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Mass-conserving solutions and non-conservative approximation to the Smoluchowski coagulation equation

By

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Abstract. The non-conservative truncation of the Smoluchowski coagulation equation is a good approximation to study the gelation phenomenon, both from a theoretical and numerical point of view. The purpose of this note is to show that it is also well-suited to approximate the Smoluchowski equation in the absence of gelation.

1. Introduction. The Smoluchowski coagulation equation is a mean-field model for the growth of clusters (particles, droplets, ...) by successive mergers, that is, two particles encounter and merge into a single one, the mass of the resulting particle being the sum of the masses of the incoming particles. When each particle in the system under consideration is fully identified by its mass, the Smoluchowski coagulation equation gives the time evolution of the mass distribution function $f = f(t, y) \geqq 0$ of particles of mass $y > 0$ at time $t \geqq 0$ and reads [6], [19]

$$\partial_t f = Q_c(f), \quad (t, y) \in \mathbb{R}_+^2, \tag{1}$$

$$f(0) = f^{in}, \quad y \in \mathbb{R}_+, \tag{2}$$

where $\mathbb{R}_+ := (0, +\infty)$ and the coagulation reaction term $Q_c(f)$ is given by

$$Q_c(f)(y) = \frac{1}{2} \int_0^y a(y_*, y - y_*) f(y_*) f(y - y_*)\, dy_* - \int_0^\infty a(y, y_*) f(y) f(y_*)\, dy_*$$

for $y \in \mathbb{R}_+$. We recall that the first term in $Q_c(f)$ accounts for the formation of particles of mass y from the coalescence of smaller particles and the last term describes the loss

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of particles of mass y after coalescence with other particles. The coalescence coefficient $a = a(y, y_*)$ gives the rate at which the coalescence of two particles with respective masses y and y_* produces a particle of mass $y + y_*$ and is a nonnegative symmetric function

$$0 \leqq a(y, y_*) = a(y_*, y), \quad (y, y_*) \in \mathbb{R}_+^2.$$

An interesting feature of the Smoluchowski coagulation equation (1), (2) lies in the time evolution of the total mass $M_1(t)$ of the particles defined by

$$M_1(t) := \int_0^\infty y\, f(t, y)\, dy, \quad t \geqq 0. \tag{3}$$

Indeed, since mass is conserved during each coalescence event, it could be expected that M_1 remains constant through time evolution. It is however well-known by now that this property fails to be true for coalescence coefficients a such that $a(y, y_*) \geqq (y\, y_*)^\alpha$ for some $\alpha > 1/2$, which grow rapidly as y and y_* become large, see [10], [16], [17], [18] and the review articles [1], [14]. The failure of mass conservation is refered to as the gelation phenomenon in the literature, and though known for some time [10], [16], [17], [18], rigorous mathematical proofs were obtained only recently [8], [11]. On the other hand, it is known that, if

$$a(y, y_*) \leqq A\, (1 + y + y_*), \quad (y, y_*) \in \mathbb{R}_+^2, \tag{4}$$

for some $A > 0$ and

$$f^{in} \in L_1^1(\mathbb{R}_+) := L^1(\mathbb{R}_+; (1 + y)\, dy) \text{ is nonnegative a.e.,} \tag{5}$$

there exists at least a mass-conserving solution f to (1), (2), that is, f satisfies

$$M_1(t) = \int_0^\infty y\, f(t, y)\, dy = \int_0^\infty y\, f^{in}(y)\, dy \tag{6}$$

for each $t \geqq 0$ [3], [7], [12], [13], [21].

