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Random and deterministic fragmentation models

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Abstract

Random and deterministic fragmentation models are considered. Their relationship is studied by deriving different forms of the kinetic fragmentation equation from the corresponding stochastic models. Results related to the problem of non-conservation of mass (phase transition into dust) are discussed. Illustrative examples are given and some open problems are mentioned.

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1 Introduction

Fragmentation models are used in many scientific and industrial areas (e.g., polymer chemistry, nuclear physics, cell biology, mining industry). A system of particles characterized by some positive quantity (mass, volume, size) is considered. The time evolution of the system is determined by a random splitting mechanism.

The study of stochastic fragmentation models was initiated by Kolmogorov [6] who gave a theoretical derivation of a distribution function that was observed experimentally for systems of mineral grains. A fragmentation equation of the form

$$\frac{\partial}{\partial t}c(t,x) = \int_x^\infty c(t,y)\,\psi(y,x)\,dy - c(t,x)\,\frac{1}{x}\int_0^x y\,\psi(x,y)\,dy \tag{1.1}$$

was studied in [8]. Here c(t, x) represents the number density of particles of mass x at time t, and ψ is a parameter determined by the fragmentation mechanism. Though these fragmentation models are relatively simple (in particular, equation (1.1) is linear), they have some interesting properties related to a phase transition. Filippov [3] studied the transformation of mass into an infinite number of particles of zero mass (called dust) in those cases where the speed of the splitting of a particle increases sufficiently rapidly with the decrease of its mass. Later this phenomenon was called "shattering" transition [7]. For more details and references related to fragmentation, we refer to the recent monographs [2] concerning stochastic models, and [1] concerning the functional analytical approach.

In this paper random and deterministic fragmentation models are considered. In Section 2 their relationship is studied by deriving different forms of the kinetic fragmentation equation from the corresponding stochastic models. In Section 3 results related to the problem of non-conservation of mass (phase transition into dust) are discussed. Illustrative examples are given and some open problems are mentioned.

2 Models

2.1 Stochastic particle models

2.1.1 Direct simulation process

The direct simulation model is based on a system of particles

$$(X_1(t), \dots, X_{N(t)}(t)), \quad t \ge 0, \quad N(0) = 1,$$
 (2.1)

where N(t) denotes the number of particles. The time evolution of the system imitates the supposed physical behaviour. Given a state (x_1, \ldots, x_N) , particles behave independently. Each particle x_i waits an exponentially distributed time with parameter $a(x_i)$ and then splits into fragments z_1, \ldots, z_k distributed according to $F(x_i, dz)$. The **fragmentation rate** a(x) is assumed to be compactly bounded on the state space of a single particle $\mathcal{X} = (0, \infty)$. The **fragmentation kernel** F(x, dz) is a probability measure on the space of clouds of fragments

$$\mathcal{Z} = \bigcup_{k=2}^{\infty} \mathcal{X}^k \,. \tag{2.2}$$

In particular, the average number of fragments is

$$n_{\text{frag}}(x) = \sum_{k=2}^{\infty} k F(x, \mathcal{X}^k).$$
(2.3)

A common assumption is the mass conservation property

$$F(x, \{z \in \mathcal{Z} : z_1 + \ldots + z_k = x\}) = 1 \qquad \forall x \in \mathcal{X}.$$

$$(2.4)$$

For studying connections between the system (2.1) and deterministic equations, it is convenient to introduce a measure-valued stochastic process. Consider the state space

$$\mathcal{Y} = \left\{ \sum_{i=1}^{N} \delta_{x_i} : N \ge 1, \quad x_i \in \mathcal{X}, \quad i = 1, \dots, N \right\},$$
(2.5)

where δ_x denotes the Dirac measure in $x \in \mathcal{X}$, with the topology of weak convergence. Define the kernel

$$q(y,\Gamma) = \sum_{i=1}^{N} \int_{\mathcal{Z}} \mathbb{1}_{\Gamma} (J_F(y,i,z)) a(x_i) F(x_i,dz), \qquad y \in \mathcal{Y},$$
(2.6)

where 1_{Γ} denotes the indicator function of a Borel set $\Gamma \in \mathcal{B}(\mathcal{Y})$, with the jump transformation

$$J_F(y, i, z) = y - \delta_{x_i} + \delta_{z_1} + \ldots + \delta_{z_k}.$$
 (2.7)

The jump process corresponding to the kernel (2.6) is called **direct simulation process**. It is represented in terms of the system (2.1) as

$$\xi(t, dx) = \sum_{i=1}^{N(t)} \delta_{X_i(t)}(dx)$$
(2.8)

and measures the number of particles with mass in a given subset of \mathcal{X} .

Let $F^{(k)}$ denote the restrictions of the fragmentation kernel F to the sets \mathcal{X}^k . Define the symmetrized restrictions

$$F_{\rm sym}^{(k)}(x, dz_1, \dots, dz_k) = \frac{1}{k!} \sum_{\pi} F^{(k)}(x, dz_{\pi(1)}, \dots, dz_{\pi(k)}), \qquad k = 2, 3, \dots, \qquad (2.9)$$

where the sum is taken over all permutations of $\{1, \ldots, k\}$, their 1-marginals

$$F_{\text{sym}}^{(k|1)}(x,dy) = F_{\text{sym}}^{(k)}(x,dy,\mathcal{X},\dots,\mathcal{X})$$
(2.10)

and the kernel

$$B(x, dy) = \sum_{k=2}^{\infty} k F_{\text{sym}}^{(k|1)}(x, dy) .$$
(2.11)

