

A NOTE ON MODELLING WITH MEASURES: TWO-FEATURES BALANCE EQUATIONS

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ABSTRACT. In this note we explain by an example what we understand by a *balance situation* and by a *balance equation in terms of measures*.

The latter ones are an attempt to *start* modelling of (not only) diffusion-reaction or mass-conservation scenarios in terms of measures rather than by derivatives and other rates.

By means of three examples this concept is extended to two-features (= two-traits-) balance situations, which, e.g., combine features like aging and physical motion in populations or physical motion and formation of polymers by means of a single model equation.

1. Introduction. In this note we introduce

- a general balance formulation based on measures and
- the concept of *two-feature* models illustrated by three examples.

The basic concept of measures is very intuitive and can (basically) be directly derived from our daily life experience. For example, it is (in most situations) clear, how we can measure, e.g., the mass or volume of an object.

The derivations of balance equations and of the basic equations of continuum mechanics very often rely on *starting* with using time-derivatives and other rates, which are much less intuitive than measures, and where it is quite unclear how one could actually measure those quantities in reality.

From a modeling point of view, it is important to rest the derivation of equations on a basis which is both as intuitive as possible and easily accessible in reality. This led us to study, as a very first attempt, the modeling of balance situations (for a basic introduction see section 1.2.) on the foundation of measures.

From a more mathematical point of view (apart from the modeling, which is the most important part for us in this paper), the derivation of equation (1) allows us to catch a first (tiny) glimpse at what can be gained by modeling with measures: If we make certain assumptions on two of the three terms in (5), we can gain more knowledge of the regularity of the third term than possible by “usual” (by just *assuming* the corresponding regularity) modeling techniques.

We focus our study at the modeling with two-feature measures (see section 1.2.) to be able to describe two different kinds of “evolution” of objects at the same time. For example (cf. section 2) we study the spatial evolution - the motion - of colloids as well as their evolution in the sense of changing structure by flocculation.

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There are many interesting open questions concerning this modeling approach, a most important and extensive one being under which *natural* conditions the mathematical assumptions allowing the modeling may actually be considered valid.

The rest of this introduction is structured as follows: In section 1.1 we introduce some notation, and in section 1.2. we explain the concepts by means of an example.

1.1. Some notation and conventions. Let $\Omega \subset \mathbb{R}^N$ be a bounded domain with Lipschitz boundary, $S := (0, T]$ - a time interval, $a > 0$, $A := [0, a]$, $M \in \mathbb{N}$, $G \subset \mathbb{R}^M$ - Lebesgue measurable, $\mathfrak{B}^M(G)$ - Borel- σ -algebra on G , λ^M - the corresponding Lebesgue measure, $\mathfrak{p}(K)$ - power set of K . We set

- $\mathfrak{A}_S := \mathfrak{B}^1(S)$, $\mathfrak{A}_\Omega := \mathfrak{B}^N(\Omega)$, $\mathfrak{A}_A := \mathfrak{B}^1(A)$, $\mathfrak{A}_K := \mathfrak{p}(K)$, $\mathfrak{A}_{\alpha\beta} := \mathfrak{A}_\alpha \otimes \mathfrak{A}_\beta$, $\alpha, \beta \in \{S, \Omega, K, A\}$, $\mathfrak{A}_{S\Omega K} := \mathfrak{A}_S \otimes \mathfrak{A}_\Omega \otimes \mathfrak{A}_K$,

- $\lambda_S := \lambda^1$, $\lambda_\Omega := \lambda^N$, $\lambda_A := \lambda^1$ and $\lambda_K := \lambda_c$ (counting measure, i.e. $\lambda_c(K') := \#$ of elements in K') are measures on their respective σ -algebras, $\lambda_{\alpha\beta} := \lambda_\alpha \otimes \lambda_\beta$ are the product measures on $\mathfrak{A}_{\alpha\beta}$, $\alpha, \beta \in \{S, \Omega, K, A\}$. H^{N-1} stands for the $(N-1)$ -dimensional surface measure.

- Normals and surface measures: Let $\Omega' \in \mathfrak{B}^N(\Omega)$ have a Lipschitz boundary $\partial\Omega'$. $n_{\Omega'}(x)$ denotes the unit outward normal at $x \in \partial\Omega'$. For any $A' = [p, q] \subseteq A$ we set $n_{A'}(p) = -1$, $n_{A'}(q) = 1$, for $p, q \in K \cap \mathbb{N}$, $K' = [p, q] \cap \mathbb{N}$, we set $n_{K'}(p) = -1$. $n_{K'}(q) = 1$. $\sigma = \sigma_{\Omega'}$ stands for the surface measure on $\partial\Omega'$. The “1D surface measures” are $\sigma_{A'}(y) := \sigma_{K'}(y) := 1$ for $y = p, q$.

Convention: We will use the word “measure” as something which measures something (notation $\widehat{\mu}$, e.g.) and as a “measure” in the measure-theoretic sense (then we drop “ $\widehat{}$ ”).

For a presentation of measure- and integration theory, we refer to the book [3].

1.2. Measure formulation of a balance situation. We illustrate this concept via an example - an (alternative) way to derive the diffusion equation: Consider a fluid filled body $\Omega \subset \mathbb{R}^3$ in which a substance X is dissolved. For simplicity we assume the fluid at rest and that there are no temperature changes. The substance X is allowed to move by diffusion. Reactions might contribute to a change of the amount of X in Ω over time $t \in S$. S stands for a basic and fixed time interval. “Amount” can be measured in a variety of ways, so let us assume the concentration of X in $x \in \Omega$ at time $t \in S$, $c(t, x)$, is measured in *mol/l*.

