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A unified framework for differential aggregations in Markovian process algebra

Max Tschaikowski, Mirco Tribastone *

Electronics and Computer Science, University of Southampton, United Kingdom

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ABSTRACT

Fluid semantics for Markovian process algebra have recently emerged as a computationally attractive approximate way of reasoning about the behaviour of stochastic models of large-scale systems. This interpretation is particularly convenient when sequential components characterised by small local state spaces are present in many independent copies. While the traditional Markovian interpretation causes state-space explosion, fluid semantics is independent from the multiplicities of the sequential components present in the model, just associating a single ordinary differential equation (ODE) with each local state. In this paper we analyse the case of a process algebra model inducing a large ODE system. Previous work, known as *exact* fluid lumpability, requires two symmetries: ODE aggregation is possible for processes that i) are isomorphic and that ii) are present with the same multiplicities. We first relax the latter requirement by introducing the notion of *ordinary* fluid lumpability, which yields an ODE system where the sum of the aggregated variables is preserved exactly. Then, we consider *approximate* variants of both notions of lumpability which make nearby processes symmetric after a perturbation of their parameters. We prove that small perturbations yield nearby differential trajectories. We carry out our study in the context of a process algebra that unifies two synchronisation semantics that are well studied in the literature, useful for the modelling of computer systems and chemical networks, respectively. In both cases, we provide numerical evidence which shows that, in practice, many heterogeneous processes can be aggregated with negligible errors.

1. Introduction

State-space explosion is a well-known problem that hinders our capability to analyse models for large-scale reactive systems that are based on an explicit discrete-state representation. The focus of this paper is on models of concurrent and parallel systems defined by process algebra, where this problem manifests itself with an exponential growth of the cardinality of the state space as a function of the number of interacting processes. Much ingenuity has gone into finding appropriate symmetries at the model level which induce a suitable coarsening of the state space that retains some information about the original one. In this respect, the classical results on bisimilarity allow to relate processes of possibly different state space sizes which are however equivalent with respect to an external observer [1].

* Corresponding author.
E-mail addresses: m.tschaikowski@soton.ac.uk (M. Tschaikowski), m.tribastone@soton.ac.uk (M. Tribastone).

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Analogous notions have been lifted to the quantitative setting, when process algebra is enriched with a stochastic semantics that maps onto a discrete-state Markov process rather than onto a labelled transition system. Here, a fundamental research question has been to define appropriate process-algebraic behavioural equivalences that induce a *meaningful* aggregation at the level of the underlying Markov chain. This has already been established for a number of Markovian process algebra. For instance, the notions of Markovian bisimulation for MTIPP [2] and strong equivalence for PEPA [3] are equivalence relations which are shown to yield a *lumped* Markov chain [4]. This is a Markov chain obtained from the original one by appropriately partitioning states, such that the probability of being in each partition block is equal to the sum of all probabilities of being in each state within the block. (See also [5] for a review of Markovian behavioural equivalences.)

With these approaches, little information is lost in the aggregation and the two stochastic processes are related exactly. Perhaps unexpectedly, however, the equivalence relations that permit such aggregations require strong symmetries at the process-algebraic level, and are essentially able to relate processes that perform the same actions at identical rates. However, there is evidence of criticism on this assumption when we insist on using models to represent actual systems. In this case, confronting reality entails that model parameterisation is difficult because measurements may be subject to noise, thereby inevitably introducing estimation errors (e.g., [6,7]). This observation has motivated a body of research into approximate reasoning about formal models of probabilistic and stochastic systems (e.g., [8–11]).

This paper follows the same line of research, by studying exact as well as approximate notions of aggregation for Markovian process algebra. However, differently from all the aforementioned literature, we target *fluid semantics*. This has recently emerged as an alternative to the classical Markovian semantics, describing the model dynamics in terms of a system of ordinary differential equations (ODEs) [12,13]. These can be interpreted as a deterministic approximation to the expectation of the Markov chain (e.g., [14–17]). When the model under consideration consists of many copies of processes in parallel, the ODE system size is independent from the multiplicities of such copies, unlike the Markovian representation, which, as discussed, suffers from state explosion.

Unfortunately, not every process algebra model enjoys a compact ODE description (e.g., [18]). Indeed, the problem of aggregating large-scale models based on ODEs has attracted the attention of researchers in a variety of other disciplines including control theory [19], theoretical ecology [20], and chemical engineering [21]. Arguably, in the process algebra literature the topic of ODE aggregation has so far received less attention than its stochastic counterpart. In [22,23] we studied a notion of behavioural equivalence for ODEs for PEPA [3]; ODE aggregations have also been investigated in [24] for rule-based models such as Kappa [25] and BioNetGen [26], for the modelling and analysis of biomolecular networks.

The goal of this paper is to extend the toolkit of ODE aggregations available for Markovian process algebra, by making the following contributions.

A unified framework for synchronisation semantics. Let us start with the observation that, in general, the development of theories in Markovian process algebra may depend on the choice of the quantitative semantics of the synchronisation operator, since this is typically defined as a function of the rates at which the operands (i.e., the synchronising processes) exhibit some behaviour. The actual choice of the function is motivated by the kinds of the systems that the language is meant to target. PEPA, for instance, can be useful for the performance evaluation of computing systems, since it has been shown to capture the semantics of other formalisms and methods such as queueing networks [27] or stochastic Petri nets [28]. Thus, the previously cited results of ODE aggregations find applicability in that domain. On the other hand, rule-based models essentially employ a semantics based on the *law of mass action*. As discussed, this is well known to be at the basis of biochemical reaction networks, though it has also been employed in epidemiological models (e.g., [29]) as well as in certain wireless networks (e.g. [30]).

Our initial starting point is to consider a unified process-algebraic framework that encompasses both kinds of interaction, in such a way that any result developed in this context finds immediate applicability to either kind of target system/semantics. To do so, we introduce and study *Fluid Extended Process Algebra* (FEPA), a lightweight extension of *Fluid Process Algebra* presented in [22]. Its characteristic trait is a generic parallel operator that is parameterised using a function of two arguments, defining the actual instance of the law of interaction to be used in the synchronisation. To show that FEPA is a conservative extension, we will first establish that the notion of *exact fluid lumpability* (EFL) presented [22] carries over. This will be used to set the stage for approximate notions of ODE aggregations, discussed later in the paper, which are defined in terms of their exact counterparts.

We take EFL as the starting point of our investigation, with the objective of extending it along two orthogonal directions. On the one hand, we define a new notion of lumpability, called *ordinary fluid lumpability* (OFL), which relaxes assumptions on certain symmetries whilst still guaranteeing exactness of the aggregated system. On the other hand, we consider approximate versions of both EFL and OFL which can yield coarser aggregations, at the cost of losing exactness. To be concrete yet informal for the purpose of overviewing our results, let us consider the process

$$\left(P_1[N_1] \parallel_K P_2[N_2] \parallel_K \cdots \parallel_K P_D[N_D]\right) \parallel_L Q[M] \tag{1}$$

where, for all $1 \leq i \leq D$, P_i is some sequential component that is replicated N_i times, and $\parallel_K$ is the (generic) parallel operator, parameterised by an action set K, in a CSP-like fashion. EFL may essentially reduce the analysis of such a model by considering the fluid trajectory of a *representative* P_i, which is shown to be equal to that of any other P_j if, for all $1 \leq i, j \leq D$, it holds that $N_i = N_j$ and P_i and P_j are isomorphic. Thus, denoting by $V_S(t)$ the ODE solution related to the

sequential component S, EFL would yield $V_{P_i}(t) = V_{P_j}(t)$ for all t. However, we notice that symmetries are required both at the level of the sequential component and at the compositional level, by ensuring that all populations have the same size.

Ordinary fluid lumpability (OFL). Similarly to EFL, ordinary fluid lumpability considers symmetry through isomorphism at the sequential level; thus, it still requires that P_i and P_j be isomorphic for all i, j. However, it allows *heterogeneity* at the compositional level: in the example above, it may yield an exactly aggregated ODE system even if $N_i \neq N_j$. However, unlike EFL, where all the trajectories of the original ODE system can be obtained from the solution of the aggregate, in OFL the aggregate gives the exact sum of the solutions of its parts, but their individual trajectories cannot be recovered. Thus, for instance, OFL would define an aggregate ODE for some variable $W_P(t)$ and show that $W_P(t) = V_{P_1}(t) + V_{P_2}(t) + \cdots + V_{P_D}(t)$. More precisely, OFL identifies an aggregate ODE system where the solution to each ODE is the linear combination of solutions of ODEs belonging to the original system. In this sense, it is similar to the approach presented in [24], where this aggregation has been cast in the context of abstract interpretation. However, there are three differences.

i) The focus in [24] is on reaction networks regulated by the law of mass action only.
ii) In [24] aggregates can be obtained by collapsing non-isomorphic biochemical species. This is useful in that application domain, where species are modelled as non-atomic entities with an internal state characterised by the simplest agents of which they are formed. This is in contrast to the modelling scenario envisaged in our FEPA, where atomic entities do not combine, but only interact with other atomic entities. More specifically, a typical modelling pattern amenable to our notions of aggregation is that of *multi-class* systems, where analogous processes (e.g., two or more kinds of infections [29]) exhibit similar behaviour, but with different rates and/or with different multiplicities.
iii) Finally, unlike [24], we also consider properties, i.e., congruence, on the compositionality of our aggregations.