Let \mathbb{E}_x denote expectation with respect to F(x, dz). Then one obtains, for appropriate test functions φ ,

$$\mathbb{E}_{x}\left[\varphi(z_{1}) + \ldots + \varphi(z_{k})\right] = \int_{\mathcal{Z}} \left[\varphi(z_{1}) + \ldots + \varphi(z_{k})\right] F(x, dz) = \sum_{k=2}^{\infty} \int_{\mathcal{X}^{k}} \left[\varphi(z_{1}) + \ldots + \varphi(z_{k})\right] F_{\text{sym}}^{(k)}(x, dz_{1}, \ldots, dz_{k})$$
$$= \sum_{k=2}^{\infty} k \int_{\mathcal{X}} \varphi(y) F_{\text{sym}}^{(k|1)}(x, dy) = \int_{\mathcal{X}} \varphi(y) B(x, dy) \quad \forall x \in \mathcal{X}.$$
(2.12)

The quantity $B(x, \Gamma)$ represents the **average number of fragments** with mass in $\Gamma \in \mathcal{B}(\mathcal{X})$, resulting from the fragmentation of a particle of mass x. In particular, the average total number of fragments (2.3) is expressed as

$$n_{\text{frag}}(x) = B(x, \mathcal{X}). \qquad (2.13)$$

Property (2.4), which means mass conservation with probability one, implies **mass** conservation on average (cf. (2.12))

$$\int_0^x y B(x, dy) = x \qquad \forall x > 0 \tag{2.14}$$

and

$$B(x, [\varepsilon, x)) < \infty \qquad \forall \, \varepsilon \in (0, x) \,. \tag{2.15}$$

2.1.2 Mass flow process

The one-dimensional jump process $\tilde{X}(t)$ corresponding to the kernel

$$\tilde{q}(x,dy) = a(x)\,\tilde{B}(x,dy)\,,\qquad x\in\mathcal{X}\,,$$
(2.16)

where

$$\tilde{B}(x,dy) = \frac{y}{x} B(x,dy), \qquad (2.17)$$

is called **mass flow process**. Note that the mass conservation property (2.14) implies

$$\int_{0}^{x} \tilde{B}(x, dy) = 1.$$
 (2.18)

Given a state $x \in \mathcal{X}$, the process \tilde{X} waits an exponentially distributed time with parameter a(x), and then jumps to a "fragment" y distributed according to the kernel (2.17). According to (2.12), one obtains

$$B(x,dy) = \int_{\mathcal{Z}} \left[\delta_{z_1}(dy) + \ldots + \delta_{z_k}(dy) \right] F(x,dz)$$
(2.19)

so that the kernel (2.17) can be represented via F in the form

$$\tilde{B}(x,dy) = \int_{\mathcal{Z}} \left[\frac{z_1}{x} \,\delta_{z_1}(dy) + \ldots + \frac{z_k}{x} \,\delta_{z_k}(dy) \right] F(x,dz) \,. \tag{2.20}$$

Thus, given $\tilde{X} = x$, the next state can be obtained as follows: first fragments z_1, \ldots, z_k are generated according to the fragmentation kernel F(x, dz); then one of the fragments is chosen with probabilities proportional to their individual masses. The quantity $\tilde{B}(x, \Gamma)$ represents the **average total mass of fragments** (normalized by x) with mass in $\Gamma \in \mathcal{B}(\mathcal{X})$, resulting from the fragmentation of a particle of mass x.

2.2 Fragmentation equations

The measure-valued function (cf. (2.8))

$$\mu(t, dx) = \mathbb{E}\xi(t, dx) \tag{2.21}$$

represents the **average number of particles** that have mass in a given subset of \mathcal{X} at time $t \geq 0$. It satisfies the **weak** form of the **fragmentation equation**

$$\frac{d}{dt} \int_{\mathcal{X}} \varphi(x) \,\mu(t, dx) = \int_{\mathcal{X}} \int_{\mathcal{Z}} \left[\varphi(z_1) + \ldots + \varphi(z_k) - \varphi(x) \right] a(x) \,F(x, dz) \,\mu(t, dx) \,,$$
(2.22)

for appropriate test functions φ . This follows from Dynkin's formula

$$\frac{d}{dt} \mathbb{E} \Phi(\xi(t)) = \mathbb{E} \mathcal{A} \Phi(\xi(t)), \qquad (2.23)$$

where (cf. (2.6))

$$\mathcal{A}\Phi(y) = \int_{\mathcal{Y}} \left[\Phi(\tilde{y}) - \Phi(y) \right] q(y, d\tilde{y})$$
(2.24)

and (cf. (2.5))

$$\Phi(y) = \int_{\mathcal{X}} \varphi(x) y(dx) = \sum_{i=1}^{N} \varphi(x_i), \qquad y \in \mathcal{Y}.$$
(2.25)

According to (2.12), equation (2.22) transforms into

$$\frac{d}{dt} \int_{\mathcal{X}} \varphi(x) \,\mu(t, dx) = \int_{\mathcal{X}} \left[\int_{\mathcal{X}} \varphi(y) \,B(x, dy) - \varphi(x) \right] a(x) \,\mu(t, dx) \,. \tag{2.26}$$

When assuming

$$\mu(t, dx) = c(t, x) dx \tag{2.27}$$

and

$$B(x, dy) = b(x, y) dy$$
, (2.28)

and removing the test functions, then one obtains from (2.26) the strong form of the fragmentation equation

$$\frac{\partial}{\partial t}c(t,x) = \int_x^\infty c(t,y)\,a(y)\,b(y,x)\,dy - a(x)\,c(t,x)\,. \tag{2.29}$$

The fragmentation kernel F enters equations (2.26), (2.29) via the kernel B (cf. (2.11)).

Remark 2.1 When a and b satisfying (cf. (2.14))

~

$$\int_0^x y \, b(x, y) \, dy = x \qquad \forall \, x > 0 \tag{2.30}$$

are given, then

$$\psi(x,y) = a(x) b(x,y) \tag{2.31}$$

transforms equation (2.29) into equation (1.1). On the other hand, given some function $\psi \geq 0$, one defines

$$a(x) = \frac{1}{x} \int_0^x y \,\psi(x, y) \,dy$$
(2.32)

and

$$b(x,y) = \frac{x}{\int_0^x u \,\psi(x,u) \,du} \,\psi(x,y)$$
(2.33)

to obtain equation (2.29) from equation (1.1). Note that the function b defined in (2.33) satisfies (2.30).