The standard diffusion-reaction equation is of the form

$$\frac{\partial c(t, x)}{\partial t} = f(t, x) + \operatorname{div}_x(-j(t, x)), \quad t \in \operatorname{int}S, \quad x \in \Omega. \quad (1)$$

A widely used example for the flux-density j is

$$j = -D\nabla_x c \quad (\text{Fick's law}). \quad (2)$$

f might stem from a mass-action law ansatz (involving c) or something else. For the following we need only the Lebesgue integrability of f , $\operatorname{div}_x j$ and $c(t, \cdot)$. We introduce the

- *amount measure* (for X) at time t : $\mu(t, \Omega') := \int_{\Omega'} c_X(t, x) dx$,
- *Flux-measure* (for X): $\mu_F(S' \times \Omega') = \int_{S'} \int_{\Omega'} -j(\tau, x) dx d\tau$,
- *Inner-production measure* (for X): $\mu_P(S' \times \Omega') = \int_{S'} \int_{\Omega'} f(\tau, x) dx d\tau$.

$\mu(t, \Omega')$ measures the amount of X in Ω' at time t , $\mu_F(S' \times \Omega')$ describes the net gain or loss of X in Ω' over the time span S' due to fluxes (here: diffusion from the outside of Ω' into Ω' through $\partial\Omega'$ or vice versa), $\mu_P(S' \times \Omega')$ describes the net gain

or loss of X over S' due to reasons located IN Ω' (that's why the name! Here it is a reaction).

$\mu(t, \cdot)$, $\mu_\xi(S' \times \cdot)$ and $\mu_\xi(\cdot \times \Omega')$, $\xi = P, F$, are measures on their respective σ -algebra for all fixed $\Omega' \in \mathfrak{B}^3(\Omega)$, $S' \in \mathfrak{B}^1(S)$ and $t \in S$. By a well-known extension procedure from Lebesgue integration theory μ_P and μ_F can be extended to the product σ -algebra $\mathfrak{A}_{S\Omega}$. Denote by $\lambda_{t,x}$ the time-space measure on $\mathfrak{A}_{S\Omega}$. Radon-Nikodym's theorem implies for all $t \in S$

$$f = \frac{d\mu_P}{d\lambda_{t,x}}, \quad \operatorname{div}_x j = \frac{d\mu_F}{d\lambda_{t,x}}, \quad c(t, \cdot) = \frac{d\mu(t, \cdot)}{\lambda^3}. \tag{3}$$

Integration of (1) over arbitrary $\Omega' \in \mathfrak{B}^3(\Omega)$, $S' \in \mathfrak{B}^1(S)$ yields

$$\int_{S'} \mu(\tau, \Omega') d\tau = \mu_P(S' \times \Omega') + \mu_F(S' \times \Omega').$$

For the particular time spans $S' := (t, t + h] \subset S$ we obtain, what we call a

Measure formulation of a balance situation

Change of X in Ω' during $S' =$ Sum of inner production and production by flux

$$\mu(t + h, \Omega') - \mu(t, \Omega') = \mu_P(S' \times \Omega') + \mu_F(S' \times \Omega'). \tag{4}$$

Note that the left-hand side does not only stand “for” the change - it *is* the change. Moreover all participants of this equation can - in principle and on appropriate subsets Ω' and S' - be measured as opposed to the expressions in (1) which are rates and, thus, not directly measurable.

(Practical) situations leading to equations like (4) we refer to as *balance situations*. They include energy balance, heat balance, mass conservation (with the corresponding μ_P being zero), even continuum mechanical formulations of Newton's law and much more ([2]).

We note that (4) can be made the point of origin for balance situations with appropriate interpretations of μ_P and μ_F . That is what we will do below.

In order to arrive at a pde like the one in (1) the quantities c and f can be axiomatically introduced via (3), supposed one postulates the corresponding absolute-continuity assumptions on the measures. The latter one is a non-physical assumption expressed in mathematical terms. The passage from (4) to (1) requires an additional assumption and goes as follows: Division of both sides of the equation in (4) by h and employment of (3) yield for all $x \in \Omega$

$$\frac{c(t + h, x) - c(t, x)}{h} = \frac{1}{h} \int_t^{t+h} f(\tau, x) - \operatorname{div}_x j(\tau, x) d\tau. \tag{5}$$

If

$$x \mapsto f(\tau, x) - \operatorname{div}_x j(\tau, x) \text{ is continuous for all } \tau, \tag{6}$$

then the localisation theorem implies the existence of

$$\lim_{h \rightarrow 0} \frac{1}{h} \int_t^{t+h} f(\tau, x) - \operatorname{div}_x j(\tau, x) d\tau = f(t, x) - \operatorname{div}_x j(t, x) \text{ for all } x \in \Omega$$

and (1) holds. Note: Modelling assumptions like (6) are difficult to motivate by arguments in terms of assumptions on the underlying measures.