Approximate aggregations. We aim to go beyond [22,24], as well as OFL, in that we also relax the requirement on the *exactness* of the aggregation. We study ε-variants of both EFL and OFL as a means to relaxing symmetries at the sequential level. These variants allow non-isomorphic processes to be aggregated if there exists a *perturbation* in the rates that makes them isomorphic. For instance, let us take $P_i \xrightarrow{(\alpha,r)} P_k$ and $P_j \xrightarrow{(\alpha,r+\varepsilon)} P_k$, for some P_k, where the edges give the usual action/rate pairs, with $r > 0$ and $\varepsilon > 0$. Then, these processes cannot be aggregated with either EFL or OFL because $\varepsilon > 0$ does not make them isomorphic. However, there exists a perturbation on the parameters of P_i and P_j that makes them isomorphic. For instance, one can take $P_j \xrightarrow{(\alpha,r)} P_k$ such that ε represents the degree of such perturbation. In fact, there exist infinitely many such perturbations. For instance, it would be possible to consider $P_i \xrightarrow{(\alpha,r+\varepsilon/2)} P_k$ and $P_j \xrightarrow{(\alpha,r+\varepsilon/2)} P_k$. In all these cases, it would hold that the model is ε-ordinarily fluid lumpable for any N_i and N_j. Clearly, the aggregated system will not be in exact correspondence with the original one. However, a theoretical bound shows that the aggregation error depends *linearly* on the intensity of the perturbation $|\varepsilon|$.

Exhibiting such near-symmetries may appear quite limiting for practical applications; however, there are models in the literature that do exhibit this characteristic. This has been recently studied in [31], where a similar notion of approximate aggregation has been presented. However, there are three main differences between [31] and the present paper:

i) The notion of aggregation in [31] is defined directly at the level of ODEs. Thus, ODE systems under considerations are not necessarily derived from a process algebra.
ii) If interpreted according to the terminology herein presented, the approach in [31] is restricted to approximate aggregations of OFL type.
iii) Being not informed by a process algebra, in [31] compositionality issues are not addressed.

Characterisation of ODE aggregations. We study the nature of such aggregations in three main ways.

i) We show that all our ODE aggregations can be induced by suitable notions of behavioural equivalence, which turn out to be congruences for FEPA.
ii) We consider the nonrestrictive notion of model well-posedness originally defined in [22]. Under this assumption, we show that processes which can be aggregated according to either EFL or OFL are related by *semi-isomorphism*. This is an extension of graph isomorphism to labelled transition systems with transition multi-sets, which does not distinguish between the multiplicity of arcs connecting two nodes whenever the total rate is the same. In this way we lift the same result in [22], developed for EFL in PEPA, to both EFL and OFL for our extended process algebra FEPA. Furthermore, under well-posedness we show that ε-EFL and ε-OFL imply the behavioural notion of ε-semi-isomorphism, the natural extension of semi-isomorphism which relates graphs up to changes in the transition rates. At the same time, however, processes that are semi-isomorphic cannot be aggregated according to EFL or OFL in general, essentially because two semi-isomorphic processes may be present in different contexts, which may impact their ODE expressions due to possibly different synchronisations.
iii) Finally, we provide some numerical evidence on the usefulness of the approximate versions of EFL and OFL, presenting model examples where even significant perturbation in the rates may yield negligible error in practice.

Paper structure. The remainder of the paper is organised as follows. Section 2 introduces FEPA, with most important definitions explained by means of a running example which will be used throughout. Section 3 presents the exact notions of ODE aggregation. It first lifts exact fluid lumpability to FEPA and then studies ordinary fluid lumpability. Section 4 considers the approximate versions, of which a numerical evaluation is presented in Section 5. Section 6 puts this paper in a broader context than analysed in this introduction, relating it to other work on ODE aggregations. Finally, Section 7 concludes. A number of technical results that are auxiliary to proving the main statements of this paper are stated and proved in Appendix A.

This paper is an extension of the workshop contribution [32], which includes proofs for all statements, more detailed explanations, and a broader discussion of related work.

2. Fluid extended process algebra

To define FEPA, we exploit the fact that fluid semantics reason about representatives of identical sequential components that are replicated in parallel without synchronisation. We call such representatives *fluid atoms*, in line with [22]. For instance, in (1), $P_1[N_1]$ will be represented in FEPA using a single fluid atom P_1 together with the information about the multiplicity of replicas, N_1, encoded in a *population function*. Therefore, overall, the model (1) would be represented by $(P_1 \parallel_K P_2 \parallel_K \cdots \parallel_K P_D) \parallel_L Q$. This information is sufficient to derive the underlying system of ODEs of the fluid semantics.

Let us first define the grammar for fluid atoms.

Definition 1. The syntax of a FEPA fluid atom is given by

$$P ::= (\alpha, r).P \mid P + P \mid A \quad \text{with } A \stackrel{\text{def}}{=} P \text{ (constant)},$$

where α is an action in the *action set* $\mathcal{A}$ and $r \in \mathbb{R}_{>0}$.

The structured operational semantics is given by the following (usual) four rules:

$$\frac{}{(\alpha, r).P \xrightarrow{(\alpha,r)} P}, \qquad \frac{P \xrightarrow{(\alpha,r)} P'}{P + Q \xrightarrow{(\alpha,r)} P'}, \qquad \frac{Q \xrightarrow{(\alpha,r)} Q'}{P + Q \xrightarrow{(\alpha,r)} Q'}, \qquad \frac{P \xrightarrow{(\alpha,r)} P'}{A \xrightarrow{(\alpha,r)} P'} \; A \stackrel{\text{def}}{=} P.$$

Note that, being based on PEPA, FEPA has no zero (or nil) process. We argue, however, that this is without loss of generality, as deadlocks can be encoded by self-loops.

Given a fluid atom P, these rules induce a labelled transition system, denoted by $dg(P)$ (the derivation graph), with nodes denoted by $ds(P)$ (the *derivative set*), and with a transition multi-set that takes into account the distinct derivations between any two fluid atoms. The formal definitions are lifted straightforwardly from PEPA [3] and FPA [22]. They are given in the same style, although we are aware of more recent and elegant approaches based on [33].

Definition 2 *(Derivative set).* The derivative set of a FEPA fluid atom P, denoted by $ds(P)$, is defined as the smallest set such that $P \in ds(P)$; and if $P' \in ds(P)$ and $P' \xrightarrow{(\alpha,r)} P''$ then $P'' \in ds(P)$.

Definition 3 *(Derivation graph).* Let $\mathcal{A}ct := \mathcal{A} \times \mathbb{R}_{>0}$ denote the set of all activities of FEPA. The derivation graph $dg(P)$ of a FEPA fluid atom P has $ds(P)$ as the set of nodes. The multi-set of transitions $\mathcal{T} \subseteq ds(P) \times \mathcal{A}ct \times ds(P)$ is the smallest multi-set that satisfies the four operational semantic rules and keeps track of all the possible ways of deriving each of its elements.

Semi-isomorphism, at the basis of our characterisation results, relates two fluid atoms whenever their derivation graphs are isomorphic up to replacing multiple transitions with the same action type between two states, with a single transition which has the same action type and a rate which is equal to the sum of all rates across such transitions.

Definition 4 *(Semi-isomorphism).* Two FEPA fluid atoms P and Q are semi-isomorphic if there is a bijection $\sigma : ds(P) \to ds(Q)$ which satisfies $\sum_{P_i \xrightarrow{(\alpha,r)} P_j} r = \sum_{\sigma(P_i) \xrightarrow{(\alpha,r)} \sigma(P_j)} r$ for all $P_i, P_j \in ds(P)$ and $\alpha \in \mathcal{A}$. We shall call such a bijection σ a semi-isomorphism.

For instance $P \stackrel{\text{def}}{=} (\alpha, r_1).P + (\alpha, r_2).P$ is semi-isomorphic to $Q \stackrel{\text{def}}{=} (\alpha, r_1 + r_2).Q$.

A FEPA model is a composition of fluid atoms, using the parallel operator $\parallel_L$. To be consistent with [22], FEPA does not feature the hiding operator.

Definition 5 *(FEPA model).* A FEPA model M is given by the grammar

$$M ::= M \parallel_L M \mid P$$

where $L \subseteq \mathcal{A}$ and P is a fluid atom. For any two distinct fluid atoms P and P' in M, we require that $ds(P) \cap ds(P') = \emptyset$.

In comparing derivative sets, equality is intended to be syntactical. The requirement on pairwise disjoint derivative sets is without loss of generality: If two distinct fluid atoms have a common derivative, it is always possible to relabel one atom with appropriate fresh constants so as to satisfy the above condition.