In analogy with (2.21), (2.8), we define the measure-valued function

$$\tilde{\mu}(t, dx) = \mathbb{E}\,\tilde{\xi}(t, dx) \quad \text{where} \quad \tilde{\xi}(t, dx) = \delta_{\tilde{X}(t)}(dx) \,.$$
(2.34)

This function represents the distribution of the process $\tilde{X}(t)$. It satisfies the **weak** form of the **mass flow equation**

$$\frac{d}{dt} \int_{\mathcal{X}} \varphi(x) \,\tilde{\mu}(t, dx) = \int_{\mathcal{X}} \left[\int_{\mathcal{X}} \varphi(y) \,\tilde{B}(x, dy) - \varphi(x) \right] a(x) \,\tilde{\mu}(t, dx) \,, \qquad (2.35)$$

for appropriate test functions φ . This follows from Dynkin's formula (2.23), with \mathcal{Y}, Φ, q replaced by \mathcal{X}, φ and \tilde{q} (cf. (2.16)), respectively. When assuming

$$\tilde{\mu}(t, dx) = \tilde{c}(t, x) \, dx \tag{2.36}$$

and (2.28), and removing the test functions, then one obtains from (2.35) the **strong** form of the **mass flow equation**

$$\frac{\partial}{\partial t}\tilde{c}(t,x) = \int_{x}^{\infty} \tilde{c}(t,y)\,a(y)\,\tilde{b}(y,x)\,dy - a(x)\,\tilde{c}(t,x)\,,\qquad(2.37)$$

where

$$\tilde{b}(x,y) = b(x,y)\frac{y}{x}.$$
(2.38)

Remark 2.2 Equations (2.26) and (2.35), as well as (2.29) and (2.37), are equivalent in the sense that their solutions can be transformed into each other via the relationships

$$\tilde{\mu}(t, dx) = \alpha \, x \, \mu(t, dx) \,, \qquad \tilde{c}(t, x) = \alpha \, x \, c(t, x) \,, \qquad \forall \, t \ge 0 \,, \tag{2.39}$$

for some $\alpha > 0$. If the solutions are unique, then a correspondence between the direct simulation process and the mass flow process can be established. Note that $\mu(0, dx)$ represents the distribution of $X_1(0)$ (cf. (2.1)), while $\tilde{\mu}(0, dx)$ is the distribution of $\tilde{X}_1(0)$. When assuming

$$\int_{\mathcal{X}} x \,\mu(0, dx) < \infty \tag{2.40}$$

and defining

$$\tilde{\mu}(0, dx) = \frac{x \,\mu(0, dx)}{\int_{\mathcal{X}} y \,\mu(0, dy)} \tag{2.41}$$

then (2.39) implies

$$\tilde{\mu}(t, dx) = \frac{1}{\int_{\mathcal{X}} y \,\mu(0, dy)} \, x \,\mu(t, dx) \qquad \forall t \ge 0 \,. \tag{2.42}$$

If

$$\mu(0, dx) = \delta_{x_0}(dx) \quad \text{for some} \quad x_0 \in \mathcal{X} \,,$$

then the initial states of both processes are the same. According to (2.21), the measure-valued function $x \mu(t, dx)$ represents the **average total mass of particles** that have mass in a given subset of \mathcal{X} at time $t \geq 0$.

2.3 Binary fragmentation

Mass conservation (2.4) implies that in a binary fragmentation model one of the two fragments is obtained as a deterministic function of the other. Thus, the general form of a binary fragmentation kernel is

$$F(x, dz) = F^{(2)}(x, dz_1, dz_2) = F^{(1)}(x, dz_1) \,\delta_{x-z_1}(dz_2) \,, \tag{2.43}$$

where $F^{(1)}$ is a probability kernel on \mathcal{X} . Introduce $F^{(1)}_{\text{sym}}$ by

$$\int_{\mathcal{X}} \varphi(y) F_{\text{sym}}^{(1)}(x, dy) = \frac{1}{2} \int_{\mathcal{X}} [\varphi(y) + \varphi(x - y)] F^{(1)}(x, dy) , \qquad (2.44)$$

for appropriate test functions φ , and note that

$$\int_{\mathcal{X}} \varphi(y) F_{\text{sym}}^{(1)}(x, dy) = \int_{\mathcal{X}} \varphi(x - y) F_{\text{sym}}^{(1)}(x, dy) \,. \tag{2.45}$$

One obtains

$$\begin{split} \int_{\mathcal{X}} \int_{\mathcal{X}} \psi(z_1, z_2) \, F_{\text{sym}}^{(2)}(x, dz_1, dz_2) &= \\ & \frac{1}{2} \int_{\mathcal{X}} \int_{\mathcal{X}} \psi(z_1, z_2) \, F^{(2)}(x, dz_1, dz_2) + \frac{1}{2} \int_{\mathcal{X}} \int_{\mathcal{X}} \psi(z_1, z_2) \, F^{(2)}(x, dz_2, dz_1) \\ &= \frac{1}{2} \int_{\mathcal{X}} \psi(z_1, x - z_1) \, F^{(1)}(x, dz_1) + \frac{1}{2} \int_{\mathcal{X}} \psi(x - z_2, z_2) \, F^{(1)}(x, dz_2) \\ &= \int_{\mathcal{X}} \psi(y, x - y) \, F_{\text{sym}}^{(1)}(x, dy) = \int_{\mathcal{X}} \int_{\mathcal{X}} \psi(z_1, z_2) \, F_{\text{sym}}^{(1)}(x, dz_1) \, \delta_{x - z_1}(dz_2) \,, \end{split}$$

for appropriate test functions $\psi\,,$ so that

$$F_{\rm sym}^{(2)}(x, dz_1, dz_2) = F_{\rm sym}^{(1)}(x, dz_1) \,\delta_{x-z_1}(dz_2) \tag{2.46}$$

and (cf. (2.11))

$$B(x, dy) = 2 F_{\text{sym}}^{(1)}(x, dy). \qquad (2.47)$$

Thus, in the binary (mass conserving) case, the function B does not only determine the average number of fragments, but also their distribution (provided the fragments are considered indistinguishable).