In order to postulate “meaningful” assumptions on μ_F , we note, that our motivating example yields

$$\mu_F(S' \times \Omega') = \int_{S'} \int_{\partial\Omega'} -j(\tau, x) \cdot n(x) d\sigma d\tau \quad (7)$$

for all $S' \in \mathfrak{B}^1(S)$ and all $\Omega' \in \mathfrak{M}_{adm}$ (set of “admitted” Ω' ’s). \mathfrak{M}_{adm} is the subset of all $\Omega' \in \mathfrak{B}^3(\Omega)$ for which the divergence theorem holds. (7) is the motivating origin for most approaches dealing with the *derivation* of the existence of flux-vector fields $j(t, \cdot) : \Omega \rightarrow \mathbb{R}^3$ for appropriately given measures μ_F . A study of the connections between j and μ_F is not in the focus of this note - rather we will assume the existence of such a j for given flux measures.

The idea to start modeling of balance situations by means of measures is - probably - not new. Nevertheless we have not been able to produce any reference which presents a *comprehensive* model of this subject. Related material geared at parts of such a balance formulation can be found in [9], [10] (“mass measure”, e.g.). A particular part - the “fluxes” (or “Cauchy interactions”, “Cauchy flows”) - is subject of intensive studies (cf. [5], [7], [3], [6] among several (but not many others.))

The situations mentioned above cover only one “feature”¹ - the amount of X , of energy, of heat, of mass or of momentum. The main intention of this paper is an introduction of the concept of *two-feature models* based on two-feature counter pieces of (4). In biology “two features” are the same as “two traits”. Our three examples deal with the two features “motion” and “evolution” (section 2), “motion” and “group formation” (section 3) and age-group formation (= “motion on an age scale”) and spatial motion (section 4). The first two examples include some discrete modeling, the third one is entirely non-discrete. Another typical example for two-feature pde’s from physics is supplied by the transport equations dealing with impulse and velocity of many-particle systems (cf. [1]) and could easily be put in the framework of a formulation in terms of measures.

2. Motion and evolution of colloidal particles (flocculation). Flocculation is the “reversible formation of aggregates in which the particles are not in physical contact” (cf. [11]). This process plays an important role in the physico-chemistry of (not only) groundwater modeling (cf. e.g. [4] or [5]).

The setting is as follows: Let $S := (0, T)$ be a time interval. Colloids of different sizes $k \in K := \{1, 2, \dots, M\}$ - where the “size-threshold“ M is fixed - move (by diffusion, advection, dispersion) in a fluid occupying a container Ω - a Lipschitz-domain $\subseteq \mathbb{R}^N$, $N = 2, 3$ - break up or get larger by adding (parts of) other colloids.

In the following, we will use the term “ k -colloid” to denote a colloid of size $k \in K$. Furthermore, for any subset $K' \subseteq K$ we say that a colloid belongs to the class K' if it has size $k \in K'$.

The domain Ω might represent the fluid-filled pore space of a porous medium or it might be a free fluid-filled space.

We consider the evolution of the different colloid sizes over time and begin with introducing, for $t \in \overline{S}$, $\Omega' \in \mathfrak{A}_\Omega$, $K' \in \mathfrak{A}_K$, the

$$\begin{aligned} & \text{amount measure } \widehat{\mu}(t, \Omega' \times K') \\ & := \text{amount of colloids in } \Omega' \text{ belonging to the size class } K' \text{ at time } t. \end{aligned}$$

¹Time t is considered as a parameter and doesn’t count as an additional feature.

The “amount” can be measured in numbers, mol or gramm, e.g., where “numbers” and “mols” might be non-integers. By the nature of the definition of this quantity, the maps

$$\begin{aligned} \mathfrak{A}_\Omega \ni \Omega' &\mapsto \widehat{\mu}(t, \Omega' \times K') \in \mathbb{R}, \quad K' \in \mathfrak{A}_K \text{ fixed,} \\ \mathfrak{A}_K \ni K' &\mapsto \widehat{\mu}(t, \Omega' \times K') \in \mathbb{R}, \quad \Omega' \in \mathfrak{A}_\Omega \text{ fixed} \end{aligned}$$

are additive. By *assuming* them to be σ -additive, we obtain measures $\widehat{\mu}(t, \cdot \times K')$ and $\widehat{\mu}(t, \Omega' \times \cdot)$, resp. Mimicking the usual construction of λ^2 by means of λ^1 we extend $\widehat{\mu}(t, \cdot \times \cdot)$ to a measure $\mu(t, \cdot)$ on $\mathfrak{A}_{\Omega K}$ - the *two-features amount measure*.

Assuming the regularity condition²

$$\mu(t, \cdot) \ll \lambda_{\Omega K} \text{ for all } t \in S \tag{8}$$

Radon-Nikodym’s theorem provides, for all $t \in S$, a concentration

$$c(t, \cdot) \in L^1_+(\Omega \times K, \mathfrak{A}_{\Omega K}, \lambda_{\Omega K}) \tag{9}$$

such that

$$\begin{aligned} \mu(t, Q') &= \int_{Q'} c(t, q) d\lambda_{\Omega K}(q) \stackrel{\text{in the special case } Q'=\Omega' \times K'}{=} \int_{\Omega'} \int_{K'} c(t, x, k) d\lambda_\Omega(x) d\lambda_K(k). \end{aligned} \tag{10}$$

Furthermore we introduce the production quantities / (signed)(pre-)measures

$$\widehat{\mu}_{P\pm}(S' \times \Omega' \times K') := \text{amount of colloids which are}$$

added to /substracted from $\Omega' \times K'$ during the intervall S'

(with additivity properties similar to those above) and

$$\widehat{\mu}_P := \widehat{\mu}_{P+} - \widehat{\mu}_{P-}.$$

Using a similar procedure as above, we obtain (signed) measures

$$\mu_{P+}, \mu_{P-}, \mu_P$$

on the σ -algebra $\mathfrak{A}_{S\Omega K}$.

