A quasi-stochastic simulation
of the general dynamics equation for aerosols

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Abstract. We propose a quasi-Monte Carlo (QMC) scheme for the simulation of the general dynamics equation (GDE) for aerosols. The mass distribution is approximated by a fixed number of weighted numerical particles. Time is discretized and a splitting approach is used. Coagulation is simulated with a stochastic particle method using quasi-random points. In addition, the particles are reordered by increasing size at every time step. Integration of condensation/evaporation and deposition is performed using a deterministic particle method. The accuracy of the scheme is assessed through several numerical experiments, in cases where an exact solution is known. The error of the QMC scheme is shown to be smaller than the error produced by the corresponding Monte Carlo (MC) scheme.

Keywords. General dynamics equation, aerosols, particle method, quasi-Monte Carlo method, low discrepancy sequences.

AMS classification. 65C05, 82C22.

1. Introduction

Aerosol formation and evolution processes include a variety of phenomena such as coagulation, fragmentation, condensation/evaporation, nucleation and deposition. Applications arise in many scientific and technological areas such as chemistry (reacting polymers), physics (colloidal particles), atmospheric aerosol studies, engineering (behavior of fuel mixtures), medicine, environment, astrophysics (dust formation in stellar environments) [27].

Many physical properties of aerosols are size dependent, so it is important to follow the aerosol size distribution. The time evolution of the concentration (or density) of aerosols undergoing coagulation, condensation/evaporation and deposition phenomena is governed by the General Dynamics Equation (GDE) for aerosols [22]:

\[
\frac{\partial c(x,t)}{\partial t} = \frac{1}{2} \int_{0}^{x} K(x-y,y)c(x-y,t)c(y,t)dy - c(x,t) \int_{0}^{+\infty} K(x,y)c(y,t)dy - \frac{\partial}{\partial x} (I_0c)(x,t) - (Rc)(x,t),
\]

for \(x > 0, t > 0\). The initial condition is \(c(x,0) = c_0(x)\), \(x > 0\). Here \(c(x,t)dx\) is the
relative number of particles whose sizes range between $x$ and $x+dx$ at time $t$, $K(x, y)$, $I_0(x, t)$ and $R(x, t)$ are, respectively, the coagulation, condensation/evaporation and deposition kernels.

The first term on the right-hand side of (1.1) represents the gain of particles of size $x$ by coagulation of two particles of size $y < x$ and $x - y$. The second term represents the loss of particles of size $x$ by coagulation with other particles. It is assumed that the coagulation kernel $K$ is positive and symmetric. The third term on the right-hand side of (1.1) describes the relaxation to an equilibrium between aerosol and gas phase. There is condensation when $I_0 \geq 0$ and evaporation if $I_0 \leq 0$. The fourth term describes aerosol loss by deposition (on ground surfaces or by sticking to rain drops), so $R \geq 0$. The pure coagulation equation (when $I_0 = R = 0$) is referred to as Smoluchowski equation: its discrete analogue was established in [26].

Analytical solutions of the GDE are available for academic cases only. Solutions of the pure coagulation equation have been obtained for bilinear kernels: $K(x, y) = \alpha + \beta(x + y) + \gamma xy$ (see [5, 1] and the references therein). To authors’ knowledge, the only exact solutions of the GDE involving more than one physical process are those reported in [19]. They are calculated for simultaneous coagulation and evaporation (without deposition: $R = 0$). They are only valid for constant or linear coagulation and evaporation kernels, and for special initial configurations. So the numerical simulation of aerosol size distribution is a research field of high interest. Deterministic numerical methods using expansions of the approximate solution on a well-chosen set of basis functions have been developed [12, 16, 9, 25]. They are not at all straightforward (one difficulty comes from the integrals on the right-hand side of the GDE) and sophisticated numerical techniques, like adaptive grid refinement or adaptive time step control are often used.