Example 1. Let us consider the FEPA model

$$Sys := (P_1 \parallel_\emptyset \ldots \parallel_\emptyset P_D) \parallel_{\{\alpha\}} Q, \tag{2}$$

with fluid atoms given by

$$P_d \stackrel{\text{def}}{=} (\alpha, r).P'_d, \qquad P'_d \stackrel{\text{def}}{=} (\beta, s).P_d, \qquad Q \stackrel{\text{def}}{=} (\alpha, u).Q', \qquad Q' \stackrel{\text{def}}{=} (\delta, w).Q, \quad 1 \leq d \leq D. \tag{3}$$

Intuitively, *Sys* considers a situation where D *independent* groups of agents, recognisable by the empty cooperation sets, synchronise with a common group of agents, of type Q, through action α. This model is a particular instance of (1), where the behaviour of the fluid atoms is defined through the constants in (3).

The next definition will be auxiliary to setting up the fluid framework. Together with the remaining definitions in this section, they are adapted from [16].

Definition 6. Let M be a FEPA model. We define then $\mathcal{G}(M)$ as the set of all fluid atoms in M; $\mathcal{B}(M)$ as the set of all atoms' derivatives, i.e., $\mathcal{B}(M) = \bigcup\{ds(P) \mid P \in \mathcal{G}(M)\}$; a *population function* $V : X \to \mathbb{R}_{\geq 0}$ with $\mathcal{B}(M) \subseteq X$; and an *initial* population function $V(0) : X \to \mathbb{R}_{\geq 0}$.

For instance, $\mathcal{G}(Sys) = \{P_1, \ldots, P_D, Q\}$, $\mathcal{B}(Sys) = \{P_d, P'_d \mid 1 \leq d \leq D\} \cup \{Q, Q'\}$. Function $V(0)$ encodes the size of the system at time $t = 0$. For instance,

$$V_{P_d}(0) = N_d, \qquad V_{P'_d}(0) = 0, \qquad V_Q(0) = N_Q, \qquad V_{Q'}(0) = 0, \tag{4}$$

states that at $t = 0$ there are N_d agents in the state P_d, no agents in the state P'_d, N_Q agents in the state Q and no agents in the state Q'.

Definition 7 *(Apparent rate).* The apparent rate of action α in a FEPA fluid atom P, denoted by $r_\alpha(P)$, is defined as follows:

$$r_\alpha\big((\beta, r).P\big) := \begin{cases} r, & \beta = \alpha, \\ 0, & \text{else}, \end{cases}$$

$$r_\alpha(A) := r_\alpha(P), \quad A \stackrel{\text{def}}{=} P$$

$$r_\alpha(P + Q) := r_\alpha(P) + r_\alpha(Q).$$

Let us recall that the intent of a fluid atom is to represent multiple independent copies of some sequential component. The notion of apparent rate gives the overall rate at which a single copy of a fluid atom is able to perform an action. In order to define the total rate at which an action is performed in a FEPA model, we turn to the forthcoming definition of parameterised apparent rate. For this, we first need to provide the semantics for interaction in FEPA. We consider two instances, distinguished by the choice of a (binary) *synchronisation function* that is hereafter denoted by ρ. Choosing $\rho = \min$ yields the semantics of PEPA; the law of mass action is instead recovered by choosing $\rho = \cdot$ (intended as multiplication). With this latter choice, FEPA can be seen as the fluid counterpart of Markovian process algebra such as [2,34], or as an alternative to process algebra for biological networks such as Bio-PEPA [15].

Definition 8 *(Parameterised apparent rate).* Let M be a FEPA model, $\alpha \in \mathcal{A}$, V a population function, and ρ the synchronisation function. The apparent rate of M with respect to V is defined as

$$r_\alpha(M_0 \parallel_L M_1, V) := \begin{cases} \min(r_\alpha(M_0, V), r_\alpha(M_1, V)), & \alpha \in L \wedge \rho = \min, \\ r_\alpha(M_0, V) \cdot r_\alpha(M_1, V), & \alpha \in L \wedge \rho = \cdot, \\ r_\alpha(M_0, V) + r_\alpha(M_1, V), & \alpha \notin L, \end{cases}$$

$$r_\alpha(P, V) := \sum_{P_i \in ds(P)} V_{P_i} r_\alpha(P_i),$$

where $r_\alpha(P_i)$ is the apparent rate of a FEPA fluid atom P_i, by Definition 7.

For instance, in (2) it holds that $r_\alpha(P_d, V) = rV_{P_d}$, which gives the apparent rate at which a population of V_{P_d} P_d-components exhibits action α. Let us remark, however, that the apparent rate for a fluid atom collects the contributions of all its local states. Thus, for instance, in a fluid atom with local states $E \stackrel{\text{def}}{=} (\alpha, r).F$ and $F \stackrel{\text{def}}{=} (\alpha, r).E$ we would have that $r_\alpha(E, V) = r(V_E + V_F)$. Now, returning back to our running example, let us assume that $D = 1$ in (2). Then $r_\alpha(P_1 \parallel_{\{\alpha\}} Q, V) = \min(rV_{P_1}, uV_Q)$ if $\rho = \min$; for $\rho = \cdot$, instead, we have that $r_\alpha(P_1 \parallel_{\{\alpha\}} Q, V) = r \cdot u \cdot V_{P_1} \cdot V_Q$. In this case, the model corresponds to a chemical reaction network with three reactions. These can be expressed, using standard notation, as follows:

$$\begin{aligned} &P_1 + Q \to P_1' + Q', && \text{with coefficient } r \cdot u,\\ &P_1' \to P_1, && \text{with coefficient } s,\\ &Q' \to Q, && \text{with coefficient } w. \end{aligned}$$

The first reaction indicates that a copy of P_1 and a copy of Q interact to become P_1' and Q', respectively. The last two reactions, instead, can be interpreted as *monomolecular reactions* where each copy spontaneously evolves without any interaction with other species.

The following quantities are used to define the vector field of the ODE system to be analysed.

Definition 9 *(Parameterised component rate).* Let M be a FEPA model, $\alpha \in \mathcal{A}$ and V a population function. The component rate of $P' \in \mathcal{B}(M)$ is parameterised by V in the following manner.

a) case $M = P$: then

$$\mathcal{R}_\alpha\big(P, V, P'\big) := V_{P'} r_\alpha\big(P'\big).$$

b) case $M = M_0 \parallel_L M_1$: if $P' \in \mathcal{B}(M_i)$, for some $i = 0, 1$, and $\alpha \notin L$ then

$$\mathcal{R}_\alpha\big(M_0 \parallel_L M_1, V, P'\big) := \mathcal{R}_\alpha\big(M_i, V, P'\big).$$

c) case $M = M_0 \parallel_L M_1$: if $P' \in \mathcal{B}(M_i)$, for some $i = 0, 1$, and $\alpha \in L$ then

$$\mathcal{R}_\alpha\big(M_0 \parallel_L M_1, V, P'\big) := \frac{\mathcal{R}_\alpha(M_i, V, P')}{r_\alpha(M_i, V)} r_\alpha(M_0 \parallel_L M_1, V).$$

Some explanation is in order. The parameterised component rate of a fluid atom P' gives the overall rate at which the fluid atom witnesses the execution of an action in the model. According to this intuition, case a) can be understood by noticing that, when restricted to a context of some fluid atom P, the parameterised component rate simply corresponds to the overall rate of that atom. Case b) is similar, in that it gives this rate in the context of a synchronisation which however does not influence the execution of the action under consideration (i.e., $\alpha \notin L$). Case c), instead, does take into account the influence of synchronisation. The fraction represents the *weight* of the α-contribution of P' with respect to the rate at which the action α can be performed by the sub-model to which P' belongs. This factor multiplies the *overall rate in the model* for action α, which depends on the other synchronising sub-model. Interestingly, we notice that in the case of $\rho = \cdot$, it holds that c) reduces to case b). That is, we have that $\mathcal{R}_\alpha(M_0 \parallel_L M_1, V, P') = \mathcal{R}_\alpha(M_i, V, P')$ even when $P' \in \mathcal{B}(M_i)$ for some $i = 0, 1$ and $\alpha \in L$. This makes the semantics consistent with the law of mass action of biochemical reaction networks. However, we must keep the above cases separate to be able to uniformly deal with either choice of ρ.

We are finally ready to provide the ODEs of the fluid semantics.

Notation. We use Newton's dot notation $\dot{V}_P$ for the derivative of V_P. To enhance readability, time t will be suppressed, e.g., $\dot{V}_P$ denotes $\dot{V}_P(t)$.

Definition 10. Let M be a FEPA model. The initial value problem for M is given by $\dot{V} = F(V)$ with initial condition $V(0)$, where

$$F_P(V) := \sum_{\alpha \in \mathcal{A}} \left(\left(\sum_{P' \in \mathcal{B}(M)} p_\alpha\big(P', P\big) \mathcal{R}_\alpha\big(M, V, P'\big) \right) - \mathcal{R}_\alpha(M, V, P) \right)$$

and

$$p_\alpha\big(P, P'\big) = \frac{1}{r_\alpha(P)} \sum_{P \xrightarrow{(\alpha, r)} P'} r$$

for all $\alpha \in \mathcal{A}$ and $P, P' \in \mathcal{B}(M)$.

