{3.37}$$

then (3.34) takes the form

$$\frac{d}{dt}\,X_t(x) \;=\; \alpha\,X_t(x) + \beta\,.$$

According to Remark 3.2, one obtains

$$X_t(x) = \exp(\alpha\,t)\left[\beta\int_0^t \exp(-\alpha\,s)\,ds + x\right] =$$
$$\exp(\alpha\,t)\left[\frac{\beta}{\alpha}\Big[1-\exp(-\alpha\,t)\Big] + x\right] = \frac{\beta}{\alpha}\Big[\exp(\alpha\,t)-1\Big] + x\,\exp(\alpha\,t)$$

so that

$$X_t^{-1}(x) = x\,\exp(-\alpha\,t) - \frac{\beta}{\alpha}\Big[1-\exp(-\alpha\,t)\Big] \tag{3.38}$$

and

$$(X_t^{-1})'(x) = \exp(-\alpha\,t)\,.$$

Note that

$$X_t^{-1}(x) > 0 \quad\Leftrightarrow\quad x > x_*(t) \quad\Leftrightarrow\quad t_*(x) > t\,, \tag{3.39}$$

where

$$x_*(t) = \frac{\beta}{\alpha}\Big[\exp(\alpha\,t)-1\Big]$$

and

$$t_*(x) = \frac{1}{\alpha}\log\left[\frac{\alpha}{\beta}\,x + 1\right]. \tag{3.40}$$

Thus, (3.36) implies

$$\mathcal{T}_I(t)f(x) = \tag{3.41}$$
$$f(X_t^{-1}(x))\,\exp(-\alpha\,t) + \int_0^{\min(t,t_*(x))} I_0(X_s^{-1}(x))\,\exp(-\alpha\,s)\,ds\,.$$

If $\alpha = 0$, then one obtains $X_t^{-1}(x) = x - \beta\,t$ and $t_*(x) = \frac{x}{\beta}$ (cf. (3.38), (3.40)) so that (3.41) takes the form

$$\mathcal{T}_I(t)f(x) = f(x-\beta\,t) + \int_0^{\min\left(t,\frac{x}{\beta}\right)} I_0(x-\beta\,s)\,ds\,. \tag{3.42}$$

**Example 3.5** *Consider the case $u = 1$ (cf. (3.37)). Let $K = 2$ and $I_0 = 1$ . Then (3.42) takes the form*

$$\mathcal{T}_I(t) f(x) = f(x-t) + \min(t, x)\,.$$

*Strang splitting (3.26) gives*

$$\begin{aligned} m_0^{\Delta t}(t_j, x) &= f_1(x - \Delta t/2) + \min(\Delta t/2, x) \\ \hat{m}_0^{\Delta t}(t_j, x) &= \hat{f}_1(x - \Delta t/2) + \min(\Delta t/2, x)\,, \end{aligned} \tag{3.43}$$

*where (cf. (3.28), (3.30))*

$$\begin{aligned} & f_1(x) = \frac{f_0(x)}{1 + f_0(x)\,\Delta t}\,, \qquad \hat{f}_1(x) = \frac{\hat{f}_0(x)}{1 + (H\hat{f}_0)(x)\,\Delta t}\,, \\ & f_0(x) = m_0^{\Delta t}(t_{j-1}, x - \Delta t/2) + \min(\Delta t/2, x)\,, \\ & \hat{f}_0(x) = \hat{m}_0^{\Delta t}(t_{j-1}, x - \Delta t/2) + \min(\Delta t/2, x)\,. \end{aligned} \tag{3.44}$$

*Note that all functions are taken to vanish for $x < 0$ . For $x \in [0, \Delta t/2)$ , one obtains from (3.43)*

$$m_0^{\Delta t}(t_j, x) = \hat{m}_0^{\Delta t}(t_j, x) = x \tag{3.45}$$

*and from (3.44)*

$$f_0(x) = \hat{f}_0(x) = x\,. \tag{3.46}$$

*For $x \in [\Delta t/2, \Delta t)$ , one obtains from (3.43) and (3.44)*

$$m_0^{\Delta t}(t_j, x) \;=\; \frac{f_0(x - \Delta t/2)}{1 + f_0(x - \Delta t/2)\,\Delta t} + \frac{\Delta t}{2} \tag{3.47}$$