Monte Carlo (MC) simulations are well developed for solving the Boltzmann equation, whose structure is closely related to that of the Smoluchowski equation. MC schemes are convenient to handle and writing codes and they can also be applied to consider multi-component systems. Several authors proposed algorithms based on the MC approach. Simulation particles are sampled from the initial number distribution; then their sizes are changed according to the GDE. Stochastic schemes for solving the pure coagulation equation are described in [4, 24, 17, 21, 11, 6]. Since simulation particles behave like real particles, they may stick together, so their number is in general a decreasing quantity (in MC methods for the Boltzmann equation, the number of particles remains constant). Hence the number of simulation particles must be artificially increased in order to make the results statistically reliable. A possibility is to run the simulation until half of the initial particle array is depleted, then fill the empty spaces in the particle array with copies of the surviving particles. Another approach is to introduce continuous refilling of the array: select a particle from the array at random and place its copy in the position vacated by coagulation [23]. A different algorithm is proposed in [2]: rather than simulating the number distribution $c(x, t)$,
scheme simulates the mass distribution $xc(x, t)$. Since the total mass is conserved by
the Smoluchowski equation, the number of simulation particles is preserved, so that a
constant statistical accuracy is maintained. Other mass-flow schemes are proposed in
[7, 10]. An application to the integration of the GDE is proposed in [3].

A drawback of MC methods is their low convergence rate. A possible way to ac-
celerate the convergence is to change the choice of the random numbers. The MC
methods use pseudo-random numbers (or vectors) which simulate i.i.d. random vari-
able with (for instance) uniform distribution. In a quasi-Monte Carlo (QMC) method,
pseudo-random numbers are replaced by quasi-random numbers or low-discrepancy
point sets, which are points “evenly distributed” (see section 2). For simulations, this
cannot be done directly as in integration problems, and special measures have to be
taken to make a proper use of the better uniformity of quasi-random points: for the
simulation of the Boltzmann equation, see [14].

A QMC scheme for the simulation of the discrete coagulation equation is proposed
in [15]. In the present work, we generalize the method to the simulation of the GDE
for aerosols. A number of weighted numerical particles are sampled from the initial
size distribution. Time is discretized into intervals and the method evolves the sizes
and weights of the particles by a fractional step iteration. The first step of the method
involves the simulation of coagulation by a MC method using quasi-random points.
Before this step, a sorting of the particles by increasing size is performed: it is shown
in [15] that this ensures better convergence for QMC schemes over MC schemes when
solving the discrete Smoluchowski equation. The second fractional step of the method
(integration of condensation/evaporation and deposition) is performed in a determi-
nistic way, by solving a system of ordinary differential equations (ODE). Despite the
non-conservative character of the GDE, the number of particles is preserved during the
simulation.

It must be stressed that stochastic methods are usually competitive to deterministic
methods in complicated settings. Sophisticated finite element methods would be more
efficient if one deals only with size changes of a one-component system involving par-
ticles of only one type, and needs high accuracy. On the other hand, MC schemes
would probably beat deterministic methods when considering multi-component sys-
tems. Nevertheless, our analysis is restricted to the simplest situation of GDE with only
one type of particles. This is a necessary preliminary to constructing QMC schemes
for engineering computation.

The paper is organized as follows. In Section 2, basic tools of QMC methods are
recalled and the new algorithm is presented. In Section 3, the efficiency of the scheme
is assessed through numerical comparison with exact solutions of the coagulation-
condensation equation. In addition, QMC results are compared with MC results in the
same special cases where an analytical solution is available. Finally, we give some
conclusions and perspectives for future work.
2. The algorithm

Stochastic methods provide solutions of the coagulation equation in the limit of the number of particles going to infinity. If direct simulation of the coagulation process is performed, the number of simulation particles will decrease. Thus, procedures are used to enrich the system to make the results statistically reliable. Since the whole mass of the system is conserved, an alternative approach is to simulate the mass flow equation whose solution is the mass (or size) distribution.

We derive a mass-flow formulation of the GDE by multiplying equation (1.1) by $x$. Using the symmetry property of $K$, we obtain the following equation for the mass distribution $f(x, t)$:

$$
\frac{\partial f}{\partial t}(x, t) = \int_0^x \tilde{K}(x - y, y) f(x - y, t) f(y, t) dy - \int_0^{\infty} \tilde{K}(x, y) f(x, t) f(y, t) dy + \left( \frac{I_0(x, t)}{x} - R(x, t) \right) f(x, t), \quad (2.1)
$$

where $\tilde{K}$ is the modified coagulation kernel defined by

$$
\tilde{K}(x, y) := \frac{K(x, y)}{y}, \quad x, y > 0.
$$

We set $f_0(x) := x c_0(x)$. Note that the last term in equation (2.1) is not conservative.