For instance, the initial value problem of (2) and (4) in the case of $\rho = \cdot$ is given by the initial condition (4) and the ODE system

$$\begin{aligned} \dot{V}_{P_d} &= -ruV_{P_d} \cdot V_Q + sV_{P'_d} & \dot{V}_{P'_d} &= -sV_{P'_d} + ruV_{P_d} \cdot V_Q \\ \dot{V}_Q &= -uV_Q \cdot \sum_{1 \le d \le D} rV_{P_d} + wV_{Q'} & \dot{V}_{Q'} &= -wV_{Q'} + uV_Q \cdot \sum_{1 \le d \le D} rV_{P_d} \end{aligned} \tag{5}$$

This also clarifies our intent of encoding the law of mass action. The rate of evolution of the interaction between distinct synchronising processes (e.g., molecules) is proportional to the product of their abundances.

Finally, let us end this section by introducing the notion of well-posedness, introduced in [22]. As discussed, this is needed to characterise ODE aggregations with respect to the structure of the fluid atoms.

Definition 11 *(Well-posedness).* A FEPA model M is said to be well-posed if and only if for all occurrences $M_1 \parallel_L M_2$ in M it holds that $\exists V_1(r_\alpha(M_1, V_1) > 0) \wedge \exists V_2(r_\alpha(M_2, V_2) > 0)$ for all $\alpha \in L$.

In essence, a model is well-posed whenever any synchronised action may be performed by both operands, for some population function. Thus, *Sys* is well-posed, but $\tilde{P} \parallel_{\{\alpha,\gamma\}} Q$, where $\tilde{P} \stackrel{\text{def}}{=} (\alpha, r).\tilde{P}' + (\gamma, r).\tilde{P}'$ and $\tilde{P}' \stackrel{\text{def}}{=} (\beta, s).\tilde{P}$, is not, since $\tilde{P}$ is hindered in performing the shared γ-action because neither Q nor Q' are capable of doing γ. We wish to point out, however, that the assumption of well-posedness is without loss of generality, since each non-well-posed model can be transformed into a well-posed one *without* changing the underlying ODE system. The corresponding procedure has been discussed in [23]. However, let us briefly sketch how this can be done in the above case. For this, is suffices to observe that by removing the γ-action in the definition of $\tilde{P}$, the ODE of the model is not affected. Thus, we may rewrite $\tilde{P} \parallel_{\{\alpha,\gamma\}} Q$ into $P_1 \parallel_{\{\alpha,\gamma\}} Q$. Since neither P_1 nor Q can perform γ-actions, $P_1 \parallel_{\{\alpha,\gamma\}} Q$ can be further rewritten into the well-posed model $P_1 \parallel_{\{\alpha\}} Q$, meaning that $P_1 \parallel_{\{\alpha\}} Q$ and $\tilde{P} \parallel_{\{\alpha\}} Q$ have (up to renaming) identical ODE systems.

3. Exact aggregations

In this section we develop the theory of ODE aggregation for FEPA. As discussed, we first overview the notion of exact fluid lumpability introduced in [22]. Although lifting it to FEPA is fairly straightforward, here we re-propose all the necessary definitions and main results because they will be instrumental in the development of its novel approximate variant in Section 4, which is defined in terms of the exact counterpart. The second part of this section is instead devoted to ordinary fluid lumpability, which is introduced here for the first time.

Exact fluid lumpability. As discussed in Section 1, EFL reduces the ODE system size by exploiting the fact that distinct fluid atoms with the same initial population function may have indistinguishable ODE solutions.

Definition 12 *(Exact fluid lumpability (EFL)).* Let M be a FEPA model and $\{\mathcal{P}^1, \ldots, \mathcal{P}^n\}$, where $\mathcal{P}^i = \{P^i_j \mid 1 \le j \le k_i\}$, be a partition of $\mathcal{G}(M)$. The partition is called *exactly fluid lumpable* if there exist bijections

$$\sigma_{P^i_j} : ds(P^i_1) \to ds(P^i_j), \quad 1 \le i \le n,\ 1 \le j \le k_i,$$

where $\sigma_{P^i_1} \equiv \mathrm{id}_{ds(P^i_1)}$, such that for all initial populations $V(0)$ which satisfy

$$V_P(0) = V_{\sigma_{P^i_j}(P)}(0), \quad \forall 1 \le i \le n\ \forall P \in ds(P^i_1)\ \forall 1 \le j \le k_i$$

the same holds for all $t \ge 0$ in the corresponding ODE solution V, i.e.

$$V_P(t) = V_{\sigma_{P^i_j}(P)}(t), \quad \forall 1 \le i \le n\ \forall P \in ds(P^i_1)\ \forall 1 \le j \le k_i\ \forall t \ge 0.$$

Exact fluid lumpability of a partition is induced by the notion of *label equivalence*, established between tuples of fluid atoms. Intuitively, relating two tuples (of the same length) (S_1, T_1) and (S_2, T_2) means that, component-wise, the fluid atoms have the same trajectories; that is, S_1 (resp., T_1), has the same ODE solution as S_2 (resp., T_2). Fluid atoms within the same tuple are coupled in the sense that matching fluid atoms have to be provided for each element of a tuple.

Definition 13 *(Label equivalence).* Let M be a FEPA model and let $\mathcal{P} = (\vec{P}^1, \ldots, \vec{P}^N)$, $\vec{P}^i = (P^i_1, \ldots, P^i_{K_i})$, be a *tuple partition* on $\mathcal{G}(M)$, that is, for each $P \in \mathcal{G}(M)$ there exist unique $1 \le i \le N$ and $1 \le k \le K_i$ with $P = P^i_k$. $\vec{P}^i$ and $\vec{P}^j$ are said to be *label equivalent*, written $\vec{P}^i \sim_{\mathcal{P}} \vec{P}^j$, if $K_i = K_j$ and there exist bijections $\sigma_k : ds(P^i_k) \to ds(P^j_k)$, where $1 \le k \le K_i$, such that for all population functions V of M and

$$V_P^\sigma := \begin{cases} V_{\sigma_k(P)}, & \exists 1 \le k \le K_i (P \in ds(P_k^i)) \\ V_{\sigma_k^{-1}(P)}, & \exists 1 \le k \le K_i (P \in ds(P_k^j)) \\ V_P, & \text{otherwise} \end{cases}$$

it holds that

a) $\mathcal{R}_\alpha(M, V, P) = \mathcal{R}_\alpha(M, V^\sigma, \sigma_k(P))$.
b) $\sum_{P'} p_\alpha(P', P)\mathcal{R}_\alpha(M, V, P') = \sum_{P'} p_\alpha(P', \sigma_k(P))\mathcal{R}_\alpha(M, V^\sigma, P')$.
c) $\mathcal{R}_\alpha(M, V, P) = \mathcal{R}_\alpha(M, V^\sigma, P)$ for all $P \in ds(P_k^l)$ with $P_k^l \notin \vec{P}^i, \vec{P}^j$.
d) $r_\alpha(M, V) = r_\alpha(M, V^\sigma)$ and $r_\alpha(P_k^i) = r_\alpha(P_k^j)$ for all $1 \le k \le K$.

Intuitively, a) the α-component rate out of P with respect to V is equal to the α-component rate out of $\sigma_k(P)$ with respect to V^σ; b) requires that the sum of α-component rates into P with respect to V is equal to the sum of α-component rates into $\sigma_k(P)$ with respect to V^σ; for c), the α-component rates of $P_k^l \notin \vec{P}^i, \vec{P}^j$ are invariant under $V \mapsto V^\sigma$; finally, for d), the α-apparent rate of M is invariant under $V \mapsto V^\sigma$.

Informally, label equivalence considers symmetries between tuples of fluid atoms. When two tuples are equivalent, related fluid atoms in the same position within their tuple will have the same fluid trajectories when initialised with the same condition. This is achieved by checking that the behaviour of such fluid atoms is invariant with respect to an exchange of the population functions according to a bijection between their derivative sets. This exchange is formalised in conditions a)–d), which require that the component rates are the same a), c), that the two atoms have the same influx up to this exchange b), and that also the apparent rates are invariant, d).

Example 2. EFL has been used to simplify replicas of composite processes [18]. For instance, let us consider the fluid atoms in Example 1, together with the constants $R_d \stackrel{\text{def}}{=} (\alpha, \tilde{r}).R'_d$, and $R'_d \stackrel{\text{def}}{=} (\gamma, \tilde{s}).R_d$. Let us take the FEPA model

$$Sys_{\mathcal{E}} := \left((P_1 \parallel_{\{\alpha\}} R_1) \parallel_\emptyset \ldots \parallel_\emptyset (P_D \parallel_{\{\alpha\}} R_D)\right) \parallel_{\{\alpha\}} Q,$$

which features D replicas of composite processes of type $P_d \parallel_{\{\alpha\}} R_d$. Let us consider now the tuple partition $\mathcal{P} := \{(P_1, R_1), \ldots, (P_D, R_D), (Q)\}$. Then, it can be shown that $(P_i, R_i) \sim_{\mathcal{P}} (P_j, R_j)$, thus formalising the intuitive idea that each replica has the same solution (if initialised with identical conditions).

Projected label equivalence establishes a relation between fluid atoms that is induced by label equivalence, which instead acts on *tuples* of atoms. In essence, it directly relates atoms which are associated with indistinguishable ODE solutions.