On the other hand, if some measure B satisfies the symmetry condition (2.45), then

$$\int_{\mathcal{X}} y B(x, dy) = \int_{\mathcal{X}} (x - y) B(x, dy) = x B(x, \mathcal{X}) - \int_{\mathcal{X}} y B(x, dy)$$

and

$$B(x,\mathcal{X}) = \frac{2}{x} \int_{\mathcal{X}} y B(x,dy) \,. \tag{2.48}$$

According to (2.48), condition (2.14) concerning mass conservation on average and the "binary condition"

$$B(x, \mathcal{X}) = 2 \qquad \forall x \in \mathcal{X} \tag{2.49}$$

are equivalent. Thus, any measure B satisfying the symmetry condition (2.45) and either the mass conservation condition (2.14) or the "binary condition" (2.49) is generated by a binary stochastic fragmentation model via (2.47) and (2.46).

When assuming

$$F^{(1)}(x, dy) = 1_{(0,x)}(y) f^{(1)}(x, y) dy, \qquad (2.50)$$

one obtains from (2.28) and (2.47) that

$$b(x,y) = 2 f_{\text{sym}}^{(1)}(x,y) = f^{(1)}(x,y) + f^{(1)}(x,x-y).$$
(2.51)

The function b is symmetric, i.e.

$$b(x,y) = b(x,x-y).$$
 (2.52)

In the case of equation (1.1), the symmetry assumption

$$\psi(x,y) = \psi(x,x-y) \tag{2.53}$$

implies symmetry of b defined in (2.33) and mass conservation (cf. (2.30)). One obtains, in analogy with (2.48),

$$\frac{1}{x} \int_0^x y \,\psi(x,y) \,dy = \frac{1}{2} \int_0^x \psi(x,y) \,dy \tag{2.54}$$

so that equation (1.1) takes the form

$$\frac{\partial}{\partial t}c(t,x) = \int_x^\infty c(t,y)\,\psi(y,x)\,dy - c(t,x)\,\frac{1}{2}\int_0^x\psi(x,y)\,dy\,.$$
(2.55)

The representations (2.32), (2.33) take the form

$$a(x) = \frac{1}{2} \int_0^x \psi(x, y) \, dy \tag{2.56}$$

and

$$b(x,y) = \frac{2}{\int_0^x \psi(x,s) \, ds} \, \psi(x,y) \tag{2.57}$$

so that (2.47) implies

$$f^{(1)}(x,y) = \frac{1}{\int_0^x \psi(x,u) \, du} \, \psi(x,y) \,. \tag{2.58}$$

Thus, in equation (2.55), the normalized function ψ represents the distribution of the fragment, while the normalization function is the doubled intensity of fragmentation.

Example 2.3 (deterministic binary fragmentation) Consider a function κ such that

$$\kappa(x) \in (0, x) \qquad \forall \, x > 0 \,,$$

and (cf. (2.43))

$$F^{(1)}(x, dy) = \delta_{\kappa(x)}(dy)$$

One obtains (cf. (2.47))

$$B(x, dy) = \delta_{\kappa(x)}(dy) + \delta_{x-\kappa(x)}(dy)$$

and (cf. (2.17))

$$\tilde{B}(x,dy) = \frac{\kappa(x)}{x} \delta_{\kappa(x)}(dy) + \left(1 - \frac{\kappa(x)}{x}\right) \delta_{x-\kappa(x)}(dy).$$
(2.59)

In the direct simulation model, a particle of mass x splits into the pieces $\kappa(x)$ and $x - \kappa(x)$. In the mass flow model, the particle x jumps into the state

$$y = \begin{cases} \kappa(x) & \text{with probability } \frac{\kappa(x)}{x} \\ x - \kappa(x) & \text{with probability } 1 - \frac{\kappa(x)}{x}. \end{cases}$$
(2.60)

When choosing

$$\kappa(x) = \frac{x}{2}$$

then the jumps in the mass flow model are deterministic, from x to $\frac{x}{2}$.

2.4 Homogeneous fragmentation

A fragmentation kernel is called homogeneous if it satisfies

$$F(x, dz) = \int_{\mathcal{S}[0,1]} \delta_{s_1 x, \dots, s_k x}(dz) F(1, ds) \qquad \forall x > 0, \qquad (2.61)$$

where F(1, ds) is a probability measure on the set of partitions

$$\mathcal{S}[0,1] = \{s_1, \dots, s_k > 0 : s_1 + \dots + s_k = 1, \quad k = 2, 3, \dots\}$$
(2.62)

of the unit interval. One obtains (cf. (2.9)-(2.11))

$$F_{\text{sym}}^{(k)}(x, dz_1, \dots, dz_k) = \frac{1}{k!} \sum_{\pi} \int_{\mathcal{S}_k[0,1]} \delta_{s_1 x, \dots, s_k x}(dz_{\pi(1)}, \dots, dz_{\pi(k)}) F^{(k)}(1, ds_1, \dots, ds_k)$$

=
$$\int_{\mathcal{S}_k[0,1]} \delta_{s_1 x, \dots, s_k x}(dz_1, \dots, dz_k) F_{\text{sym}}^{(k)}(1, ds_1, \dots, ds_k),$$

$$F_{\rm sym}^{(k|1)}(x,dy) = \int_0^1 \delta_{u\,x}(dy) \, F_{\rm sym}^{(k|1)}(1,du)$$

and

$$B(x, dy) = \int_0^1 \delta_{ux}(dy) B(1, du). \qquad (2.63)$$

The mass conservation condition (2.14) reduces to

$$\int_0^1 u B(1, du) = 1.$$
 (2.64)