The efficiency of a QMC scheme depends on the quality of the quasi-random points that are used: they must form a low-discrepancy point set. We recall from [18] some basic notations and concepts. If $s \geq 1$ is a fixed dimension, then $I_s := [0, 1)^s$ is the $s$-dimensional unit cube and $\lambda_s$ denotes the $s$-dimensional Lebesgue measure. For a point set $U = \{u_0, \ldots, u_{N-1}\} \subset I_s$, we define the local discrepancy by:

$$
D_N(J, U) := \frac{A(J, U)}{N} - \lambda_s(J),
$$

where $A(J, U)$ is the number of $k$ with $u_k \in J$. The discrepancy of $U$ is:

$$
D_N(U) := \sup_{J \in \mathcal{J}} |D_N(J, U)|,
$$

where $\mathcal{J}$ is the family of all subintervals of $I_s$. The star discrepancy of $U$ is:

$$
D^*_N(U) := \sup_{J \in \mathcal{J}^*} |D_N(J, U^*)|,
$$

where $\mathcal{J}^*$ is the family of all subintervals of $I_s$ with one vertex at the origin. The idea of $(t, m, s)$-nets is to consider point sets $U$ for which $D_N(J, U) = 0$ for a large family
of intervals $J$. Such point sets should have a small discrepancy. For an integer $b \geq 2$, an elementary interval in base $b$ is an interval of the form

$$\prod_{i=1}^{s} \left[ \frac{a_i}{b^{d_i}}, \frac{a_i + 1}{b^{d_i}} \right],$$

with integers $d_i \geq 0$ and $0 \leq a_i < b^{d_i}$ for $1 \leq i \leq s$. If $0 \leq t \leq m$ are integers, a $(t, m, s)$-net in base $b$ is a set $U$ of $b^m$ points in $I^s$ such that $D_N(J, U) = 0$ for every elementary interval $J$ in base $b$ such that $\lambda_s(J) = b^t - m$. If $b \geq 2$ and $t \geq 0$ are integers, a sequence $U = \{u_0, u_1, \ldots\}$ of points in $I^s$ is a $(t, s)$-sequence in base $b$ if for all integers $n \geq 0$ and $m > t$,

$$U^n := \{u_p : nb^m \leq p < (n+1)b^m\} \quad (2.2)$$

is a $(t, m, s)$-net in base $b$.

For the simulation of equation (2.1), we choose integers $b \geq 2$, $m \geq 1$ and we set $N = b^m$. For $x^* > 0$, let $\delta_{x^*}(x)$ denote the Dirac measure located at $x^*$. The scheme determines discrete times: $0 = t_0 < t_1 < \cdots < t_n < \cdots$ and uses an approximation of the solution at each time $t_n$ with a sum of $N$ weighted particles:

$$f_n^N(x) := \frac{1}{N} \sum_{0 \leq k < N} w_k^N \delta_{x^*_k}(x) \approx f_n^N(x) := f(x, t_n), \quad (2.3)$$

where the weights $w_k^N$ and sizes $x^*_k$ of the particles at time $t_n$ are positive numbers. We set

$$(W^n, X^n) := \{(w_k^N, x^*_k) : 0 \leq k < N\}.$$

### 2.1. Initialization

Without loss of generality, we suppose that the initial mass distribution function satisfies:

$$\int_0^{+\infty} f_0(x) dx = 1. \quad (2.4)$$

We start with an approximation $f_0^N(x)$ of the probability measure $f_0(x)dx$: we set $w_k^0 = 1$ for $0 \leq k < N$ and we sample $N$ points $x_0^0, x_1^0, \ldots, x_{N-1}^0$ from $f_0(x)dx$. This can be done by choosing

$$x^0_k = F_0^{-1}(v_k), \quad 0 \leq k < N, \quad (2.5)$$

where

$$F_0(x) := \int_0^x f_0(y) dy \quad \text{and} \quad v_k := \frac{2k + 1}{2N}, \quad 0 \leq k < N.$$
Assuming that we have computed an approximation \( f_N^n(x) \) at time \( t_n \), we compute an approximation \( f_N^{n+1}(x) \) at time \( t_{n+1} := t_n + \Delta t_n \). This is done by a splitting method: the original evolutionary problem is reduced to a pair of problems describing the coagulation on the one side and the condensation/evaporation and deposition on the other side. Following [3], we introduce the time scale of each physical process (with a kernel \( \neq 0 \)).