The usual way to construct such a solution relies on the so-called *conservative* approximation of (1), which is defined as follows: given a positive integer $n \geqq 1$, we set

$$f_n^{in}(y) := f^{in}(y)\, \mathbf{1}_{(0,n)}(y), \quad a_n^c(y, y_*) := a(y, y_*)\, \mathbf{1}_{(0,n)}(y + y_*), \tag{7}$$

and consider the integro-differential equation

$$\partial_t \bar{f}_n(t, y) = \frac{1}{2} \int_0^y a(y - y_*, y_*) \bar{f}_n(t, y_*) \bar{f}_n(t, y - y_*)\, dy_* - \int_0^{n-y} a(y, y_*) \bar{f}_n(t, y) \bar{f}_n(t, y_*)\, dy_*, \quad (t, y) \in \mathbb{R}_+ \times (0, n), \tag{8}$$

$$\bar{f}_n(0) = f_n^{in}, \quad y \in (0, n). \tag{9}$$

Observe that (8) follows from (1) after replacing a by a_n^c. Under the assumptions (4), (5), the existence and uniqueness of a nonnegative solution $\bar{f}_n \in \mathcal{C}([0,+\infty); L^1(0,n))$ to (8), (9) are easily obtained by a classical fixed point argument. In addition, $\bar{f}_n$ satisfies a truncated version of the mass conservation (6), namely,

$$\int_0^n y\ \bar{f}_n(t,y)\,dy = \int_0^n y\ f^{in}(y)\,dy, \quad t \geqq 0\,. \tag{10}$$

Thanks to the growth condition (4), it is then possible to extract a subsequence $(\bar{f}_{n_k})$ of $(\bar{f}_n)$ such that $(\bar{f}_{n_k})$ converges towards a solution f to (1), (2) in $\mathcal{C}_w([0,T]; L^1_1(\mathbb{R}_+))$ for each $T > 0$ [13]. A straightforward consequence of this convergence and (10) is that the solution f to (1), (2) thus obtained is mass-conserving, that is, satisfies (6). We recall here that $\mathcal{C}_w([0,T]; L^1_1(\mathbb{R}_+))$ denotes the space of weakly continuous functions from $[0,T]$ to $L^1_1(\mathbb{R}_+)$ and that a sequence (g_n) converges to g in $\mathcal{C}_w([0,T]; L^1_1(\mathbb{R}_+))$ if

$$\lim_{n\to+\infty} \sup_{t\in[0,T]} \left| \int_0^\infty (1+y)(g_n(t,y) - g(t,y))\varphi(y)\,dy \right| = 0$$

for every $\varphi \in L^\infty(\mathbb{R}_+)$.

There are however other approximations to the Smoluchowski coagulation equation (1) which differ from the *conservative* approximation (8) and we refer to [2], [4] for a detailed discussion of this issue. Of particular interest to study the onset of gelation is the *non-conservative* approximation, which is defined as follows: given a positive integer $n \geqq 1$, we set

$$f_n^{in}(y) := f^{in}(y)\,\mathbf{1}_{(0,n)}(y), \quad a_n^{nc}(y,y_*) := a(y,y_*)\,\mathbf{1}_{(0,n)}(y)\,\mathbf{1}_{(0,n)}(y_*), \tag{11}$$

and consider the integro-differential equation

$$\begin{aligned} \partial_t f_n(t,y) = {} & \frac{1}{2}\int_0^y a(y-y_*,y_*) f_n(t,y_*) f_n(t,y-y_*)\,dy_* \\ & - \int_0^n a(y,y_*)\ f_n(t,y)\ f_n(t,y_*)\,dy_*, \quad (t,y) \in \mathbb{R}_+ \times (0,n), \end{aligned} \tag{12}$$

$$f_n(0) = f_n^{in}, \quad y \in (0,n). \tag{13}$$

Here again, notice that (13) follows from (1) after replacing a by a_n^{nc}. Similarly as for (8), (9), the existence and uniqueness of a nonnegative solution $f_n \in \mathcal{C}([0,+\infty); L^1(0,n))$ to (12), (13) are easily established by a classical fixed point argument. But f_n satisfies