“Addition” to $\Omega' \times K'$, modeled by μ_{P+} can happen by addition *inside* of $\Omega' \times K'$ as well as by fluxes *into* $\Omega' \times K'$. A similar remark applies to subtraction and μ_{P-} .

Thus we have the net-production (signed)(pre-)measures (again assuming additivity)

$$\begin{aligned} \widehat{\mu}^{int}(S' \times \Omega' \times K') &:= \widehat{\mu}_+^{int}(S' \times \Omega' \times K') - \widehat{\mu}_-^{int}(S' \times \Omega' \times K'), \\ \widehat{\mu}^{flux}(S' \times \Omega' \times K') &:= \widehat{\mu}_+^{flux}(S' \times \Omega' \times K') - \widehat{\mu}_-^{flux}(S' \times \Omega' \times K') \end{aligned}$$

which, by the same procedure as above, yield the signed measures μ^{int} and μ^{flux} on $\mathfrak{A}_{S\Omega K}$. Note, that in the given context,

$$\mu_P := \mu^{int} + \mu^{flux}.$$

The regularity assumption

$$\mu^{int} \ll \lambda_{S\Omega K}$$

²The measure on the right hand side is sometimes called a “comparison measure”.

excludes the production of colloids on sets of $\lambda_{S\Omega K}$ -measure zero. Moreover it assures the existence of the Radon-Nikodym density of the internal production

$$f^{int} := \frac{d\mu^{int}}{d\lambda_{S\Omega K}}.$$

In order to get a reasonable idea for a representation of the flux measure we consider the special case $Q' = \Omega' \times K'$ with, say, $K' = \{a, a + 1, \dots, b\} \in \mathfrak{A}_K$.

The boundary “surface“

$$\mathfrak{F} := (\Omega' \times \{a\}) \cup (\Omega' \times \{b + 1\}) \cup (\partial\Omega \times K')$$

is the location of any interaction with the outside of Q' ³.

We distinguish two locations on \mathfrak{F} to enter or leave Q' - one via $\mathfrak{F}_1 = (\Omega' \times \{a\}) \cup (\Omega' \times \{b + 1\})$, the other one through $\mathfrak{F}_2 := \partial\Omega \times K'$.

Flux through \mathfrak{F}_2 is physical flux due to the motion of colloids of class K' into or out of Ω' through $\partial\Omega$.

Flux through \mathfrak{F}_1 is flux through the “class boundary”, independently of motion or collisions of colloids. This means that (parts of) colloids leave the classes $\{a\}$ or $\{b\}$ into the adjacent classes $\{a - 1\}$ or $\{b + 1\}$ respectively or (parts of) colloids from classes $\{a - 1\}$ or $\{b + 1\}$ enter the classes $\{a\}$ or $\{b\}$ respectively.

The only possible reason for this flux is the break-off of *one* particle of a certain colloid, since this is the only scenario in which there is an exchange of parts of colloids between *adjacent* classes without physical motion.

Note that we do not include the formation of k -colloids due to collision of $(k - 1)$ - and 1-colloids into the flux, as such a collision requires physical motion

The unit-outward normal field $\mathbf{n} = \mathbf{n}(x, k)$ on \mathfrak{F} can be split into two orthogonal components (visualising the set $\partial\Omega \times K'$ as a cylinder with base Ω), $\mathbf{n} = \mathbf{n}_\Omega + \mathbf{n}_K$, $\mathbf{n}_\Omega = (n_\Omega, 0)$, $\mathbf{n}_K = (0, n_K)$ respectively, where $n_K(x, a) = -1$, $n_K(x, b) = +1$ and $n_\Omega = n_\Omega(x, k)$ is the unit-outward normal on $\partial\Omega$.

Borrowing from the theory of Cauchy interactions⁴, we obtain⁵ for all $t \in \bar{S}$ the existence of two vector fields

$$\begin{aligned} j_\Omega(t, \cdot) &: \Omega \times K \rightarrow \mathbb{R}^N, \\ j_K(t, \cdot) &: \Omega \times K \rightarrow \mathbb{R}, \end{aligned}$$

where we agree on the convention that the flux entering class k from class $k - 1$ is given by $j_K(t, x, k)$ and that the flux leaving class k to class $k + 1$ is given by $j_K(t, x, k + 1)$. From this definition it immediately follows that $j_K(t, x, 1) = j_K(t, x, M + 1) = 0$, since the maximal colloid size is given by M .

We also obtain signed measures μ_Ω^{flux} and μ_K^{flux} such that

$$\mu^{flux} = \mu_\Omega^{flux} + \mu_K^{flux}$$

³The definition of the boundary surface corresponds to the idea that class k lies *between* the numbers k and $k + 1$.

⁴We abstain from presenting any such theory and refer to [10], [6] and [8], e.g. The settings in all these approaches differ slightly from each other. The crucial assumptions center around assumptions re. estimates for F_Ω^{flux} . Translated into the given situation they read as: There is a constant $c_0 > 0$ such that $|F_\Omega(S' \times \partial\Omega' \times K')| \leq c_0 |S'| H^{N-1}(\partial\Omega')$ for all admitted Ω' , all $K' \subseteq K$ and all intervals $S' \subseteq S$. “admitted” means that Ω' is of finite perimeter or a Lipschitz domain. The crucial point is that these theories assure the existence of a flux density j_Ω .