- For coagulation:
  \[
  \tau_k^n := \min_{0 \leq k, \ell < N} \frac{1}{K(x_k^n, x_\ell^n) u_\ell^n}.
  \]

- For condensation/evaporation:
  \[
  \tau_{c/e}^n := \min_{0 \leq k < N} \frac{x_k^n}{|I_0(x_k^n, t_n)|}.
  \]

- For deposition:
  \[
  \tau_d^n := \min_{0 \leq k < N} \frac{1}{R(x_k^n, t_n)}.
  \]

The smallest time scale is usually due to coagulation. To ensure an accurate integration of all processes, the time step \( \Delta t_n \) is chosen such that

\[
\Delta t_n \leq \varepsilon \min(\tau_k^n, \tau_{c/e}^n, \tau_d^n),
\]

for a sufficiently small quantity \( \varepsilon > 0 \) (for instance \( \varepsilon = 0.1 \)).

For the QMC approximation of the coagulation process, we need a low-discrepancy sequence \( U := \{u_0, u_1, \ldots\} \subset I^3 \). If the point set \( U^N \) is defined as in (2.2), we use it for the coagulation during the time interval \([t_n, t_{n+1}]\). If \( \pi \) denotes the projection from \( I^3 \) to \( I^2 \) defined by \( \pi(x_1, x_2, x_3) = (x_1, x_2) \), we assume

\[
\forall n \geq 0 \quad \pi(U^n) \text{ is a } (0, m, 2)\text{-net in base } b. \tag{2.7}
\]

### 2.2. Coagulation

We follow the algorithm devised in [15] for the approximation of Smoluchowski’s coagulation equation.

#### 2.2.1 Sorting of the particles

The first step is to relabel the particles so that

\[
x_0^n \leq x_1^n \leq \cdots \leq x_{N-1}^n.
\]

This type of sort was first introduced and motivated in [13]. It guarantees theoretical convergence. The idea is to match the sizes of the particles with the low-discrepancy point set \( \pi(U^n) \).
2.2.2 Integration of coagulation

We want to solve the pure mass-flow coagulation equation

\[
\frac{\partial f}{\partial t}(x, t) = \int_0^x \tilde{K}(x - y, y) f(x - y, t) f(y, t) dy - \int_0^{+\infty} \tilde{K}(x, y) f(x, t) f(y, t) dy,
\]

over the time interval \([t_n, t_{n+1}]\) with initial data \(f_n^N(x)\). Let \(\mathcal{M}^+\) denote the set of all nonnegative measurable functions on \((0, +\infty)\). Equation (2.9) can be given the form

\[
\frac{d}{dt} \int_0^{+\infty} f(x, t) \sigma(x) dx = \int_0^{+\infty} \int_0^{+\infty} \tilde{K}(x, y) f(x, t) f(y, t) (\sigma(x + y) - \sigma(x)) dy dx,
\]

for any \(\sigma \in \mathcal{M}^+\). We discretize (2.10) using an explicit Euler scheme: we define a measure \(g_n^{N+1}(x)\) by

\[
\int_0^{+\infty} g_n^{N+1}(x) \sigma(x) := \int_0^{+\infty} f_n^N(x) \sigma(x) + \Delta t_n \int_0^{+\infty} \int_0^{+\infty} \tilde{K}(x, y) f_n^N(x) \otimes f_n^N(y) (\sigma(x + y) - \sigma(x)).
\]

Hence

\[
\int_0^{+\infty} g_n^{N+1}(x) \sigma(x) = \frac{1}{N} \sum_{0 \leq k < N} \left( 1 - \frac{\Delta t_n}{N} \sum_{0 \leq \ell < N} \tilde{K}(x_k^n, x_\ell^n) w_\ell^n \right) w_k^n \sigma(x_k^n) + \frac{\Delta t_n}{N^2} \sum_{0 \leq k, \ell < N} \tilde{K}(x_k^n, x_\ell^n) w_k^n w_\ell^n \sigma(x_k^n + x_\ell^n).
\]