The average number of fragments (2.13) takes the form

$$n_{\rm frag}(x) = \int_0^1 B(1, du)$$
 (2.65)

and does not depend on x. It follows from (2.63) that (cf. (2.17))

$$\tilde{B}(x,dy) = \frac{y}{x} \int_0^1 \delta_{ux}(dy) B(1,du) = \int_0^1 \delta_{ux}(dy) u B(1,du).$$
(2.66)

Assuming

$$B(1, du) = b(1, u) \, du$$

one obtains

$$\int_0^x \varphi(y) B(x, dy) = \int_0^1 \varphi(u x) b(1, u) du = \int_0^x \varphi(v) b\left(1, \frac{v}{x}\right) \frac{1}{x} dv$$

so that (cf. (2.28))

$$b(x,y) = \frac{1}{x} b\left(1,\frac{y}{x}\right)$$
(2.67)

and (cf. (2.38))

$$\tilde{b}(x,y) = \frac{1}{x} b\left(1,\frac{y}{x}\right) \frac{y}{x}.$$
(2.68)

Example 2.4 ([4]) Consider

$$F(1,ds) = \frac{1}{2} \,\delta_{\frac{1}{2},\frac{1}{2}}(ds_1,ds_2) + \frac{1}{2} \,\delta_{\frac{1}{2},\frac{1}{4},\frac{1}{4}}(ds_1,ds_2,ds_3)$$

and

$$\hat{F}(1,ds) = \frac{3}{4} \,\delta_{\frac{1}{2},\frac{1}{2}}(ds_1,ds_2) + \frac{1}{4} \,\delta_{\frac{1}{4},\frac{1}{4},\frac{1}{4},\frac{1}{4}}(ds_1,ds_2,ds_3,ds_4) \,.$$

Note that

$$F_{\text{sym}}(1, ds) = \frac{1}{2} \delta_{\frac{1}{2}, \frac{1}{2}}(ds_1, ds_2) + \frac{1}{6} \left[\delta_{\frac{1}{2}, \frac{1}{4}, \frac{1}{4}}(ds_1, ds_2, ds_3) + \delta_{\frac{1}{4}, \frac{1}{2}, \frac{1}{4}}(ds_1, ds_2, ds_3) + \delta_{\frac{1}{4}, \frac{1}{4}, \frac{1}{2}}(ds_1, ds_2, ds_3) \right]$$

and $\hat{F}_{sym}(1, ds) = \hat{F}(1, ds)$. It is obvious that $F_{sym}(1, ds) \neq \hat{F}_{sym}(1, ds)$. One obtains (cf. (2.11))

$$\begin{split} B(1,du) &= 2 F_{\text{sym}}^{(2|1)}(1,du) + 3 F_{\text{sym}}^{(3|1)}(1,du) = \delta_{\frac{1}{2}}(du) + \frac{1}{2} \left[\delta_{\frac{1}{2}}(du) + 2 \delta_{\frac{1}{4}}(du) \right] \\ &= \frac{3}{2} \delta_{\frac{1}{2}}(du) + \delta_{\frac{1}{4}}(du) \end{split}$$

and

$$\hat{B}(1, du) = 2 \,\hat{F}_{\rm sym}^{(2|1)}(1, du) + 4 \,\hat{F}_{\rm sym}^{(4|1)}(1, du) = B(1, du) \,.$$

Thus, in this example the fragmentation equations for both kernels are identical, but the distributions of the random clouds of fragments differ. In particular, the probability of having k = 2, 3, 4 fragments cannot be determined from B.

Example 2.5 (power law) Consider

$$b(x,y) = C(x) y^{\beta}.$$

Mass conservation condition (2.14) implies

$$C(x) = \frac{x}{\int_0^x y^{\beta+1} \, dy} = \frac{\beta+2}{x^{\beta+1}} \,, \qquad \beta > -2 \,,$$

so that

$$b(x,y) = \frac{\beta + 2}{x^{\beta+1}} y^{\beta}$$
(2.69)

and (2.67) holds. The average number of fragments (2.65) is

$$\int_0^1 b(1,u) \, du = \begin{cases} \frac{\beta+2}{\beta+1} \in [2,\infty) & \text{if } -1 < \beta \le 0\\ \\ \infty & \text{if } -2 < \beta \le -1 \end{cases}$$

Example 2.6 (homogeneous binary fragmentation) Consider a probability measure P on (0, 1) and (cf. (2.43))

$$F^{(1)}(x, dy) = \int_0^1 \delta_{ux}(dy) P(du).$$

One obtains (cf. (2.44), (2.47))

$$B(1, du) = 2 P_{\text{sym}}(du).$$

The choice

$$P(du) = \delta_c(du)$$
 for some $c \in (0, 1)$

corresponds to the deterministic fragmentation with $\kappa(x) = c x$ (cf. Example 2.3). If P has a density p, then one obtains

$$b(1, u) = p(u) + p(1 - u)$$

Note that both p(u) = 1 and p(u) = 2u give the same b(1, u) = 2 that corresponds to the power law case with $\beta = 0$.