*and*

$$\hat{m}_0^{\Delta t}(t_j, x) \;=\; \frac{\hat{f}_0(x - \Delta t/2)}{1 + (H\hat{f}_0)(x - \Delta t/2)\,\Delta t} + \frac{\Delta t}{2}\,. \tag{3.48}$$

*If (cf. (2.3))*

$$x - \Delta t/2 \in [x_{l-1}, x_l) \subset [0, \Delta t/2)\,, \qquad \text{for some} \quad l = 1, \ldots, L\,, \tag{3.49}$$

*then is follows from (3.46) that (cf. (2.6), (2.23))*

$$(H\hat{f}_0)(x - \Delta t/2) = \frac{x_{l-1} + x_l}{2}\,. \tag{3.50}$$

*Consider $x = x_{l-1} + \Delta t/2$ such that (3.49) is satisfied and $x_{l-1} > \Delta t/4$ . This choice is possible for sufficiently small $\Delta x$ . Then (3.46)–(3.48) and (3.50) imply*

$$\begin{aligned} & m_0^{\Delta t}(t_j, x) - \hat{m}_0^{\Delta t}(t_j, x) = \\ & \qquad \frac{\Delta t\, f_0(x - \Delta t/2)\Big[(H\hat{f}_0)(x - \Delta t/2) - f_0(x - \Delta t/2)\Big]}{\Big[1 + f_0(x - \Delta t/2)\,\Delta t\Big]\Big[1 + (H\hat{f}_0)(x - \Delta t/2)\,\Delta t\Big]} \\ & = \quad \frac{\Delta t\, x_{l-1}\left[\frac{x_{l-1} + x_l}{2} - x_{l-1}\right]}{\Big[1 + x_{l-1}\,\Delta t\Big]\Big[1 + (x_{l-1} + x_l)\,\Delta t/2\Big]} \ge \frac{\Delta t^2/4\ \Delta x/2}{\Big(1 + \Delta t^2/2\Big)^2} \end{aligned}$$

*so that*

$$\|m_0^{\Delta t}(t_j) - \hat{m}_0^{\Delta t}(t_j)\|_\infty \quad \geq \quad C(\Delta t)\,\Delta x\,. \tag{3.51}$$

*According to (3.45), (3.47) and (3.48), the steady state in the region $x \in [0, \Delta t - \Delta x]$ is reached after one time step. Thus, (3.51) implies*

$$\liminf_{\Delta x \to 0} \frac{\|m_{0,\infty}^{\Delta t} - \hat{m}_{0,\infty}^{\Delta t}\|_\infty}{\Delta x} \quad > \quad 0$$

*so that (3.2) follows (cf. (3.24)).*

## 3.3 Cell averages

Here we consider the case $\Delta t > 0$ . According to Example 3.5, the second order convergence (2.15) of Theorem 2.1 does not hold in general. However, the norm (2.9) is rather strong with respect to $x$ . It is of interest to understand if second order convergence holds, when a weaker distance is used. Such a distance is obtained by using cell averages, since (cf. (2.23), (2.28))

$$\|Hc_\infty^{\Delta t} - H\hat{c}_\infty^{\Delta t}\| \quad \leq \quad \|c_\infty^{\Delta t} - \hat{c}_\infty^{\Delta t}\|\,. \tag{3.52}$$

Let $K = 2$ and $I_0 = 1$ . Numerical estimates of the quantities

$$\|Hm_{0,\infty}^{\Delta t} - H\hat{m}_{0,\infty}^{\Delta t}\|_\infty \tag{3.53}$$

are provided in Figure 1. These results indicate that there is indeed second order convergence, if $u$ is constant (as in Example 3.5), but in general there is only first order convergence. This implies (3.3), since (cf. (2.9))

$$\|Hm_{0,\infty}^{\Delta t} - H\hat{m}_{0,\infty}^{\Delta t}\|_\infty \quad \leq \quad \|Hc_\infty^{\Delta t} - H\hat{c}_\infty^{\Delta t}\|\,.$$