⁵With respect to the preceding footnote one could, more precisely, say “we assume“.

and

$$\begin{aligned} \mu_{\Omega}^{flux}(S' \times \Omega' \times K') &= \int_{S'} \int_{\mathfrak{F}_2} -j_{\Omega}(t, x, k) \cdot n_{\Omega}(x, k) d\lambda_K(k) d\sigma_{\partial\Omega}(x) d\lambda_S(t), \\ \mu_K^{flux}(S' \times \Omega' \times K') &= \int_{S'} \int_{\mathfrak{F}_1} -j_K(t, x, k) n_K(x, k) d\lambda_K(k) d\lambda_{\Omega}(x) d\lambda_S(t) \end{aligned}$$

for all $S' \in \mathfrak{A}_S$ and $\Omega' \in \mathfrak{A}_{\Omega}$, where $\sigma_{\partial\Omega}$ is the surface measure on $\partial\Omega$.

The physical meaning of these measures is the net-production of colloids in $\Omega' \times K'$ during the time-set (not necessarily an interval) S' via fluxes through the boundaries \mathfrak{F}_2 respectively \mathfrak{F}_1 .

Introducing the discrete partial derivative (with respect to the class size)

$$\partial_{CS}^d j_K(t, x, k) := j_K(t, x, k + 1) - j_K(t, x, k), \quad k \in K$$

we calculate

$$\begin{aligned} &\int_{S'} \int_{Q'} -\partial_{CS}^d j_K(t, x, k) d\lambda_K(k) d\lambda_{\Omega}(x) d\lambda_S(t) \\ &= \int_{S'} \int_{\Omega'} \int_{K'} -\partial_{CS}^d j_K(t, x, k) d\lambda_K(k) d\lambda_{\Omega}(x) d\lambda_S(t) \\ &= \int_{S'} \int_{\Omega'} \sum_{n=a}^b -\partial_{CS}^d j_K(t, x, n) d\lambda_{\Omega}(x) d\lambda_S(t) \\ &= \int_{S'} \int_{\Omega'} \sum_{n=a}^b (j_K(t, x, n) - j_K(t, x, n + 1)) d\lambda_{\Omega}(x) d\lambda_S(t) \\ &= \int_{S'} \int_{\Omega'} (j_K(t, x, a) - j_K(t, x, b + 1)) d\lambda_{\Omega}(x) d\lambda_S(t). \end{aligned}$$

Using the outward unit vectors $n_K(x, a) = -1$ and $n_K(x, b + 1) = +1$ we can write

$$\begin{aligned} &\int_{S'} \int_{Q'} -\partial_{CS}^d j_K(t, x, k) d\lambda_K(k) d\lambda_{\Omega}(x) d\lambda_S(t) \\ &= \int_{S'} \int_{\Omega'} (-j_K(t, x, a) n_K(x, a) - j_K(t, x, b + 1) n_K(x, b + 1)) d\lambda_{\Omega}(x) d\lambda_S(t) \\ &= \int_{S'} \int_{\Omega'} \int_{\{a, b+1\}} -j_K(t, x, k) n_K(x, k) d\lambda_K(k) d\lambda_{\Omega}(x) d\lambda_S(t) \\ &= \int_{S'} \int_{\mathfrak{F}_1} -j_K(t, x, k) n_K(x, k) d\lambda_K(k) d\lambda_{\Omega}(x) d\lambda_S(t). \end{aligned}$$

Recalling the definitions $\mu^{flux} = \mu_{\Omega}^{flux} + \mu_K^{flux}$, $\mathfrak{F}_2 := \partial\Omega \times K'$ we can now - using the divergence theorem of Gauss in the integral over \mathfrak{F}_2 - write

$$\begin{aligned} \mu^{flux}(S' \times Q') &= \int_{S'} \int_{Q'} -\operatorname{div}_x j_{\Omega}(t, x, k) d\lambda_K(k) d\lambda_{\Omega}(x) d\lambda_S(t) \\ &\quad + \int_{S'} \int_{Q'} -\partial_{CS}^d j_K(t, x, k) d\lambda_K(k) d\lambda_{\Omega}(x) d\lambda_S(t). \end{aligned} \tag{11}$$

We formulate the following intuitive ‘‘Balance principle’’:

$$\boxed{\begin{aligned} \mu(t + h, \Omega' \times K') - \mu(t, \Omega' \times K') &= \mu_P((t, t + h) \times \Omega' \times K'), \\ \forall t, t + h \in \bar{S}, \forall \Omega', \forall K'. \end{aligned}} \tag{12}$$

Using the integral representations in the balance principle (12) and Fubini’s theorem yields for all $Q' = \Omega' \times K'$ that

$$\begin{aligned} \int_{Q'} c(t+h, q) - \int_{Q'} c(t, q) d\lambda_{\Omega K}(q) &= \int_t^{t+h} \int_{Q'} f^{int}(\tau, q) d\lambda_{\Omega K}(q) d\lambda_S(\tau) \\ &+ \int_t^{t+h} \int_{Q'} -\operatorname{div}_x j_{\Omega}(t, x, k) d\lambda_K(k) d\lambda_{\Omega}(x) d\lambda_S(t) \\ &+ \int_t^{t+h} \int_{Q'} -\partial_{CS}^d j_K(t, x, k) d\lambda_K(k) d\lambda_{\Omega}(x) d\lambda_S(t). \end{aligned}$$