2.2.3 QMC approximation

For \(0 \leq k, \ell < N\), we denote by \(c_{k, \ell}\) the indicator function of the elementary interval in base \(b\):

\[
\left[ \frac{k \cdot N + 1}{N} \right] \times \left[ \frac{\ell \cdot N + 1}{N} \right].
\]

Let \(\chi_{k, \ell}^n\) be the indicator function of the interval

\[
[0, \Delta t_n \tilde{K}(x_k^n, x_\ell^n) w_\ell^n],
\]
which is well defined, by assumption (2.6). For \( \sigma \in \mathcal{M}^+ \), we set

\[
C^n_{\sigma}(u) := \sum_{0 \leq k, \ell < N} c_{k, \ell}(u_1, u_2) \left( \left(1 - \chi^n_{k, \ell}(u_3)\right) w^n_k \sigma(x^n_k) + \chi^n_{k, \ell}(u_3) w^n_k \sigma(x^n_k + x^n_\ell) \right),
\]

for \( u = (u_1, u_2, u_3) \in I^3 \). Then

\[
\int_0^{+\infty} g^{n+1}_N(x) \sigma(x) = \int_{I^3} C^n_{\sigma}(u) du. \tag{2.12}
\]

We define

\[
\tilde{f}^n_N(x) := \frac{1}{N} \sum_{0 \leq k < N} w^n_k \delta_{x^n_k}(x)
\]

by performing a QMC integration:

\[
\int_0^{+\infty} \tilde{f}^n_N(x) \sigma(x) = \frac{1}{N} \sum_{nN \leq p < (n+1)N} C^n_{\sigma}(u_p). \tag{2.13}
\]

This can be reworded as follows. For \( x > 0 \), let \( \lfloor x \rfloor \) denote the greatest integer \( \leq x \) and put \( k(u) := \lfloor Nu \rfloor \), for \( u \in I \). It follows from (2.7) that the mappings:

\[
p \in \{nN, nN + 1, \ldots, (n + 1)N - 1\} \rightarrow k(u, 1),
\]

\[
p \in \{nN, nN + 1, \ldots, (n + 1)N - 1\} \rightarrow k(u, 2)
\]

are one-to-one. In addition, the pairs \( \{(k(u, 1), k(u, 2)) : nN \leq p < (n + 1)N\} \) are “evenly distributed” over the grid \( \{0, 1, \ldots, N-1\} \times \{0, 1, \ldots, N-1\} \). Eq. (2.13) means:

\[
\tilde{x}^n_{k(u, 1)} = \begin{cases} 
  x^n_{k(u, 1)} + x^n_{k(u, 2)} & \text{if } u_{p, 3} < \Delta t_u \tilde{K}(x^n_{k(u, 1)}, x^n_{k(u, 2)}) w^n_{k(u, 2)}, \\
  x^n_{k(u, 1)} & \text{otherwise.}
\end{cases}
\tag{2.14}
\]

### 2.3. Condensation/evaporation and deposition

We want to solve the linear hyperbolic equation of the first order

\[
\frac{\partial f}{\partial t}(x, t) + \frac{\partial}{\partial x} \left( I_0 f(x, t) - \left( \frac{I_0(x, t)}{x} - R(x, t) \right) f(x, t) \right) = 0, \tag{2.15}
\]

over the time interval \( [t_n, t_{n+1}] \) with initial data \( \tilde{f}^n_N(x) \). We use a deterministic particle method [20]. We put

\[
a(x, t) := \frac{I_0(x, t)}{x} - R(x, t).
\]
For \( x > 0, \tau > 0 \), let \( \xi(t; x, \tau) \) denote the solution of the differential equation:

\[
\frac{d\xi}{dt}(t) = I_0(\xi(t), t), \quad t > \tau,
\]

\( \xi(\tau) = x. \) (2.16)