Example 2.7 (log-normal distribution) The mass flow process in discrete time can be represented in the form (cf. (2.66))

$$\tilde{X}(t) = \tilde{X}_0 \prod_{i=1}^t u_i, \qquad t = 1, 2, \dots,$$

where u_1, u_2, \ldots are independent identically distributed random variables with distribution u B(1, du) on (0, 1). Note that

$$\log \tilde{X}(t) = \log \tilde{X}_0 + \sum_{i=1}^t \log u_i.$$
 (2.70)

If

$$\alpha := \int_0^1 (\log u) \, u \, B(1, du) > -\infty \,, \tag{2.71}$$

then (2.70) and the law of large numbers imply

$$\mathbb{P}\left(\lim_{t\to\infty}\frac{\log \tilde{X}(t)}{t} = \alpha\right) = 1.$$

If (2.71) holds and

$$\sigma^{2} := \int_{0}^{1} (\log u)^{2} u B(1, du) - \alpha^{2} < \infty,$$

then (2.70) and the central limit theorem imply

$$\lim_{t \to \infty} \mathbb{P}\left(\frac{\log \tilde{X}(t) - \alpha t}{\sqrt{\sigma^2 t}} < x\right) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^x \exp\left(-\frac{y^2}{2}\right) dy.$$

Note that (cf. (2.34), (2.42), (2.21))

$$\begin{split} \mathbb{P}\left(\log \tilde{X}(t) < x\right) &= \mathbb{P}\left(\tilde{X}(t) < e^x\right) = \int_0^{e^x} \tilde{\mu}(t, dy) = \frac{1}{\int_{\mathcal{X}} y \,\mu(0, dy)} \int_0^{e^x} y \,\mu(t, dy) \\ &= \frac{\mathbb{E} \int_0^{e^x} y \,\xi(t, dy)}{\mathbb{E} \int_0^{\infty} y \,\xi(0, dy)} = \frac{\mathbb{E} \sum_{i: X_i(t) < e^x} X_i(t)}{\mathbb{E} X_1(0)} \\ &= \frac{1}{\mathbb{E} X_1(0)} \,\mathbb{E} \sum_{i: \log X_i(t) < x} X_i(t) \,, \end{split}$$

which is the average total mass of those particles having the logarithm of their mass less than x, normalized by the average total mass in the system. Kolmogorov [6] obtained a similar distribution property by studying the appropriately normalized quantity

$$\mathbb{E}\sum_{i:\log X_i(t) < x} 1,$$

which is the average total number of those particles having the logarithm of their mass less than x.

3 Results concerning mass conservation

Here we study the problem whether the identities

$$\int_0^\infty x \, c(t,x) \, dx = \int_0^\infty x \, c(0,x) \, dx \, ,$$

in terms of the solution of equation (2.29), or

$$\int_0^\infty x \,\xi(t, dx) = \int_0^\infty x \,\xi(0, dx) = X_1(0) \,,$$

in terms of the stochastic process (2.8), are fulfilled for all $t \ge 0$. It turns out that these mass conservation properties do not hold for certain fragmentation models.

3.1 Non-conservative solutions

The classical paper covering the topic of mass conservation for fragmentation models is [3]. Filippov starts from the direct simulation model determined by the functions $\tilde{B}(x, (0, y))$ (cf. (2.20)), which represent the (normalized by x) average total mass of fragments of mass less than y originating from the breakage of a particle of mass x. Studying quantities that represent the average sum of masses of particles of mass less than x (cf. Remark 2.2), the mass flow equation (2.35) is derived. Indeed, with test functions $\varphi(y) = 1_{(0,x)}(y)$, equation (2.35) takes the form

$$\begin{split} \frac{\partial}{\partial t} \,\tilde{\mu}(t,(0,x)) &= \int_0^\infty \left[\tilde{B}(y,(0,x)) - \mathbf{1}_{(0,x)}(y) \right] a(y) \,\tilde{\mu}(t,dy) \\ &= \int_x^\infty a(y) \,\tilde{B}(y,(0,x)) \,\tilde{\mu}(t,dy) \,, \end{split}$$

which is identical to [3, eq. (2)]. Based on this equation, the mass flow process is introduced. Finally, in Section 9b, the following necessary and sufficient condition for mass conservation in the homogeneous case is given.

Theorem 3.1 Let the fragmentation rate a be bounded on compacts and converge monotonically to $+\infty$ as $x \to 0$. Assume

$$\tilde{B}(x,(0,y)) = f\left(\frac{y}{x}\right) \tag{3.1}$$

and

$$\int_{0}^{1} \frac{f(\lambda)}{\lambda} d\lambda < \infty \,. \tag{3.2}$$

Then a necessary and sufficient condition for mass conservation is

$$\int_0^{\delta} \frac{1}{x \, a(x)} \, dx = \infty \qquad \text{for some} \quad \delta > 0 \,. \tag{3.3}$$

A very general homogeneous fragmentation model is studied in [4], where also precise conditions for mass conservation are proved. When restricting the model to the situation considered in this paper, the corresponding result reduces to the following.

Theorem 3.2 Let the fragmentation rate a be continuous and decreasing near zero. Consider the function (cf. (2.62))

$$\Phi(q) = \int_{\mathcal{S}[0,1]} \left(1 - \sum_{i=1}^{k} s_i^{q+1} \right) F(1, ds), \qquad q \ge 0,$$
(3.4)

and assume

$$\Phi'(0+) < \infty \,. \tag{3.5}$$

Then (3.3) is a necessary and sufficient condition for mass conservation.

Note that assumption (3.1) implies

$$f(\lambda) = \tilde{B}(1, (0, \lambda)) = \int_0^\lambda u B(1, du), \qquad 0 < \lambda \le 1,$$
(3.6)

so that

$$\int_{0}^{1} \frac{f(\lambda)}{\lambda} d\lambda = \int_{0}^{1} \frac{1}{\lambda} \int_{0}^{\lambda} u B(1, du) d\lambda = \int_{0}^{1} \int_{0}^{1} \frac{1}{\lambda} 1_{(0,\lambda)}(u) u d\lambda B(1, du)$$
$$= \int_{0}^{1} \int_{u}^{1} \frac{1}{\lambda} u d\lambda B(1, du) = \int_{0}^{1} |\log u| u B(1, du).$$
(3.7)

Function (3.4) takes the form (cf. (2.9)-(2.11))

$$\Phi(q) = 1 - \sum_{k=2}^{\infty} \int \left(\sum_{i=1}^{k} s_i^{q+1}\right) F^{(k)}(1, ds_1, \dots, ds_k)$$