Definition 14 *(Projected label equivalence).* Fix a FEPA model M and a tuple partition $\mathcal{P}$ of $\mathcal{G}(M)$. Two fluid atoms $P_1, P_2 \in \mathcal{G}(M)$ are projected label equivalent, $P_1 \approx_{\mathcal{P}} P_2$, if $\vec{P}^i \sim_{\mathcal{P}} \vec{P}^j$ and $k_i = k_j$ in the unique assignment $P_1 = P_{k_i}^i$, $P_2 = P_{k_j}^j$.

Therefore, in the running example we have that $P_1 \approx_{\mathcal{P}} P_2$, $R_1 \approx_{\mathcal{P}} R_2$, and so on.

Following [22], we are finally ready to extend EFL to FEPA, showing that the following result is also valid for semantics based on the law of mass action via $\rho = \cdot$.

Theorem 1. *Fix a FEPA model M and a tuple partition $\mathcal{P}$ of $\mathcal{G}(M)$. Then, $\sim_{\mathcal{P}}$ is a congruence relation with respect to $\parallel_L$, $\approx_{\mathcal{P}}$ is an equivalence relation on $\mathcal{G}(M)$ and $\mathcal{G}(M)/\approx_{\mathcal{P}}$ is exactly fluid lumpable.*

Proof. It is sufficient to note that the proofs of Theorems 2, 3 and 4 from [22] carry over in the case of $\rho = \cdot$. □

For instance, it holds that $\mathcal{G}(Sys_{\mathcal{E}})/\approx_{\mathcal{P}}$ yields the exactly fluid lumpable partition $\{\{P_1, \ldots, P_D\}, \{R_1, \ldots, R_D\}, \{Q\}\}$. This result gives us a tool which aggregates ODE systems to smaller ones. In Example 2, for instance, this permits recovering the solution of an ODE system of size $4D + 2$ by solving an aggregated ODE system of size $4 + 2$.

Furthermore, the characterisation of EFL can be shown also when $\rho = \cdot$.

Theorem 2. *Fix a well-posed FEPA model M, a tuple partition $\mathcal{P} = \{\vec{P}^1, \ldots, \vec{P}^N\}$ on $\mathcal{G}(M)$ and assume that $\vec{P}^i \sim_{\mathcal{P}} \vec{P}^j$. Then, P_k^i is semi-isomorphic to P_k^j for all $1 \le k \le K_i$.*

Proof. Let us fix a set of bijections $\sigma_l : ds(P_l^i) \to ds(P_l^j)$, $1 \le l \le K_i$, which establishes $\vec{P}^i \sim_{\mathcal{P}} \vec{P}^j$ and some $1 \le k \le K_i$. We will show that σ_k is a semi-isomorphism between P_k^i and P_k^j. For this, we fix some $P', P'' \in ds(P_k^i)$, an $\alpha \in \mathcal{A}$, define

$$V_P := \begin{cases} 1, & P \in \mathcal{B}(M) \wedge P \notin ds(P_k^i) \\ 1, & P = P' \\ 0, & P \in ds(P_k^i) \setminus \{P'\} \end{cases}$$

and assume first that $r_\alpha(P') > 0$. Under this assumption, it can be shown by means of structural induction on M that V satisfies $\mathcal{R}_\alpha(M, V, P') > 0$, cf. Lemma 1. Property b) of Definition 13 yields then

$$\sum_{P \in ds(P_k^i)} p_\alpha\big(P, P''\big)\mathcal{R}_\alpha(M, V, P) = \sum_{P \in ds(P_k^i)} p_\alpha\big(\sigma_k(P), \sigma_k\big(P''\big)\big)\mathcal{R}_\alpha\big(M, V^\sigma, \sigma_k(P)\big)$$

which implies (together with the definition of V)

$$p_\alpha\big(P', P''\big)\mathcal{R}_\alpha\big(M, V, P'\big) = p_\alpha\big(\sigma_k\big(P'\big), \sigma_k\big(P''\big)\big)\mathcal{R}_\alpha\big(M, V^\sigma, \sigma_k\big(P'\big)\big).$$

Since a) implies $\mathcal{R}_\alpha(M, V, P') = \mathcal{R}_\alpha(M, V^\sigma, \sigma_k(P'))$ and $\mathcal{R}_\alpha(M, V, P')$ is known to be positive, we infer $p_\alpha(P', P'') = p_\alpha(\sigma_k(P'), \sigma_k(P''))$. This and d) show then the desired equality

$$\sum_{P' \xrightarrow{(\alpha, r)} P''} r = \sum_{\sigma_k(P') \xrightarrow{(\alpha, r)} \sigma_k(P'')} r.$$

Instead, if $r_\alpha(P') = 0$, property d) implies $r_\alpha(\sigma_k(P')) = 0$ and the above equality trivially holds. □

The reverse implication does not hold in general. For instance, let us consider $P \stackrel{\text{def}}{=} (\alpha, r).Q$, $Q \stackrel{\text{def}}{=} (\beta, s).P$, and P' a primed copy of P. Then we have that P is (semi-)isomorphic to P' however the two fluid atoms cannot be related by a projected label equivalence in the model $P \parallel_{\{\alpha\}} P'$.

Using the last theorem, one can show that, under the condition of well-posedness, different exactly fluid lumpable partitions can be merged.

Theorem 3. *Fix a well-posed FEPA model M and a set of tuple partitions $S = \{\mathcal{P}_1, \ldots, \mathcal{P}_m\}$ of $\mathcal{G}(M)$. Then, the partition $\mathcal{G}(M)/(\approx_{\mathcal{P}_1} \cup \cdots \cup \approx_{\mathcal{P}_m})^*$ is exactly fluid lumpable.*

Proof. It is sufficient to note that the proof of Theorem 5 from [22] applies when $\rho = \cdot$. □

The importance of the above theorem is rooted in the fact that there exist EFL partitions that cannot be inferred using Theorem 1, see [22].

Remark 1. In what follows, we will assume that an EFL partition is established as in Theorem 1.

Ordinary fluid lumpability. EFL considers a partition of fluid atoms such that elements in the same part have the *same solution*. Instead, in ordinary fluid lumpability (OFL) *the sum of the solutions* of elements within the same part are fully recovered from the solution of a (smaller) ODE system consisting of one single ODE for a representative element of each part.

Definition 15 *(Ordinary fluid lumpability (OFL)).* Let M be a FEPA model and let $\{\mathcal{P}^1, \ldots, \mathcal{P}^n\}$ be a partition of $\mathcal{G}(M)$. The partition is called *ordinarily fluid lumpable* if there exist bijections

$$\sigma_{P_j^i} : ds\big(P_1^i\big) \to ds\big(P_j^i\big), \quad 1 \le i \le n,\ 1 \le j \le k_i$$

such that $\sigma_{P_1^i} \equiv \mathrm{id}_{ds(P_1^i)}$ and for all $\alpha \in \mathcal{A}$, $1 \le i \le n$, V and

$$V_P^\sigma := \begin{cases} \sum_{1 \le j \le k_i} V_{\sigma_{P_j^i}(P)}, & \exists 1 \le i \le n (P \in ds(P_1^i)) \\ 0, & \text{otherwise} \end{cases}$$

it holds that

i) $\sum_{1 \le j \le k_i} \mathcal{R}_\alpha(M, V, \sigma_{P_j^i}(P)) = \mathcal{R}_\alpha(M, V^\sigma, P)$ for all $P \in ds(P_1^i)$.
ii) $\sum_{1 \le j \le k_i} \sum_{P' \in ds(P_1^i)} p_\alpha(\sigma_{P_j^i}(P'), \sigma_{P_j^i}(P))\mathcal{R}_\alpha(M, V, \sigma_{P_j^i}(P')) = \sum_{P' \in ds(P_1^i)} p_\alpha(P', P)\mathcal{R}_\alpha(M, V^\sigma, P')$ for all $P \in ds(P_1^i)$.
iii) $r_\alpha(M, V) = r_\alpha(M, V^\sigma)$ and $r_\alpha(P_1^i) = r_\alpha(P_j^i)$ for all $1 \le j \le k_i$.

Intuitively, *i)* requires that the α-component rates out of $\sigma_{P^i_1}(P), \ldots, \sigma_{P^i_{k_i}}(P)$ are linear in V; *ii)* requires that the α-component rates into $\sigma_{P^i_1}(P), \ldots, \sigma_{P^i_{k_i}}(P)$ are linear in V; finally *iii)* requires that the α-apparent rate of M is linear in V.

We can now define and relate the lumped ODE system to the original one.

Theorem 4 *(ODE lumping). Let M be a FEPA model, $\{\mathcal{P}^1, \ldots, \mathcal{P}^n\}$ an ordinarily fluid lumpable partition of $\mathcal{G}(M)$, and V the ODE solution of M for a given initial condition $V(0)$. Define*

$$W_P := \sum_{1 \le j \le k_i} V_{\sigma_{P^i_j}(P)}, \quad 1 \le i \le n,\ P \in ds\big(P^i_1\big)$$

and

$$\overline{W}_P := \begin{cases} W_P, & \exists 1 \le i \le n (P \in ds(P^i_1)) \\ 0, & \text{otherwise} \end{cases}$$

for all $P \in \mathcal{B}(M)$. Then, W is the unique solution of the ODE system

$$\begin{aligned} \dot{W}_P &= \sum_{\alpha \in \mathcal{A}} \Bigg(\sum_{P' \in ds(P^i_1)} p_\alpha\big(P', P\big) \mathcal{R}_\alpha\big(M, \overline{W}, P'\big) - \mathcal{R}_\alpha\big(M, \overline{W}, P\big) \Bigg), \\ W_P(0) &= \sum_{1 \le j \le k_i} V_{\sigma_{P^i_j}(P)}(0), \end{aligned} \tag{6}$$

where $1 \le i \le n$ and $P \in ds(P^i_1)$. Hence,

$$\sum_{1 \le j \le k_i} V_{\sigma_{P^i_j}(P)}, \quad 1 \le i \le n,\ P \in ds\big(P^i_1\big),$$

can be recovered by solving the lumped ODE system (6).