$$\begin{aligned} \int_0^n y\ f_n(t,y)\,dy = {} & \int_0^n y\ f^{in}(y)\,dy \\ & - \frac{1}{2}\int_0^t \int_0^n \int_{n-y}^n (y+y_*)\,a(y,y_*)\ f_n(s,y)\ f_n(s,y_*)\,dy_* dy ds \end{aligned} \tag{14}$$

for $t \geqq 0$ instead of (10). Proceeding along the lines of [13], one can also prove that, if

$$\lim_{y_* \to +\infty} \sup_{y \in (0,R)} \frac{a(y, y_*)}{y_*} = 0 \quad \text{for each} \quad R > 0\,,$$

there are a subsequence (f_{n_k}) of (f_n) and a solution f to (1), (2) such that (f_{n_k}) converges towards f in $\mathcal{C}_w([0, T]; L^1(\mathbb{R}_+))$ for each $T > 0$. The convergence being with respect to a weaker topology, we can only conclude from (14) that f satisfies

$$\int_0^\infty y\, f(t, y)\, dy \leqq \int_0^\infty y\, f^{in}(y)\, dy, \quad t \geqq 0.$$

Thus, if a satisfies additionally the growth condition (4) and in the absence of a general uniqueness result for (1), it is not known whether the solution to (1), (2) constructed with the *non-conservative* approximation (13), (12) is mass-conserving or not.

Nevertheless, numerical simulations which we performed recently in [9] seem to indicate that the answer to this question is positive and the purpose of this note is to provide a proof of this fact. More precisely, we have the following result:

Theorem 1. *Assume that the coalescence coefficient a and the initial datum f^{in} satisfy* (4) *and* (5)*, respectively. For $n \geqq 1$, we denote by f_n the solution to* (13), (12). *Then there are a subsequence (f_{n_k}) of (f_n) and a mass-conserving solution f to* (1), (2) *such that*

$$f_{n_k} \longrightarrow f \quad in \quad \mathcal{C}_w([0, T]; L^1_1(\mathbb{R}_+)) \tag{15}$$

for each $T > 0$.

By a mass-conserving solution f to (1), (2), we mean a nonnegative function

$$f \in \mathcal{C}_w([0, +\infty); L^1(\mathbb{R}_+)) \cap L^\infty(0, +\infty; L^1_1(\mathbb{R}_+))$$

satisfying (6) and

$$\int_0^\infty (f(t, y) - f^{in}(y))\, \varphi(y)\, dy$$
$$= \int_0^t \int_0^\infty \int_0^\infty a(y, y_*)(\varphi(y + y_*) - \varphi(y) - \varphi(y_*))\, f(s, y)\, f(s, y_*)\, dy_* dy ds$$

for every $t \geqq 0$ and $\varphi \in L^\infty(\mathbb{R}_+)$.

The proof of Theorem 1 requires two steps: we first proceed as in the proof of [13, Theorem 2.5] to show that there are a subsequence (f_{n_k}) of (f_n) and a solution f to (1), (2) such that the convergence (15) holds true. The second step is to justify that f is actually a mass-conserving solution to (1), (2) and this does not solely follow from (15) as for the *conservative* approximation (8), (9). Indeed, we shall additionally prove that the second term in the right-hand side of (14) vanishes in the limit $n \to +\infty$. This fact will follow from a suitable moment estimate (see (24) below).

2. Proof of Theorem 1. Since $f^{in} \in L^1_1(\mathbb{R}_+)$ by (5), a refined version of the de la Vallée-Poussin theorem [5], [15] ensures the existence of two nonnegative and convex functions Φ_1 and Φ_2 in $\mathcal{C}^2([0, +\infty))$ such that Φ_1' and Φ_2' are concave,

$$\Phi_i(0) = 0\,, \quad \lim_{r\to+\infty} \frac{\Phi_i(r)}{r} = +\infty, \quad i = 1, 2, \tag{16}$$

and

$$\int_0^\infty \Phi_1(1+y)\, f^{in}(y)\, dy < +\infty \quad \text{and} \quad \int_0^\infty \Phi_2(f^{in}(y))\, dy < +\infty. \tag{17}$$

Let us recall here some properties of nondecreasing and convex functions with concave first derivatives (such as Φ_1 and Φ_2) which will be needed in the sequel.