= $1 - \sum_{k=2}^{\infty} \int \left(\sum_{i=1}^{k} s_i^{q+1}\right) F^{(k)}_{\text{sym}}(1, ds_1, \dots, ds_k)$ (3.8)
= $1 - \sum_{k=2}^{\infty} k \int_0^1 u^{q+1} F^{(k|1)}_{\text{sym}}(1, du) = 1 - \int_0^1 u^{q+1} B(1, du)$

so that

$$\Phi'(q) = \int_0^1 |\log u| \, u^{q+1} \, B(1, du) \,. \tag{3.9}$$

Function (3.9) is non-negative, decreasing and finite, for all q > 0, since the function $|\log u| u^q$ is bounded on (0, 1). According to (3.7) and (3.9), both assumptions (3.2) and (3.5) are equivalent and take the form (cf. (2.70))

$$\int_{0}^{1} |\log u| \, u \, B(1, du) < \infty \,. \tag{3.10}$$

According to (2.64), condition (3.10) can be written as

$$\mathbb{E} \left| \log \xi \right| < \infty, \qquad (3.11)$$

where ξ is a random variable with distribution u B(1, du) on (0, 1). Sufficient conditions are

$$\mathbb{E}\,\xi^{-\varepsilon} = \int_0^1 u^{1-\varepsilon}\,B(1,du) < \infty\,, \qquad \text{for some} \quad \varepsilon > 0\,,$$

and, in particular, the finiteness of the average number of fragments (2.65),

$$\int_0^1 B(1, du) < \infty.$$

In the power law case (2.69) one obtains

$$B(1, du) = (\beta + 2) u^{\beta} du$$

so that (3.10) is fulfilled for all $\beta > -2$. Note that, for any $c \in (0, 1)$,

$$\int_0^c \frac{1}{x |\log x|^{\gamma}} \, dx < \infty \qquad \forall \, \gamma > 1$$

and

$$\int_0^c \frac{1}{x |\log x|^{\gamma}} \, dx = \infty \qquad \forall \, \gamma \le 1 \, .$$

This allows one to construct examples such that (3.11) does not hold.

3.2 Explosion properties

Consider a locally compact separable metric space \mathcal{Y} and a compactly bounded kernel $q(y, d\tilde{y})$ on \mathcal{Y} . Let Y_0, Y_1, \ldots be a Markov chain in \mathcal{Y} with the transition kernel

$$\frac{1}{\lambda(y)} q(y, d\tilde{y}), \qquad (3.12)$$

where

$$\lambda(y) = q(y, \mathcal{Y}). \tag{3.13}$$

Let T_0, T_1, \ldots be a sequence of independent random variables exponentially distributed with parameter 1 and independent of (Y_k) . Define jump times

$$\tau_0 = 0$$
 $\tau_l = \sum_{k=0}^{l-1} \frac{T_k}{\lambda(Y_k)}$ $l = 1, 2, \dots$

and explosion time

$$\tau_{\infty} = \lim_{l \to \infty} \tau_l \,.$$

The **minimal jump process** (cf., e.g., [9, p.69]) is a process on the one-point compactification $\mathcal{Y} \cup \{\Delta\}$ defined as

$$Y^{\Delta}(t) = \begin{cases} Y_l : & \tau_l \le t < \tau_{l+1} \\ \Delta : & t \ge \tau_{\infty} \end{cases}$$

The minimal jump process is called **regular** if

$$\mathbb{P}\left(\tau_{\infty}=\infty\right)=1$$

and explosive if

 $\mathbb{P}\left(\tau_{\infty}<\infty\right)>0\,.$

Up to the explosion time its time evolution is the same as for a standard jump process. Given a state y, the process waits an exponentially distributed time with parameter $\lambda(y)$ and jumps to \tilde{y} according to the distribution (3.12).

A necessary and sufficient condition for regularity is

$$\mathbb{P}\left(\sum_{k=0}^{\infty} \frac{1}{\lambda(Y_k)} = \infty\right) = 1.$$
(3.14)

Thus, boundedness of λ is sufficient for regularity. In order to get explosion, λ should be unbounded and (Y_k) should converge to Δ with an appropriate speed.

The following results were proved in [10].

Theorem 3.3 Assume the fragmentation rate satisfies

$$a(x) \geq \frac{C}{x^{\alpha}} \quad \forall x > 0 \quad for some \quad \alpha > 0 \quad and \quad C > 0.$$
 (3.15)

Then the direct simulation process explodes almost surely, for any initial distribution.

Theorem 3.4 Assume (3.15) and

$$\int_0^x \left(\frac{y}{x}\right)^{\alpha} \tilde{B}(x, dy) \leq \gamma < 1 \qquad \forall x > 0.$$
(3.16)

Then the mass flow process explodes almost surely, for any initial distribution.

In the homogeneous case, condition (3.16) takes the form (cf. (2.66))

$$\int_0^1 u^{\alpha+1} B(1, du) < 1$$

and is fulfilled for all $\alpha > 0$.

The following example illustrates that the assertion of Theorem 3.4 might be wrong, if assumption (3.16) does not hold.

Example 3.5 ([10]) Consider deterministic binary fragmentation (cf. Example 2.3) with

$$\kappa(x) = \begin{cases} \frac{x}{2} + \frac{1}{4} & \text{if } x > \frac{1}{2} \\ \\ \frac{x}{2} & \text{otherwise.} \end{cases}$$

Condition (3.16) takes the form (cf. (2.59))

$$\left(\frac{\kappa(x)}{x}\right)^{\alpha+1} + \left(1 - \frac{\kappa(x)}{x}\right)^{\alpha+1} \le \gamma < 1 \qquad \forall x > 0$$

and is not fulfilled for $x \searrow \frac{1}{2}$. If $x_0 > \frac{1}{2}$, then the sequence

$$x_k = \frac{1}{2} + \frac{2x_0 - 1}{2^{k+1}}$$
 $k = 0, 1, \dots$

satisfies $\lim_{k\to\infty} x_k = \frac{1}{2}$. Thus, there is no explosion on this trajectory, for any compactly bounded fragmentation rate. On the other hand, there is a transition from x_k to

$$\kappa(x_k) = \frac{1}{4} + \frac{2x_0 - 1}{2^{k+2}} + \frac{1}{4} = x_{k+1}$$

with probability $\frac{\kappa(x_k)}{x_k}$ (cf. (2.60)). The trajectory of "slowest decay" (x_k) has a non-zero probability

$$\lim_{k \to \infty} \frac{\kappa(x_0)}{x_0} \frac{\kappa(x_1)}{x_1} \dots \frac{\kappa(x_k)}{x_k} = \frac{1}{x_0} \lim_{k \to \infty} \kappa(x_k) = \frac{1}{2 x_0}.$$

Thus, for $x_0 > \frac{1}{2}$, the mass flow process does not explode almost surely.