The measure solution of (2.15), with initial data \( \tilde{f}_N(x) \) is given by:

\[
\tilde{f}_N(x, t) = \frac{1}{N} \sum_{0 \leq k < N} w_k^n \exp \left( \int_{t_n}^t a(\xi(s; \tilde{x}_k^n, t_n), s) \, ds \right) \delta_{\xi(t; \tilde{x}_k^n, t_n)}(x). \] (2.17)

If the Cauchy problem (2.16) can be solved exactly and if the integral in (2.17) has a closed-form expression, we define:

\[
f_{n+1}^{n+1}(x) := \tilde{f}_N(x, t_{n+1}). \]

This yields

\[
x_{k}^{n+1} = \xi(t_{n+1}; \tilde{x}_k^n, t_n),
\] (2.18)

\[
w_{k}^{n+1} = w_k^n \exp \left( \int_{t_n}^{t_{n+1}} a(\xi(t; \tilde{x}_k^n, t_n), t) \, dt \right). \] (2.19)

We may equivalently define a weight functions \( w_k(t) \) as the solution of the differential equation:

\[
\frac{dw_k}{dt}(t) = a(\xi(t; \tilde{x}_k^n, t_n), t)w_k(t), \quad t > t_n,
\]

\( w_k(t_n) = w_k^n. \) (2.20)

and set \( w_{k}^{n+1} := w_k(t_{n+1}). \) Except in very special cases, the solutions of the Cauchy problems (2.16) and (2.20) have to be determined numerically by means of ODE solvers. When using an explicit Euler scheme, we obtain:

\[
x_{k}^{n+1} = \tilde{x}_k^n + \Delta t_n I_0(\tilde{x}_k^n, t_n),
\] (2.21)

\[
w_{k}^{n+1} = w_k^n + \Delta t_n a(\tilde{x}_k^n, t_n)w_k^n. \] (2.22)

By assumption (2.6), the weights \( w_{k}^{n+1} \) and sizes \( x_{k}^{n+1} \) are positive numbers.

3. Numerical examples

The aim of this section is to numerically validate the QMC method described above and to compare it with the MC scheme described in [3]. We restrict our experiments to cases where an exact solution is known, so that we can compare the errors induced
by both approaches. These errors depend on the number of the simulation particles as well as on the lengths of the time steps used.

We define a measure of error which tells how well the particle distribution $f_n^N(x)$ approximates the exact solution $f^n(x)$. If $(W, X) = \{(w_0, x_0), \ldots, (w_{N-1}, x_{N-1})\}$ is a weighted point set in $(0, +\infty)^2$ and if $f$ is a non-negative and measurable function on $(0, +\infty)$, we define the star $f$-discrepancy of $(W, X)$ by:

$$D^\star_N(W, X; f) := \sup_{x>0} \left| \frac{1}{N} \sum_{0 \leq k < N} w_k 1_{(0,x)}(x_k) - \int_0^x f(y)dy \right|,$$

where $1_{(0,x)}$ denotes the indicator function of the interval $(0, x)$. Analytical solutions of the GDE are available only for few kernels and initial distributions. For constant or linear coagulation and condensation kernels and assuming $R = 0$, explicit solutions are given in [19], with the initial distribution

$$c_0(x) = e^{-x}. \quad (3.1)$$

In these cases, we can compute the error $D^\star_N(W^n, X^n; f^n)$ of the algorithm and we can compare it with the error given by the MC scheme.

Moments of the concentration distribution are defined as follows:

$$M_m(t) := \int_0^{+\infty} x^m c(x, t) dx,$$

for positive integer values of $m$. At time $t_n$, the moment $M_m(t_n)$ is approximated according to (2.3) as

$$M^m_{m,N} = \frac{1}{N} \sum_{0 \leq k < N} w_k^n (x_k^n)^{m-1}. \quad (3.2)$$

We examine the accuracy of this approximation. In our experiments, the number base $b$ is taken to be 3 and the low discrepancy sequence $U$ is a $(0,3)$-sequence in base 3 constructed by Faure [8].