Lemma 2. *For $(r, r_*) \in \mathbb{R}_+^2$, we have*

$$\Phi_2(r) \leqq r\, \Phi_2'(r) \leqq 2\, \Phi_2(r), \tag{18}$$

$$0 \leqq \Phi_1(r + r_*) - \Phi_1(r) - \Phi_1(r_*) \leqq 2\, \frac{r\, \Phi_1(r_*) + r_*\, \Phi_1(r)}{r + r_*}. \tag{19}$$

The inequalities (18) and (19) follow from [12, Lemma A.1] and [12, Lemma A.2], respectively.

We next recall that, for $n \geqq 1$ and $\varphi \in L^\infty(\mathbb{R}_+)$, the solution f_n to (13), (12) satisfies

$$\begin{aligned} &\int_0^n \varphi(y)(f_n(t,y) - f_n^{in}(y))\, dy \\ &\quad = \frac{1}{2} \int_0^t \int_0^n \int_0^n D_\varphi(y, y_*)\, a(y, y_*)\, f_n(s, y)\, f_n(s, y_*)\, dy_* dy ds, \end{aligned} \tag{20}$$

where

$$D_\varphi(y, y_*) := \varphi(y + y_*)\, \mathbf{1}_{(0,n)}(y + y_*) - \varphi(y) - \varphi(y_*), \quad (y, y_*) \in (0, n)^2. \tag{21}$$

The assertion (20) follows from (13) after multiplication by $\varphi(y)$, integration over $(0, t) \times (0, n)$ and application of the Fubini theorem to the first term of the right-hand side. A straightforward consequence of (5), (11) and (20) with $\varphi(y) = y$ and $\varphi(y) = 1$ is that, for each $n \geqq 1$,

$$\sup_{t \geqq 0} \int_0^n (1 + y)\, f_n(t, y)\, dy \leqq \int_0^\infty (1 + y)\, f^{in}(y)\, dy. \tag{22}$$

In the following, we denote by C any positive constant depending only on A, f^{in}, Φ_1 and Φ_2. The dependence of C upon additional parameters will be indicated explicitly. We also extend $f_n(t)$ to $\mathbb{R}_+$ by setting $f_n(t, y) = 0$ for $y \geqq n$.

Owing to (17) and (20), we may study the behaviour of f_n for large values of y.

Lemma 3. *For $T > 0$, there is a constant $C(T)$ depending on T such that, for every $n \geqq 1$,*

$$\sup_{t \in [0,T]} \int_0^n \Phi_1(1 + y)\, f_n(t, y)\, dy \leqq C(T), \tag{23}$$

$$\int_0^T \int_0^n \int_{n-y}^n \Phi_1(1 + y_*)\, a(y, y_*)\, f_n(s, y)\, f_n(s, y_*)\, dy_* dy ds \leqq C(T). \tag{24}$$

Proof. We take $\varphi(y) = \Phi_1(1 + y)$, $y \in (0, n)$, in (20) and use (11) and (17) to obtain

$$\int_0^n \Phi_1(1 + y)\, f_n(t, y)\, dy \leqq C + \frac{1}{2} \int_0^t (\mathcal{I}_n(s) + \mathcal{J}_n(s))\, ds, \tag{25}$$

where

$$\mathcal{I}_n(s) := \int_0^n \int_0^{n-y} D_1(y, y_*)\, a(y, y_*) f_n(s, y) f_n(s, y_*)\, dy_* dy$$

$$\mathcal{J}_n(s) := \int_0^n \int_{n-y}^n D_1(y, y_*)\, a(y, y_*)\, f_n(s, y)\, f_n(s, y_*)\, dy_* dy$$

$$D_1(y, y_*) := \Phi_1(1 + y + y_*)\, \mathbf{1}_{(0,n)}(y + y_*) - \Phi_1(1 + y) - \Phi_1(1 + y_*).$$