Proof. It can be shown that the ODE system is Lipschitz, cf. Propositions 1 and 2. Consequently, the lumped ODE system (6) is Lipschitz too and the theorem of Picard–Lindelöf asserts then that (6) has a unique solution. Moreover, for all $1 \le i \le n$ and $P \in ds(P^i_1)$, it holds that

$$\begin{aligned} \dot{W}_P &= \sum_{1 \le j \le k_i} \dot{V}_{\sigma_{P^i_j}(P)} = \sum_{1 \le j \le k_i} \sum_{\alpha \in \mathcal{A}} \Bigg[-\mathcal{R}_\alpha\big(M, V, \sigma_{P^i_j}(P)\big) + \sum_{P' \in ds(P^i_1)} p_\alpha\big(\sigma_{P^i_j}(P'), \sigma_{P^i_j}(P)\big) \mathcal{R}_\alpha\big(M, V, \sigma_{P^i_j}(P')\big) \Bigg] \\ &\overset{i),ii)}{=} \sum_{\alpha \in \mathcal{A}} \Bigg(\sum_{P' \in ds(P^i_1)} p_\alpha\big(P', P\big) \mathcal{R}_\alpha\big(M, V^\sigma, P'\big) - \mathcal{R}_\alpha\big(M, V^\sigma, P\big) \Bigg) \\ &= \sum_{\alpha \in \mathcal{A}} \Bigg(\sum_{P' \in ds(P^i_1)} p_\alpha\big(P', P\big) \mathcal{R}_\alpha\big(M, \overline{W}, P'\big) - \mathcal{R}_\alpha\big(M, \overline{W}, P\big) \Bigg) \end{aligned}$$

and $W_P(0) = \sum_{1 \le j \le k_i} V_{\sigma_{P^i_j}(P)}(0)$. This yields the claim. □

For instance, let us consider again Example 1. It can be shown that the partition $\{\{P_1, \ldots, P_D\}, \{Q\}\}$ is an OFL partition of *Sys*. According to the above theorem, the aggregated ODE system, of size 4, is given by

$$\begin{aligned} \dot{W}_P &= -ruW_P \cdot W_Q + sW_{P'} & \dot{W}_{P'} &= +ruW_P \cdot W_Q - sW_{P'} \\ \dot{W}_Q &= -ruW_P \cdot W_Q + wW_{Q'} & \dot{W}_{Q'} &= +ruW_P \cdot W_Q - wW_{Q'} \end{aligned}$$

with initial condition

$$W_P(0) = \sum_{d=1}^{D} V_{P_d}(0) = \sum_{d=1}^{D} N_d$$

$$W_{P'}(0) = \sum_{d=1}^{D} V_{P'_d}(0) = 0$$

$$W_Q(0) = V_Q(0) = M$$
$$W_{Q'}(0) = V_{Q'}(0) = 0$$

It holds that $W_P(t) = \sum_{d=1}^{D} V_{P_d}(t)$, but each individual solution, $V_{P_d}(t)$, cannot be recovered.

The next theorem can be regarded as a congruence property of OFL with respect to the parallel composition of FEPA.

Theorem 5. *Fix two FEPA models M_1, M_2 and let $\{\mathcal{P}^1, \ldots, \mathcal{P}^n\}$ and $\{\mathcal{P}^{n+1}, \ldots, \mathcal{P}^{n+m+1}\}$ be ordinarily fluid lumpable partitions of $\mathcal{G}(M_1)$ and $\mathcal{G}(M_2)$, respectively. Then, thanks to the set of bijections*

$$\sigma_{P_j^i} : ds\big(P_1^i\big) \to ds\big(P_j^i\big), \quad 1 \le i \le n+m+1,\ 1 \le j \le k_i,$$

the partition $\{\mathcal{P}^1, \ldots, \mathcal{P}^n\} \cup \{\mathcal{P}^{n+1}, \ldots, \mathcal{P}^{n+m+1}\}$ of $\mathcal{G}(M_1 \parallel_L M_2)$ is also ordinarily fluid lumpable.

Proof. Let us fix an arbitrary V of $M = M_1 \parallel_L M_2$. Then, in the case of $\alpha \in L$ it holds that

$$\begin{aligned} r_\alpha(M_1 \parallel_L M_2, V) &= \rho\big(r_\alpha(M_1, V), r_\alpha(M_2, V)\big) \\ &\overset{iii)}{=} \rho\big(r_\alpha\big(M_1, V^\sigma\big), r_\alpha\big(M_2, V^\sigma\big)\big) = r_\alpha\big(M_1 \parallel_L M_2, V^\sigma\big), \end{aligned}$$

whereas, in the case of $\alpha \notin L$

$$\begin{aligned} r_\alpha(M_1 \parallel_L M_2, V) &= r_\alpha(M_1, V) + r_\alpha(M_2, V) \\ &\overset{iii)}{=} r_\alpha\big(M_1, V^\sigma\big) + r_\alpha\big(M_2, V^\sigma\big) = r_\alpha\big(M_1 \parallel_L M_2, V^\sigma\big). \end{aligned}$$

Let us assume without loss of generality that $P_1^i \in \mathcal{G}(M_1)$. Then, if $\alpha \in L$, for all $P \in ds(P_1^i)$ it holds that

$$\begin{aligned} \sum_{1\le j\le k_i} \mathcal{R}_\alpha\big(M, V, \sigma_{P_j^i}(P)\big) &= \sum_{1\le j\le k_i} \frac{\mathcal{R}_\alpha(M_1, V, \sigma_{P_j^i}(P))}{r_\alpha(M_1, V)} r_\alpha(M_1 \parallel_L M_2, V) \\ &\overset{iii)}{=} \sum_{1\le j\le k_i} \frac{\mathcal{R}_\alpha(M_1, V, \sigma_{P_j^i}(P))}{r_\alpha(M_1, V^\sigma)} r_\alpha\big(M_1 \parallel_L M_2, V^\sigma\big) \\ &\overset{ii)}{=} \sum_{1\le j\le k_i} \frac{\mathcal{R}_\alpha(M_1, V^\sigma, \sigma_{P_j^i}(P))}{r_\alpha(M_1, V^\sigma)} r_\alpha\big(M_1 \parallel_L M_2, V^\sigma\big) \\ &= \sum_{1\le j\le k_i} \mathcal{R}_\alpha\big(M, V^\sigma, \sigma_{P_j^i}(P)\big) \end{aligned}$$

and

$$\begin{aligned} &\sum_{1\le j\le k_i} \sum_{P'\in ds(P_1^i)} p_\alpha\big(\sigma_{P_j^i}(P'), \sigma_{P_j^i}(P)\big) \mathcal{R}_\alpha\big(M, V, \sigma_{P_j^i}(P')\big) \\ &= \sum_{1\le j\le k_i} \sum_{P'\in ds(P_1^i)} p_\alpha\big(\sigma_{P_j^i}(P'), \sigma_{P_j^i}(P)\big) \frac{\mathcal{R}_\alpha(M_1, V, \sigma_{P_j^i}(P'))}{r_\alpha(M_1, V)} r_\alpha(M, V) \\ &\overset{iii)}{=} \sum_{1\le j\le k_i} \sum_{P'\in ds(P_1^i)} p_\alpha\big(\sigma_{P_j^i}(P'), \sigma_{P_j^i}(P)\big) \frac{\mathcal{R}_\alpha(M_1, V, \sigma_{P_j^i}(P'))}{r_\alpha(M_1, V^\sigma)} r_\alpha\big(M, V^\sigma\big) \\ &\overset{ii)}{=} \sum_{1\le j\le k_i} \sum_{P'\in ds(P_1^i)} p_\alpha\big(\sigma_{P_j^i}(P'), \sigma_{P_j^i}(P)\big) \frac{\mathcal{R}_\alpha(M_1, V^\sigma, \sigma_{P_j^i}(P'))}{r_\alpha(M_1, V^\sigma)} r_\alpha\big(M, V^\sigma\big) \\ &= \sum_{1\le j\le k_i} \sum_{P'\in ds(P_1^i)} p_\alpha\big(\sigma_{P_j^i}(P'), \sigma_{P_j^i}(P)\big) \mathcal{R}_\alpha\big(M, V^\sigma, \sigma_{P_j^i}(P')\big). \end{aligned}$$

As similar calculations show that for $P_1^i \in \mathcal{G}(M_1)$ and for all $P \in ds(P_1^i)$

$$\sum_{1\le j\le k_i} \mathcal{R}_\alpha\big(M, V, \sigma_{P_j^i}(P)\big) = \sum_{1\le j\le k_i} \mathcal{R}_\alpha\big(M, V^\sigma, \sigma_{P_j^i}(P)\big)$$

and

$$\sum_{1\le j\le k_i}\sum_{P'\in ds(P_1^i)} p_\alpha\big(\sigma_{P_j^i}(P'),\sigma_{P_j^i}(P)\big)\mathcal{R}_\alpha\big(M,V,\sigma_{P_j^i}(P')\big)$$
$$=\sum_{1\le j\le k_i}\sum_{P'\in ds(P_1^i)} p_\alpha\big(\sigma_{P_j^i}(P'),\sigma_{P_j^i}(P)\big)\mathcal{R}_\alpha\big(M,V^\sigma,\sigma_{P_j^i}(P')\big)$$

in the case of $\alpha\notin L$, the proof is complete. □

Finally, similarly to EFL, the next theorem characterises OFL with respect to semi-isomorphism.