3.3 Comments

Theorems 3.3, 3.4 provide less precise conditions for non-conservation of mass, compared to the necessary and sufficient condition (3.3), but they cover the case of non-homogeneous fragmentation. In this situation certain phenomena may occur that are not possible in the homogeneous case. Example 3.5 shows that even power like growth at zero of the fragmentation intensity is not sufficient for almost sure explosion of the mass flow process. Due to the special structure of the function κ , the mass flow process stays above $\frac{1}{2}$ with a positive probability, while the direct simulation process always produces enough particles below $\frac{1}{2}$ leading to explosion. In addition, Example 3.5 provides a fragmentation model, where the property

$$\lim_{t \to \infty} \int_0^\infty x \, c(t, x) \, dx = 0$$

related to "total loss of mass" does not seem to be fulfilled. This might be of independent interest.

The relationship between regularity of the stochastic model and mass-conservation for the corresponding deterministic equation is (more or less) straightforward for the mass flow process. But it is less obvious for the direct simulation process, where explosion can either mean that some particles reach 0 or that the number of particles reaches ∞ . More specifically, one obtains from (2.6) that (cf. (3.13))

$$\lambda(y) = \sum_{i=1}^{N} a(x_i), \quad y \in \mathcal{Y}.$$

If a is bounded by C_a , then

$$\sum_{k=0}^{\infty} \frac{1}{\lambda(Y_k)} \geq \sum_{k=0}^{\infty} \frac{1}{C_a \left(1 + \zeta_1 + \dots + \zeta_k\right)},$$

where ζ_i is the number of fragments created at the *i*-th jump. If the number of fragments is bounded, then condition (3.14) is fulfilled and regularity follows. A similar argument seems to work for bounded *a*, when the expected number of fragments is finite, but it is not obvious what happens for an infinite expected number of fragments.

The fragmentation equation can have non-conservative solutions even when the fragmentation rate is bounded at zero. Straightforward computations show that the function

$$c(t,x) = \frac{e^t}{(1+x)^3} \qquad t \ge 0, \quad x > 0,$$
 (3.17)

satisfies equation (2.29) with the parameters a(x) = x and $b(x, y) = \frac{2}{x}$ that correspond to the power law case (2.69) with $\beta = 0$. Note that multiplying equation (2.29) by x and integrating over $(0, \infty)$ implies mass conservation

$$\frac{d}{dt}\int_0^\infty x\,c(t,x)\,dx=0$$

provided that the term

$$\int_0^\infty x \int_x^\infty c(t,y) \, a(y) \, b(y,x) \, dy \, dx = \int_0^\infty \int_0^y x \, c(t,y) \, a(y) \, b(y,x) \, dx \, dy \\ = \int_0^\infty y \, a(y) \, c(t,y) \, dy$$

is finite. However, this is not the case for the function (3.17). It turns out that there exists also a mass-conserving solution in the above example (cf., e.g., [1, Section 8.1.2]). Note that the solutions studied in Theorems 3.1, 3.2 are unique. This is proved using an initial state with compact support as opposed to (3.17).

One may ask which kernels B and b occurring in the kinetic equations (2.26) and (2.29) are admissible in the sense that there exists a corresponding fragmentation kernel F. A complete answer was given in the particular case of binary fragmentation. But it seems that this problem has not been studied in full generality even for the power law fragmentation model. Note that the property

$$F\left(x, \left\{z \in \mathcal{Z} : \sum_{i=1}^{k} z_i \, \mathbf{1}_{(0,y)}(z_i) \ge \sum_{i=1}^{k} (x-z_i) \, \mathbf{1}_{(x-y,x)}(z_i) \right\}\right) = 1 \quad (3.18)$$

holds for all $y < \frac{x}{2}$. Indeed, due to mass conservation (2.4), there is at most one fragment bigger than x - y. If there is no such fragment, then the right-hand side of the inequality in (3.18) is zero. If there is one fragment $z_1 \ge x - y$, then (due to mass conservation) the sum of the other fragments is $x - z_1 \le y$ so that both sides equal $x - z_1$. Property (3.18) implies condition

$$\int_0^y u B(x, du) \ge \int_{x-y}^x (x-u) B(x, du) \qquad \forall y < \frac{x}{2}$$

which is used in the literature to characterize admissible functions B. The problem of admissibility does not exist for the mass flow model, since the kernel from the kinetic equation directly defines the stochastic process. This model is very attractive both for theoretical studies and for numerical purposes. However, the mass flow model is restricted to the scalar case, while the direct simulation model covers the case of multi-dimensional states.

Concerning real world examples for the transformation into dust, Filippov notes that "in actual physical processes this does not occur, since for very small masses new properties are exhibited, which are not taken into account in our scheme". However, when introducing a truncation (positive smallest mass of particles), then the model can provide a "good approximation to real processes". It is interesting to study the shattering phenomenon in a discrete mass model [5]. Starting with 1 particle of mass n one studies the time when the total mass of sufficiently small particles reaches O(n). This is in analogy with the approach to gelation in coagulating systems, where one starts from n particles of mass 1 and studies the time when the largest component reaches O(n). Both the truncation and the discrete approach would also be appropriate for numerical investigations of the phase transition.

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