By multiplying by $\frac{1}{h}$ and passing to the limit $h \rightarrow 0$ we can now deduce the following equation (the classical continuity equation with a slightly different interpretation of the entries)

$$\frac{\partial c}{\partial t}(t, x, k) + (\operatorname{div}_x j_{\Omega}(t, x, k) + \partial_{CS}^d j_K(t, x, k)) = f^{int}(t, x, k).$$

We identify the terms as follows (motivated by the coagulation-fragmentation equation, see e.g [5, p.4]):

Let b_k be the fragmentation rate of k -colloids and let furthermore d_{ki} be the breakage distribution which describes the mass-fraction of k -colloids due to breakage of i -colloids. Then

$$\partial_{CS}^d j_K(t, x, k) = d_{k-1,k} b_k c(t, x, k) - d_{k,k+1} b_{k+1} c(t, x, k+1)$$

and

$$\begin{aligned} f^{int}(t, x, k) &= \frac{1}{2} \sum_{i+j=k, 1 \leq i, j \leq M} \beta_{ij} c(t, x, i) c(t, x, j) \\ &- \sum_{i=1}^M \beta_{ki} c(t, x, k) c(t, x, i) + \sum_{i>k+1}^M d_{ki} b_i c(t, x, i) - \sum_{1 \leq i < k-1} d_{ik} b_k c(t, x, k) \end{aligned}$$

where β_{ij} is the “connection-rate” of colliding colloids of sizes i and j .

3. Dynamic group formation and -dissolution in a population. In this section we look into the following social-interaction scenario⁶: Let $M \in \mathbb{N}$ be given. A very large number of people moves in a room Ω , a bounded domain in \mathbb{R}^2 , and forms groups of size k (“ k -groups”), $k \in K := \{1, 2, 3, \dots, M-1, M\}$. The “formations” are supposed to happen by groups joining or group splitting. We restrict ourselves to the following special case: At any given time and location a change of group size is assumed to be accomplishable only by either a single member leaving the group or an outsider joining a group. In the first case a k -group turns into two groups - a $(k-1)$ -group and a 1-group. In the second one two groups form one larger group, resp.

Let $k \in K' \subseteq K$. We say “a person belongs to a K' -group”, if it is a member of a k -group.

Following the lines of section 2, let $t \in \bar{S}$, $\Omega' \in \mathfrak{A}_{\Omega}$ and $K' \in \mathfrak{A}_K$ and introduce

$$\hat{\mu}(t, \Omega' \times K') := \text{number of people in } \Omega' \text{ which belong at time } t \text{ to the } K' \text{-group.} \tag{13}$$

⁶Also cf. [7] in which there is far more information on the underlying evacuation problem (on which the present setting is based on).

By nature of their definition, the maps $\Omega' \mapsto \widehat{\mu}(t, \Omega' \times K')$ and $K' \mapsto \widehat{\mu}(t, \Omega' \times K')$ are additive and non-negative. Postulating/assuming them to be σ -additive, the extension procedure indicated in section 2 yields a measure $\mu(t, \cdot)$ on $\mathfrak{A}_{\Omega K}$ for all $t \in \overline{S}$.

By requiring

$$\mu(t, \cdot) \ll \lambda_{\Omega K} \quad \text{for all } t \in \overline{S}, \quad (14)$$

we obtain a non-negative Radon-Nikodym density $c(t, \cdot) := \frac{d\mu(t, \cdot)}{d\lambda_{\Omega K}}$ and exclude population concentrations on sets of measure zero.

For the special case $Q' := \Omega' \times K' \in \mathfrak{A}_{\Omega} \times \mathfrak{A}_K$ we have

$$\mu(t, Q') = \int_{\Omega' \times K'} c(t, x, k) d\lambda_{\Omega K}. \quad (15)$$

In the given context the motion of the people as well as the change of group size by joining and dissolution are *the* contributing factors to a change of $c(t, \cdot, \cdot)$. This gives rise to the introduction of *production measures* $\mu_P, \mu_{P\pm}$ on $Y := S \times \Omega \times K$: Let

$$Y' := S' \times \Omega' \times K' \in \mathfrak{A}_{S\Omega K}. \quad (16)$$

“Positive production” is modelled by

$$\begin{aligned} \mu_{P+}(Y') := & \text{number of people which are added} \\ & \text{to } \Omega' \times K' \text{ during } S', \end{aligned} \quad (17)$$

“negative production”, μ_{P-} , is introduced in analogy and the “net production” is

$$\mu_P := \mu_{P+} - \mu_{P-}. \quad (18)$$

We specify μ_P by introducing two “production measures” - a *flux measure* μ^{flux} and an *inner-production measure* μ^{int} such that

$$\mu_P = \mu^{int} + \mu^{flux}. \quad (19)$$

We begin with μ^{flux} : Let $\Omega' \times K' \in \mathfrak{A}_{\Omega} \times \mathfrak{A}_K$ and denote the “physical flux into Ω' ” by “physical” or “spatial motion” of the people by

$$\begin{aligned} F_{\Omega+}^{flux} = F_{\Omega+}^{flux}(S' \times \partial\Omega' \times K') := & \text{number of people belonging} \\ & \text{to the } K'\text{-group and crossing through } \partial\Omega' \text{ into } \Omega' \text{ during } S'. \end{aligned} \quad (20)$$

Analogously we introduce $F_{\Omega-}^{flux} = F_{\Omega-}^{flux}(S' \times \partial\Omega' \times K')$ as the corresponding loss to $\Omega' \times K'$. Such fluxes might be given as some sort of a diffusion or advection flux, e.g. Finally we introduce the

$$\text{total } \Omega\text{-flux measure } F_{\Omega}^{flux} := F_{\Omega+}^{flux} - F_{\Omega-}^{flux}. \quad (21)$$