Theorem 6. *Fix a well-posed FEPA model M and assume that the partition $\{\mathcal{P}^1,\dots,\mathcal{P}^n\}$ of $\mathcal{G}(M)$ is ordinarily fluid lumpable. Then, P_1^i is semi-isomorphic to P_j^i for all $2\le j\le k_i$ and $1\le i\le n$.*

Proof. Let us fix arbitrary $P_0,P_1\in ds(P_1^i)$ and $\alpha\in\mathcal{A}$. Let us first assume that $r_\alpha(\sigma_{P_j^i}(P_0))>0$. Then, Lemma 1 asserts that the population function

$$W_P=\begin{cases}1, & P\in ds(P_j^i)\wedge P=\sigma_{P_j^i}(P_0)\\ 0, & P\in ds(P_j^i)\wedge P\neq\sigma_{P_j^i}(P_0)\\ 1, & P\notin ds(P_j^i)\end{cases}$$

satisfies $\mathcal{R}_\alpha(M,W,\sigma_{P_j^i}(P_0))>0$ and *i*) yields

$$0<\sum_{1\le l\le k_i}\mathcal{R}_\alpha\big(M,W,\sigma_{P_l^i}(P_0)\big)\overset{i)}{=}\mathcal{R}_\alpha\big(M,W^\sigma,P_0\big).$$

Since $r_\alpha(P_0)=r_\alpha(\sigma_{P_j^i}(P_0))>0$ because of property *iii*), it holds that $\mathcal{R}_\alpha(M,\widehat{V},P_0)>0$ for

$$\widehat{V}_P:=\begin{cases}1, & P\in ds(P_1^i)\wedge P=P_0\\ 0, & P\in ds(P_1^i)\wedge P\neq P_0\\ W_P^\sigma, & P\notin ds(P_1^i)\end{cases}$$

This is shown as Lemma 3 in Appendix A. Using

$$V_P:=\begin{cases}1, & P\in ds(P_j^i)\wedge P=\sigma_{P_j^i}(P_0)\\ 0, & P\in ds(P_j^i)\wedge P\neq\sigma_{P_j^i}(P_0)\\ 0, & P\in ds(P_1^i)\\ W_P^\sigma, & P\notin ds(P_1^i)\wedge P\notin ds(P_j^i)\end{cases}$$

we infer

$$\mathcal{R}_\alpha\big(M,V,\sigma_{P_j^i}(P_0)\big)=\sum_{1\le l\le k_i}\mathcal{R}_\alpha\big(M,V,\sigma_{P_l^i}(P_0)\big)\overset{i)}{=}\mathcal{R}_\alpha\big(M,V^\sigma,P_0\big)$$

and

$$\begin{aligned}p_\alpha\big(\sigma_{P_j^i}(P_0),\sigma_{P_j^i}(P_1)\big)\mathcal{R}_\alpha\big(M,V,\sigma_{P_j^i}(P_0)\big)&=\sum_{P'\in ds(P_1^i)}p_\alpha\big(\sigma_{P_j^i}(P'),\sigma_{P_j^i}(P_1)\big)\mathcal{R}_\alpha\big(M,V,\sigma_{P_j^i}(P')\big)\\&=\sum_{1\le l\le k_i}\sum_{P'\in ds(P_1^i)}p_\alpha\big(\sigma_{P_l^i}(P'),\sigma_{P_l^i}(P_1)\big)\mathcal{R}_\alpha\big(M,V,\sigma_{P_l^i}(P')\big)\\&\overset{ii)}{=}\sum_{P'\in ds(P_1^i)}p_\alpha\big(P',P_1\big)\mathcal{R}_\alpha\big(M,V^\sigma,P'\big)\\&=p_\alpha(P_0,P_1)\mathcal{R}_\alpha\big(M,V^\sigma,P_0\big).\end{aligned}$$

Hence, as the equality $\mathcal{R}_\alpha(M,V^\sigma,P_0)=\mathcal{R}_\alpha(M,\widehat{V},P_0)>0$ implies $p_\alpha(P_0,P_1)=p_\alpha(\sigma_{P_j^i}(P_0),\sigma_{P_j^i}(P_1))$, *iii*) yields the desired equality

$$\sum_{P_0 \xrightarrow{(\alpha,r)} P_1} r = \sum_{\sigma_{P_j^i}(P_0) \xrightarrow{(\alpha,r)} \sigma_{P_j^i}(P_1)} r.$$

If, instead, $r_\alpha(\sigma_{P_j^i}(P_0)) = 0$, the above equality follows from *iii*). □

Well-posedness is needed in Theorems 2 and 6. Let $\tilde{P}_d \stackrel{\text{def}}{=} (\alpha, r).\tilde{P}'_d + (\gamma, r/d).\tilde{P}'_d$ and $\tilde{P}'_d \stackrel{\text{def}}{=} (\beta, s).\tilde{P}_d$, i.e. $\tilde{P}_i$ and $\tilde{P}_j$ are not semi-isomorphic. Then, $((\tilde{P}_1 \parallel_{\{\alpha\}} R_1) \parallel_\emptyset \ldots \parallel_\emptyset (\tilde{P}_D \parallel_{\{\alpha\}} R_D)) \parallel_{\{\alpha,\gamma\}} Q$ and $(\tilde{P}_1 \parallel_\emptyset \ldots \parallel_\emptyset \tilde{P}_D) \parallel_{\{\alpha,\gamma\}} Q$ are ill-posed, while $(\tilde{P}_i, R_i) \sim_{\mathcal{P}} (\tilde{P}_j, R_j)$ and $\{\{\tilde{P}_1, \ldots, \tilde{P}_D\}, \{Q\}\}$ are fluid lumpable.

Although EFL and OFL lead to aggregations of the original ODE system, we wish to point out that both notions are intrinsically different, due to two reasons. First, EFL makes assumptions on the initial conditions, whereas OFL does not. Second, and more important, EFL allows to recover the solution of the original ODE systems, whereas OFL makes only statements about sums of the original ODE system.

4. Fluid ε-lumpability

We now study aggregations for models where certain fluid atoms can be made elements of the same partition block after a suitable perturbation of their parameters. In the case of EFL, we must allow for perturbation that affect both the rate parameters and the initial populations of the fluid atoms, because this notion of lumpability requires symmetries in both cases. In the case of OFL, instead, we only consider perturbations on rate parameters because there is no requirement on identical initial populations for fluid atoms that are to be aggregated.

At the basis of our investigation is the following comparison theorem which relates two ODE systems of the same size, where the vector field is made dependent on a vector of parameters, here denoted by ζ and ξ. Thus, for some norm $\|\cdot\|$, we interpret $\varepsilon = \|\xi - \zeta\|$ as the intensity of the perturbation on the rates of the same model. The two ODE systems may also have different initial conditions $\underline{x}_\zeta$ and $\underline{x}_\xi$, and we let $\delta = \|\underline{x}_\xi - \underline{x}_\zeta\|$. As discussed, this is needed to define our approximate version of EFL. The theorem states that, on a fixed time interval $[0; t]$, the distance between the two solutions depends *linearly* on both ε and δ. The presence of the perturbation on the initial conditions makes this result different from the one in [31], which instead concerns approximate aggregations only of OFL type.

Theorem 7. *Consider the ODE systems*

$$\begin{cases} \dot{x}_\zeta = f(\zeta, x_\zeta) \\ x_\zeta(0) = \underline{x}_\zeta \end{cases} \qquad \begin{cases} \dot{x}_\xi = f(\xi, x_\xi) \\ x_\xi(0) = \underline{x}_\xi \end{cases}$$

where f is assumed to be Lipschitz continuous in some domain $\mathcal{D} \subseteq \mathbb{R}^{n+m}$, both with respect to x and with respect to ζ with Lipschitz constant L_ζ and K_x respectively, that is

$$\begin{aligned} &\left\| f(\zeta, x) - f\left(\zeta, x'\right) \right\| \leq L_\zeta \left\| x - x' \right\|, \quad (\zeta, x), \left(\zeta, x'\right) \in \mathcal{D}, \\ &\left\| f(\zeta, x) - f\left(\zeta', x\right) \right\| \leq K_x \left\| \zeta - \zeta' \right\|, \quad (\zeta, x), \left(\zeta', x\right) \in \mathcal{D}. \end{aligned}$$

Let us assume further that both ODE systems have a solution on $[0; t]$, where $t > 0$, which remains in $\mathcal{D}$, and that $K := \sup_{0 \leq s \leq t} K_{x_\xi(s)} < \infty$. Then

$$\left\| x_\zeta(t) - x_\xi(t) \right\| \leq \left(\frac{\varepsilon K}{L_\zeta} + \delta \right) e^{L_\zeta t} - \frac{\varepsilon K}{L_\zeta}$$

if $\varepsilon = \|\xi - \zeta\|$ and $\delta = \|\underline{x}_\zeta - \underline{x}_\xi\|$.