On the one hand, if $y + y_* \leqq n$, we infer from (19), the monotonicity of Φ_1 and (4) that

$$\begin{aligned} & a(y, y_*)\, D_1(y, y_*) \\ & \leqq a(y, y_*)\, (\Phi_1(2 + y + y_*) - \Phi_1(1 + y) - \Phi_1(1 + y_*)) \\ & \leqq 2a(y, y_*)\, \frac{(1 + y)\, \Phi_1(1 + y_*) + (1 + y_*)\, \Phi_1(1 + y)}{2 + y + y_*} \\ & \leqq 2A((1 + y)\, \Phi_1(1 + y_*) + (1 + y_*)\, \Phi_1(1 + y)). \end{aligned}$$

Using (22), we end up with

$$\mathcal{I}_n(s) \leqq C \int_0^n \Phi_1(1+y)\, f_n(s,y)\, dy.$$

On the other hand, if $y + y_* > n$, we have $D_1(y, y_*) = -\Phi_1(1+y) - \Phi_1(1+y_*)$ and thus

$$\mathcal{J}_n(s) = -2 \int_0^n \int_{n-y}^n a(y,y_*)\, \Phi_1(1+y_*)\, f_n(s,y)\, f_n(s,y_*)\, dy_* dy \leqq 0.$$

Inserting the estimates for $\mathcal{I}_n(s)$ and $\mathcal{J}_n(s)$ in (25) and using the Gronwall lemma yield (23) and (24). □

We next proceed along the lines of [13, Lemma 3.3 & Lemma 3.5] to prove the following result.

Lemma 4. *For any $T > 0$ and $R > 0$, there is a constant $C(T, R)$ such that*

$$\sup_{t\in[0,T]} \int_0^R \Phi_2\left(f_n(t,y)\right) dy \leqq C(T,R),$$

$$\sup_{t\in[0,T]} \left| \frac{d}{dt} \int_0^R f_n(t,y)\varphi(y) dy \right| \leqq C(T,R)\, \|\varphi\|_{L^\infty(0,R)}$$

for every $n \geqq 1$ and $\varphi \in L^\infty(0, R)$.

Proof. It follows from (13) and the non-negativity of a and f_n that

$$\frac{d}{dt}\int_0^R \Phi_2(f_n)\, dy \leqq \frac{1}{2}\int_0^R \int_0^{R-y_*} a(y,y_*)\, \Phi_2'(f_n(y+y_*))\, f_n(y)\, f_n(y_*)\, dy dy_* .$$

We now use (4) and the inequality

$$\Phi_2'(r)\, r_* \leqq \Phi_2(r_*) + r\, \Phi_2'(r) - \Phi_2(r) \leqq \Phi_2(r_*) + \Phi_2(r), \quad r, r_* \geqq 0,$$

which is a consequence of (18) and the convexity of Φ_2 to deduce that

$$\begin{aligned}
&\frac{d}{dt}\int_0^R \Phi_2(f_n)\, dy \\
&\quad \leqq \frac{1}{2}\int_0^R \int_0^{R-y_*} a(y,y_*)\{\Phi_2(f_n(y+y_*)) + \Phi_2(f_n(y_*))\}\, f_n(y)\, dy dy_* \\
&\quad \leqq A(1+R) \left(\int_0^R f_n(y)\, dy\right) \left(\int_0^R \Phi_2(f_n(y))\, dy\right),
\end{aligned}$$