### 3.1. Constant coagulation and linear condensation

Here

$$K(x, y) := 1 \quad \text{and} \quad I_0(x, t) := x.$$

Then

$$c(x, t) = \frac{M_0(t)^2}{M_1(t)} \exp \left( -\frac{M_0(t)}{M_1(t)} x \right), \quad (3.3)$$

where the first moments are as follows:

$$M_0(t) = \frac{2}{t+2}, \quad M_1(t) = e^t,$$

$$M_2(t) = (t+2)e^{2t}, \quad M_3(t) = \left( \frac{3}{2}t^2 + 6t + 6 \right) e^{3t}. \quad (3.4)$$
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Figure 1. Constant coagulation and linear condensation. Averaged discrepancy for MC (left) vs. QMC (right) simulations for \( P = 100, 200, 400, 800, 1600 \) and 3 200 time steps.

We compute the solution up to time \( T = 1.0 \) with \( N \) particles (varying from \( 3^4 \) to \( 3^{13} \)) and \( P \) time steps (varying from \( 1 \times 100 \) to \( 2^5 \times 100 \)), with \( \Delta t_n := T/P \) for every \( n \).

In order to reduce scatter, we graph the averaged discrepancy, which is defined by:

\[
D^\ast_{N,P} := \frac{1}{100} \sum_{h=1}^{100} D^\ast_N(W^{hn}, X^{hn}, f^{hn}),
\]

where \( n = P/100 \). Figure 1 is a plot of the averaged discrepancy as a function of \( N \) on a log-log scale. We see that both schemes give an approximation of the mass distribution that converges towards the exact solution as \( N \) and \( P \) increase. In addition, QMC simulations achieve faster convergence of the error to zero than MC computations: for the same discretization parameters \( N \) and \( \Delta t \), the error of the QMC method is always smaller than the error of the MC scheme. The faster convergence of QMC is more tangible for small time steps. For large time steps, the improvement of the statistical error related to the number of simulation particles is hidden by the error induced by coarse time discretization.

Next we choose a time step small enough so that time discretization error is insignificant relative to the MC or QMC error. The results are displayed in Figure 2. The best (in the sense of least squares) straight line fit to the log-log plot of the data gives for \( P = 3200 \):

\[
D^\ast_{N,P}(MC) = O(N^{-0.51}) \quad \text{and} \quad D^\ast_{N,P}(QMC) = O(N^{-0.64}). \quad (3.5)
\]

The results displayed in Figure 2 show that, for \( N \geq 3^8 = 6561 \), the error of the QMC
method using $N$ simulation particles is smaller than the error of the MC method with $3N$ particles. If $N \geq 3^{11} = 177,147$, the QMC error is even smaller than the MC error using $9N$ particles. The situation is different if we compare the computation times, because the sorting algorithm of QMC induces an extra cost. In our experiments, the QMC method is approximately three times longer than the MC scheme using the same number of simulation particles (may be the codes are not optimized). If $P = 3200$, the improvement factor:

$$f_{N,P} := \frac{D_{N,P}^*(\text{QMC})}{D_{3N,P}^*(\text{MC})}$$

ranges from 0.73 (for $N = 3^8$) to 0.49 (for $N = 3^{12}$): it indicates the reduction of MC error when using a QMC calculation with the same computation cost.

The averaged absolute error on the $m$-th moment $M_m(t)$ is calculated as follows:

$$E_{N,P}^m := \frac{1}{100} \sum_{h=1}^{100} \left| M_{m,N}^{hN} - M_m(t_{hn}) \right|.$$  

Figure 3 shows the curves of the averaged error on the second moment as a function of $N$ on a log-log scale. Both methods converge to the exact moment, as $N \to \infty$ and $P \to \infty$. Additionally, it is clear that the QMC method enjoys better convergence properties than the MC scheme: with a few exceptions, the error of the QMC method is smaller than the error of the MC scheme with the same $N$ and $\Delta t$; but the faster convergence of QMC is more sensible for small time steps. When $P = 3200$ and
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Figure 3. Constant coagulation and linear condensation. Averaged absolute error on the second moment for MC (left) vs. QMC (right) simulations for \( P = 100, 200, 400, 800, 1600 \) and 3200 time steps.

\[ N \geq 3^9 = 19,683, \text{ the error of the QMC method using } N \text{ simulation particles is smaller than the error of the MC method with } 9N \text{ particles.} \]

The results for the averaged error on the third moment are displayed in Figure 4. The conclusions are similar to those drawn for the approximation of the second moment.