Borrowing again from theories of Cauchy interactions we obtain for all $t \in S$ and $k \in K$ a flux density

$$j_{\Omega}(t, \cdot, k) : \Omega \rightarrow \mathbb{R}^N \quad (22)$$

such that for all intervalls $S' \subseteq S$, $\Omega' \in \mathfrak{A}_{\Omega}$ with Lipschitz boundary and all $K' \subseteq K$:

$$\begin{aligned} \mu_{\Omega}^{flux}(S' \times \Omega' \times K') := & F_{\Omega}^{flux}(S' \times \partial\Omega' \times K') \\ = & \int_{S'} \int_{\Omega'} \int_{\partial K'} -j_{\Omega}(t, x, k) \cdot n_{\Omega} d\sigma_{\Omega} d\lambda_{\Omega} d\lambda_S. \end{aligned} \quad (23)$$

A second flux is introduced along the group-size scale K in the following way (and very reminiscent to the flux in the colloid setting in section 2): Let

$$p, q \in \mathbb{N}, \quad K' := [p, q] \cap \mathbb{N} \quad (24)$$

and set

$$\begin{aligned} \mu_{K^+}^{flux}(S' \times \Omega' \times K') &:= F_{\Omega^+}^{flux}(S' \times \Omega' \times \{p\}) \\ &:= \text{increase during } S' \text{ of the number of people in } \Omega' \text{ belonging} \\ &\text{to the } K' \text{-group by joining of a } (p-1) \text{-group with a 1-group (in } \Omega'). \end{aligned} \tag{25}$$

Analogously we introduce

$$\begin{aligned} \mu_{K^-}^{flux}(S' \times \Omega' \times K') &:= F_{\Omega^-}^{flux}(S' \times \Omega' \times \{q\}) \\ &:= \text{decrease during } S' \text{ of the number of people in } \Omega' \text{ belonging} \\ &\text{to the } K' \text{-group by splitting of a } q \text{-group into a 1-group} \\ &\text{and a } (q-1) \text{-group (in } \Omega'). \end{aligned} \tag{26}$$

Finally we introduce the

$$\text{total-}K\text{-flux measure } \mu_K^{flux} := \mu_{K^+}^{flux} - \mu_{K^-}^{flux}.$$

Let K' be as in (24). We call (p, q) the *ordered discrete boundary of K'* (notation: $\partial_{od}K'$). Moreover, the discrete partial derivative $\partial_{GS}^d j_K$ is introduced as in section 2. Also as in section 2 we introduce a flux density, the *K -flux density*

$$j_K(t, \cdot, \cdot) : \Omega \times K \rightarrow \mathbb{R}$$

such that

$$\begin{aligned} \mu_K^{flux}(S' \times \Omega' \times K') &= \int_{S'} \int_{\Omega'} \int_{\partial_{od}K'} -j_K(t, x, k) n_{K'}(k) d\sigma_K d\lambda_\Omega d\lambda_S \\ &= \int_{S'} \int_{\Omega'} \int_{K' - \{q\}} -\partial_{GS}^d j_K(t, x, k) d\lambda_K d\lambda_\Omega d\lambda_S. \end{aligned} \tag{27}$$

As in section 2: (27) does also hold for arbitrary $K' \subseteq K$.

Often one has an

$$\begin{aligned} &\text{integral representation for } \mu^{int} : \\ \mu^{int}(Y') &= \int_{Y'} f^{int}(t, x, y) d\lambda_{S\Omega K} \quad \text{for all } Y' \in \mathfrak{A}_{S\Omega A}. \end{aligned} \tag{28}$$

The motivations leading to (28) are similar to the corresponding ones in section 2.

Also along the lines of section 2 we see: If c , j_Ω and j_K are sufficiently smooth, then one has

$$\frac{\partial c}{\partial t} + [\text{div}_x j_\Omega + \partial_{GS}^d j_K] = f^{int} \quad \text{in } Y. \tag{29}$$

We conclude this section with a **specification** of j_Ω , j_K and f^{int} . Since there is an almost total analogy to section 2, we keep this short: Set

$$\begin{aligned} f^{int}(t, x, 1) &:= - \sum_{i=1}^{M-1} \beta_i c(t, x, i) c(t, x, 1) - \beta_1 c(t, x, 1) c(t, x, 1) + \sum_{i=3}^M \alpha_i c_i(t, x, i), \\ f^{int}(t, x, k) &:= -\beta_k c(t, x, k) c(t, x, 1) + \beta_{k-1} c(t, x, k-1) c(t, x, 1) \\ &\quad \text{for } k = 2, \dots, M-1, \\ f^{int}(t, x, M) &:= +\beta_{M-1} c(t, x, M-1) c(t, x, 1). \end{aligned}$$

$\alpha_k \in [0, 1]$ describes the likelihood under which a single member of a k -group separates from his group. $\beta_k c(t, x, k) c(t, x, 1)$ models the density of the number of people being removed from a k -group by interaction with a 1-group. Finally we specify $j_K(t, x, \cdot)$ as

$$\begin{aligned} j_K(t, x, 1) &:= \alpha_2 c(t, x, 2), \\ j_K(t, x, k) &:= -\alpha_k c(t, x, k) \quad \text{for } k = 2, \dots, M, \\ j_K(t, x, M+1) &:= 0. \end{aligned}$$

In [7] the spatial fluxes are Fickian diffusion fluxes, i.e.

$$j_\Omega(t, x, k) = -D_k \nabla_x c(t, x, k).$$

If the crowd were driven by advection-type, attractive or repulsive fluxes, one needs to choose j_Ω appropriately.