whence

$$\frac{d}{dt}\int_0^R \Phi_2(f_n)\,dy \leqq C(R)\int_0^R \Phi_2(f_n(y))\,dy$$

by (22). The Gronwall lemma then entails the first estimate in Lemma 4. We next readily infer from (4) and (22) that, for $\varphi \in L^\infty(0,R)$,

$$\begin{aligned}\left|\frac{d}{dt}\int_0^R f_n(t,y)\,\varphi(y)\,dy\right| &\leqq \frac{A}{2}(1+R)\left(\int_0^R f_n(t,y)\,dy\right)^2 \|\varphi\|_{L^\infty(0,R)}\\ &+ A\int_0^{\min\{R,n\}}\int_0^n (1+y+y_*)\,f_n(t,y)\,f_n(t,y_*)\,dy_*dy\,\|\varphi\|_{L^\infty(0,R)}\\ &\leqq C(R)\,\|\varphi\|_{L^\infty(0,R)},\end{aligned}$$

and the proof of Lemma 4 is complete. □

Owing to (16), (22), (23) and Lemma 4, we may use the Dunford-Pettis and the Arzelà-Ascoli theorems to conclude that (f_n) is relatively compact in $\mathcal{C}_w([0,T];L_1^1(\mathbb{R}_+))$ for each $T>0$. There are thus a subsequence of (f_n) (not relabeled) and a nonnegative function $f \in \mathcal{C}_w([0,+\infty);L_1^1(\mathbb{R}_+))$ such that

$$f_n \longrightarrow f \quad \text{in} \quad \mathcal{C}_w([0,T];L_1^1(\mathbb{R}_+)) \tag{26}$$

for each $T>0$. It is now a standard matter to show that (4), (13), (12) and (26) ensure that f is a solution to (1), (2) [13], [20].

It remains to show that f is mass-conserving. For that purpose, we notice that, if $y+y_*>n$, then either $y>n/2$ or $y_*>n/2$ so that $\Phi_1(1+y)+\Phi_1(1+y_*)\geqq\Phi_1(n/2)$, thanks to the non-negativity and monotonicity of Φ_1. Therefore, since $y+y_*\leqq 2n$,

$$\begin{aligned}&\frac{1}{2}\int_0^t\int_0^n\int_{n-y}^n (y+y_*)\,a(y,y_*)\,f_n(s,y)\,f_n(s,y_*)\,dy_*dyds\\ &\leqq \frac{n}{\Phi_1(n/2)}\int_0^t\int_0^n\int_{n-y}^n \Phi_1(n/2)\,a(y,y_*)f_n(s,y)\,f_n(s,y_*)\,dy_*dyds\\ &\leqq \frac{n}{\Phi_1(n/2)}\int_0^t\int_0^n\int_{n-y}^n (\Phi_1(1+y)+\Phi_1(1+y_*))\\ &\quad\cdot a(y,y_*)f_n(s,y)\,f_n(s,y_*)\,dy_*dyds\end{aligned}$$

$$\leqq \frac{2n}{\Phi_1(n/2)} \int_0^t \int_0^n \int_{n-y}^n \Phi_1(1+y_*)\, a(y,y_*)\, f_n(s,y) f_n(s,y_*)\, dy_* dy ds$$

$$\leqq \frac{2n}{\Phi_1(n/2)}\, C(t)$$

by (24). Owing to (16), we may let $n \to +\infty$ in the above inequality to conclude that

$$\lim_{n\to+\infty} \frac{1}{2} \int_0^t \int_0^n \int_{n-y}^n (y+y_*)\, a(y,y_*)\, f_n(s,y)\, f_n(s,y_*)\, dy_* dy ds = 0\,.$$

Recalling (11), (14) and (26), we may then pass to the limit as $n \to +\infty$ in (14) to obtain that

$$\int_0^\infty y\, f(t,y)\, dy = \int_0^\infty y\, f^{in}(y)\, dy,$$

which completes the proof of Theorem 1.

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