3.2. Linear coagulation and linear condensation

In this case

\[ K(x, y) := x + y \quad \text{and} \quad I_0(x, t) := x. \]

Then

\[ c(x, t) = \frac{M_0(t)}{x \sqrt{1 - M_0(t)}} \exp \left( -\frac{2 - M_0(t)}{M_1(t) x} \right) I_1 \left( 2 \sqrt{\frac{1 - M_0(t)}{M_1(t)}} x \right), \tag{3.6} \]

where \( I_1 \) is the modified Bessel function of the first kind of order one. Here the first moments are as follows:

\[ M_0(t) = \exp(1 - e^t), \quad M_1(t) = e^t, \quad M_2(t) = 2 \exp(2e^t + 2t - 2). \tag{3.7} \]

We compute the solution up to time \( T = 0.5 \) with \( N \) particles (varying from \( 3^4 \) to \( 3^{12} \)) and \( P \) time steps (varying from \( 1 \times 100 \) to \( 2^4 \times 100 \)), with \( \Delta t_n := T/P \) for every \( n \).

The average discrepancy is computed as in the first model problem. We see in Figure 5 that both methods converge and that the QMC method is superior to the MC scheme: for the same discretization parameters \( N \) and \( \Delta t \), the error of the QMC method is
always smaller than the error of the MC scheme. Once again, the faster convergence of QMC is more sensible for small time steps.

The gain in the rate of convergence is illustrated in Figure 6. As in the first example, if the time step is chosen small enough, the log-log scale allows the plot of an error of order $O(N^{-q})$ to appear as a straight line with slope $-q$: for $P = 1600$, one has

$$D^*_{N,P}(MC) = O(N^{-0.51}) \quad \text{and} \quad D^*_{N,P}(QMC) = O(N^{-0.65}).$$

The results depicted in Figure 6 show that, if $N \geq 3^7 = 2187$, the error of the QMC approach using $N$ simulation particles is smaller than the error of the MC approach with $3N$ particles. In this example, if $P = 1600$, the improvement factor $f_{N,P}$ ranges from 0, 87 (for $N = 3^7$) to 0, 35 (for $N = 3^{11}$).

The averaged relative error on the $m$-th moment $M_m(t)$ is calculated as follows:

$$E^m_{N,P} := \frac{1}{100} \sum_{h=1}^{100} \left| \frac{M^h_{m,N} - M_m(t_{hn})}{M_m(t_{hn})} \right|.$$
Figure 5. Linear coagulation and linear condensation. Averaged discrepancy for MC (left) vs. QMC (right) simulations for $P = 100, 400, 800$ and $1600$ time steps.

Figure 6. Linear coagulation and linear condensation. Linear fits to the averaged discrepancy as a function of $N$ for $P = 1600$ time steps: comparison of MC and QMC simulations.
4. Conclusion

We have presented an algorithm for solving the GDE for aerosols. We use a fractional step scheme in time and we reduce the original evolutionary problem to a sequence of problems describing the coagulation, the condensation/evaporation and the deposition respectively. The approach is to approximate the mass distribution of the aerosols with a large number of weighted particles. A stochastic particle method is used to simulate the aggregation process: the sizes of the particles may vary but the weights remain unchanged. Since the standard Monte Carlo method converges slowly, we have considered an improvement to this method by using quasi-random numbers in place of pseudo-random numbers. To make an optimal use of the greater uniformity of quasi-random sequences, we reorder the particles by size at each time step. We simulate the condensation/evaporation and deposition processes with a deterministic particle method. The sizes and weights of the particles are calculated through the integration over a time step of an ODE system. With this method, the number of simulation particles is preserved. We test our scheme by comparing the numerical results with two known exact solutions to the coagulation-condensation equation. In both cases, the results of the scheme have been found to reproduce the exact mass distribution and its first moments. Moreover, by making use of low-discrepancy sequences, a remarkable gain of efficiency has been achieved over a standard MC simulation. One difficulty (which is shared with corresponding MC schemes) is the choice of the time step, which must be sufficiently small to ensure the feasibility of the scheme and accurate integration of all physical processes. Further investigation will be required to solve
this problem. It must be stressed that the accuracy of QMC method has been stated on elementary test problems, with simple kernels. The validation of QMC approach must be pursued in more realistic settings.

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