Note: With $c_k(t, x) := c(t, x, k)$, $f_k(t, x) := f(t, x, k)$, $j_k(t, x) := j_\Omega(t, x, k)$ one obtains a system of pde's for c_k with spatial fluxes j_k and right-hand sides f_k , $k = 1, \dots, M$.

4. Age-groups moving in a habitat. Much of the following is in almost complete analogy to the preceding two sections with one exception: the second feature is not discrete.

Let Ω be a habitat occupied by some population B , $a > 0$ an upper bound for the realisable ages of the B 's ($a = 180$ years for humans, $a = 2$ days for the common mayfly, $a = 20$ years for rabbits, e.g.), set $A = [0, a]$, $S := [0, T]$ (time interval) and assume $\Omega \subseteq \mathbb{R}^N$ to be bounded and measurable, $N = 2, 3$. The B 's get older and they might move, for instance by advection or by a diffusion-like mechanism or they might be driven by an attractant or repellent. The aging issue can be considered as a flux from one age group to the "next" one whereas advection etc. constitutes a flux *in* Ω . We introduce, for $\Omega' \in \mathfrak{B}^N(\Omega)$, $A' \in \mathfrak{B}^1(A)$, $t \in \bar{S}$, the

$$\begin{aligned} & \widehat{\mu}(t, \Omega' \times A') = \text{age group population measure} \\ & \text{amount of } B' \text{ in } \Omega' \text{ belonging to the age group } A'. \end{aligned}$$

Following the arguments in section 2 we obtain a measure $\mu(t, \cdot)$ on $\mathfrak{A}_{\Omega A} := \mathfrak{B}^N(\Omega) \otimes \mathfrak{B}^1(A)$ for all $t \in \bar{S}$. Set $\lambda_A := \lambda^1$ on $\mathfrak{B}^1(A)$, $\lambda_{\Omega A} := \lambda_\Omega \otimes \lambda_A$ and $Q := \Omega \times A$. The regularity assumption $\mu(t, \cdot) \ll \lambda_{\Omega A}$ yields a Radon-Nikodym density $c(t, \cdot) := \frac{d\mu(t, \cdot)}{d\lambda_{\Omega A}} \in L^1_+(Q)$. We introduce $\mu_P := \mu^{flux} +$, where $\mu^{int} := \mu_P - \mu^{flux}$ and $\mu^{flux} := \mu_\Omega^{flux} + \mu_A^{flux}$. μ^{int} and μ^{flux} are introduced as in the previous section where K gets replaced by A : In particular we set $\mu_A^{flux} = \mu_{A+}^{flux} - \mu_{A-}^{flux}$, where

$$\begin{aligned} & \widehat{\mu_{A\pm}^{flux}}(S' \times \Omega' \times A') := \text{number of } B' \text{ s in } \Omega', \\ & \text{which enter/leave } A' \text{ during } S' \text{ from/to the outside of } A', \end{aligned}$$

and

$$\widehat{\mu_A^{int}}(S' \times \Omega' \times A') := \text{number of } B' \text{ s in the age group } A' \text{ which are produced in } \Omega' \text{ during } S'.$$

A special case: Let $A' := [p, q] \subseteq A$. Then

$$\begin{aligned} & \widehat{\mu_{A+}^{flux}}(S' \times \Omega' \times A') := F_{A+}(S' \times \Omega' \times \{p\}) := \text{number of } B' \text{ s in } \Omega' \\ & \text{which pass during } S' \text{ the age } p. \end{aligned}$$

$\widehat{\mu_{A-}}$ is analogously introduced. In analogy to the preceding examples we can introduce (or obtain) flux-density vectors $j_\Omega(t, \cdot) = j_\Omega(t, x, y)$ and $j_A(t, \cdot) = j_A(t, x, y)$ such that for all $S' \times \Omega' \times A' \in \mathfrak{A}_{S\Omega A}$

$$\begin{aligned} & \mu_\Omega^{flux}(S' \times \Omega' \times A') = \int_{S' \times \Omega' \times A'} -\text{div}_x j_\Omega(t, x, y) d\lambda_{S\Omega A} \\ & \text{and} \\ & \mu_A^{flux}(S' \times \Omega' \times A') = \int_{S' \times \Omega' \times A'} -\partial_{GS} j_A(t, x, y) d\lambda_{S\Omega A}. \end{aligned}$$

$j_\Omega(t, \cdot)$ models physical motion inside of Ω , $j_A(t, \cdot)$ stands for motion in A . "Getting older" provides a natural example for the latter and is expressed by $j_A(t, x, y) :=$

$1c(t, x, y)$ - a complete analogon of advection fluxes! With the (definition-/postulate-)procedure indicated in section 2, $\widehat{\mu}^{flux}$ and $\widehat{\mu}_A^{int}$ can be extended to measures μ^{flux} and μ_A^{int} on $\mathfrak{A}_{\Omega A}$, resp. Assuming (28) and assuming sufficient regularity of the participating terms we arrive at

$$\frac{\partial c}{\partial t} + \operatorname{div}_{xy} j_{\Omega A} = f^{int}.$$

Note: Births are modelled by a boundary condition at $a = 0$ to be imposed on $j_A(t, x, 0)$.

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