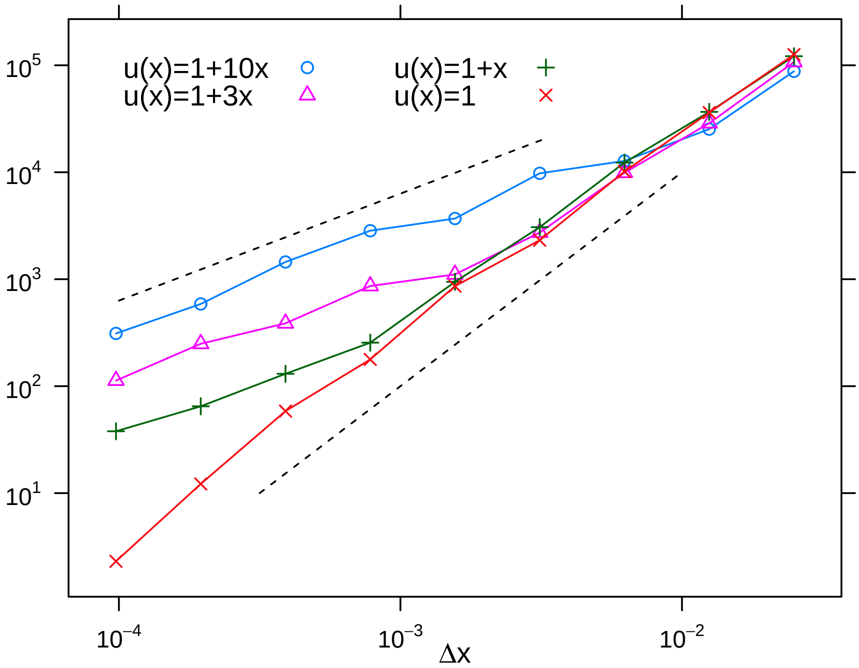


Figure 1: Error (3.53) for the cell averages of the zeroth moments (3.4). Dashed lines indicate first and second order.

# 4 Comments

Theorem 2.1 provides second order convergence with respect to cell size. The assumption of non-vanishing advection cannot be skipped, as Example 3.4 shows. The assumption of a bounded coagulation rate is essential for the present proof technique. The result might remain true at least for sublinear (non-gelling) coagulation kernels. The second order convergence is quite surprising, when taking into account that the spatial smoothing function (2.6) is not even continuous and the norm (2.9) is rather strong with respect to the position. Originally, we expected to get second order only with respect to a weaker distance measuring the difference of cell averages (cf. (3.52)). The result holds for the limiting equations with no time splitting error. For practical purposes, the time step should be sufficiently small in order to observe second order convergence with respect to cell size. This assumption is quite reasonable, since splitting should not allow particles to travel too far without having a chance to coagulate.

The main purpose of this paper was to understand the approximation error with respect to cell size. In order to make the derivations more transparent, we considered a relatively simple model. Some generalizations are straightforward. In particular, the result of Theorem 2.1 holds for more general type spaces, e.g., $\mathcal{Y} = (0,\infty)^k$, or $\mathcal{Y} = \{1,2,\ldots\}^k$, or combinations of discrete and continuous components. This is important to cover various applications (cf. [PW12]), since the main motivation for developing stochastic particle methods is their ability to treat high dimensional type spaces efficiently. Moreover, the result holds when the right-hand side of equation (1.1) is extended by linear terms, e.g., those representing surface growth in certain soot models (cf. [PWK11]). It also holds for the stochastic weighted algorithm introduced in [PW12], since that algorithm has the same limiting equation as one of the direct simulation algorithms considered here (cf. (2.8)). The proof of Theorem 2.1 works for non-equidistant grids, when $\Delta x$ is defined as the maximum grid size. Finally, Theorem 2.1 is expected to hold in the transient case as well, but the present proof technique is restricted to the steady state equations.

Other generalizations of the model are more challenging. In particular, it would be of considerable interest to cover a multi-dimensional position space and to include more general transport mechanisms. A problem, which we hope to address in the near future, is to understand the joint behaviour of cell size and time step error. This would allow us to give quantitative recommendations about the choice of these parameters.

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