Proof. We first show a modified version of Gronwall's inequality. To be more specific, let c_1, c_2, c_3 be positive constants and u a continuous function on $0 \leq t < \infty$ such that

$$u(t) \leq c_3 + c_2 t + c_1 \int_0^t u(s) ds \tag{7}$$

Then, it holds that

$$u(t) \leq \left(\frac{c_2}{c_1} + c_3 \right) e^{c_1 t} - \frac{c_2}{c_1}.$$

The inequality condition (7) can be written as

$$u(t) + \frac{c_2}{c_1} \leq \left(\frac{c_2}{c_1} + c_3\right) + c_1 \int_0^t \left(u(s) + \frac{c_2}{c_1}\right) ds.$$

As this yields together with $\tilde{u}(s) := u(s) + \frac{c_2}{c_1}$, $\tilde{\alpha} := \frac{c_2}{c_1} + c_3$ and $\tilde{v}(s) := c_1$

$$\tilde{u}(t) \leq \tilde{\alpha} + \int_0^t \tilde{u}(s)\tilde{v}(s) ds,$$

Gronwall's inequality ensures $\tilde{u}(t) \leq \tilde{\alpha} \cdot e^{\int_0^t \tilde{v}(s) ds}$ and we infer the auxiliary statement. Equipped with this, we observe that

$$\begin{aligned}
\left\| x_\zeta(t) - x_\xi(t) \right\| &\leq \|\underline{x}_\zeta - \underline{x}_\xi\| + \left\| \int_0^t f\left(\zeta, x_\zeta(s)\right) - f\left(\xi, x_\xi(s)\right) ds \right\| \\
&\leq \delta + \left\| \int_0^t f\left(\zeta, x_\zeta(s)\right) - f\left(\zeta, x_\xi(s)\right) ds \right\| + \left\| \int_0^t f\left(\zeta, x_\xi(s)\right) - f\left(\xi, x_\xi(s)\right) ds \right\| \\
&\leq \delta + L_\zeta \int_0^t \left\| x_\zeta(s) - x_\xi(s) \right\| ds + \varepsilon K t.
\end{aligned}$$

Thus, the claim follows from the auxiliary statement in the case of $u(s) := \|x_\zeta(s) - x_\xi(s)\|$, $c_3 := \delta$, $c_1 := L_\zeta$ and $c_2 := \varepsilon K$. □

Our goal is now to cast the fluid semantics of FEPA to the setting established in Theorem 7. To do so, we formally introduce the notion of perturbation on rates on FEPA models, achieved by enumerating all possible syntactic occurrences of rates in a model and by considering an operation of substitution.

Definition 16. For a FEPA model M, let $\nu(M)$ denote the vector of distinct occurrences of action rates in M, written $\nu(M) = (x_1, \ldots, x_i, \ldots, x_{|\nu(M)|})$. Then, for a $\xi \in \mathbb{R}_{>0}^{|\nu(M)|}$, the model $M(\xi)$ arises from M by replacing each x_i with ξ_i.

Theorem 7 can be applied to FEPA by proving that FEPA models induce globally Lipschitz ODE systems and have bounded ODE solutions.

Theorem 8. *Fix a FEPA model M, a $\zeta \in \mathbb{R}_{>0}^{|\nu(M)|}$, a population function $V^\zeta(0)$ and $c, t > 0$. Then, there exist $C_1, C_2 > 0$ such that $\|V^\xi(0)\|, \|\xi\| \leq c$ implies*

$$\max_{0 \leq s \leq t} \left\| V^\xi(s) - V^\zeta(s) \right\| \leq C_1 \|\xi - \zeta\| + C_2 \left\| V^\xi(0) - V^\zeta(0) \right\|,$$

where V^ξ and V^ζ refer to the ODE solutions of $M(\xi)$ and $M(\zeta)$, respectively.

Proof. Let us define the drift by

$$F_P(\xi, V) := \sum_{\alpha \in \mathcal{A}} \left(\sum_{P' \in \mathcal{B}(M)} p_\alpha(P', P) \mathcal{R}_\alpha(M, V, P') - \mathcal{R}_\alpha(M, V, P) \right).$$

Then, in the case of $\rho = \min$, we claim that $F(\xi, \cdot)$ and $F(\cdot, V)$ are globally Lipschitz. This is proven as Proposition 1 in the appendix. Then, given that K_V denotes the Lipschitz constant of $F(\cdot, V)$ for some fixed V, it holds that $\sup_{\|V\| \leq c} K_V < \infty$ for all $c > 0$. If, instead, $\rho = \cdot$, the function $F(\cdot, \cdot)$ is easily identified as locally Lipschitz. This is proven as Proposition 2 in the appendix. Then it can be shown by means of structural induction on M that

i) For all $P \in \mathcal{B}(M)$ there exists a nonnegative function ζ such that $\dot{V}_P \geq -V_P \zeta(V)$.
ii) For all $P \in \mathcal{G}(M)$ it holds that $\sum_{P' \in ds(P)} \dot{V}_{P'} = 0$.

Since *i)* ensures that $V_P \geq 0$ for all $P \in \mathcal{B}(M)$ and *ii)* yields the conservation of mass, this yields $\|V(t)\|_\infty \leq c$ for all $t \geq 0$, provided that $c := \max_{P \in \mathcal{G}(M)} \sum_{P' \in ds(P)} V_{P'}(0)$. Using this auxiliary statements, the overall claim readily follows from Theorem 7. □

Let us remark that the above result states that the perturbations on the rate parameters and on the initial conditions yield separate additive contributions to the aggregation error. While the former kind of perturbation can be related to analogous approximate aggregations for Markov chains, e.g., [4], the latter does not have a stochastic counterpart to the best of our knowledge. This is because altering the initial population of agents leads to a generator matrix of different size, while a perturbation on the rates preserves the matrix structure. In the fluid semantics, instead, both cases do not alter the structure of the ODE system, but only its parameters. Let us also notice that, in the above theorem, $M(\zeta)$ is arbitrary but fixed, whereas $M(\xi)$ varies. In general, the ODE system of $M(\xi)$ has the same size as that of $M(\zeta)$. Thus, we now focus on the more interesting situation where $M(\zeta)$ has either an exactly or an ordinarily fluid lumpable partition.

Definition 17 *(Fluid ε-lumpability).* Fix a FEPA model M and $\xi \in \mathbb{R}_{>0}^{|\nu(M)|}$. If $M(\zeta)$ has an exactly/ordinarily fluid lumpable partition $\{\mathcal{P}^1, \ldots, \mathcal{P}^n\}$ for some $\zeta \in \mathbb{R}_{>0}^{|\nu(M)|}$, $M(\xi)$ is said to be $\|\xi - \zeta\|$-exactly/ordinarily fluid lumpable with respect to some norm $\|\cdot\|$.

For instance, let us take $D = 2$ and, with obvious ordering of the rate occurrences, $\zeta = (r, s, r, s, u, w)$, for which the model (2) admits EFL whenever $V_{P_1}(0) = V_{P_2}(0)$ and $V_{P'_1}(0) = V_{P'_2}(0)$. Consider now the same model, where the rates are replaced with $\xi = (r + \varepsilon_1, s + \varepsilon_2, r, s, u, w)$. This model is ε-exactly fluid lumpable with $\varepsilon = \|(\varepsilon_1, \varepsilon_2, 0, 0, 0, 0)\|$. In general, an exactly/ordinarily fluid lumpable partition admits an infinity of ε-lumpable partitions; ε gives the measure of how close a given model is to error-free lumping.

Both ε-EFL and ε-OFL enjoy congruence.

Theorem 9 *(Congruence). Fix two FEPA models M_1, M_2 and assume that $\{\mathcal{P}_k^1, \ldots, \mathcal{P}_k^{n_k}\}$ is $\|\xi_k - \zeta_k\|$-exactly/ordinarily fluid lumpable in $\mathcal{G}(M_k(\xi_k))$ for some $\xi_k, \zeta_k \in \mathbb{R}_{>0}^{|\nu(M_k)|}$, and $k = 1, 2$. Then, for any $L \subseteq \mathcal{A}$, $\bigcup_{k=1}^{2}\{\mathcal{P}_k^1, \ldots, \mathcal{P}_k^{n_k}\}$ is $\|(\xi_1, \xi_2) - (\zeta_1, \zeta_2)\|$-exactly/ordinarily fluid lumpable in $\mathcal{G}(M_1 \parallel_L M_2)$.*

Proof. Theorem 1 shows the case of exact fluid lumpability, whereas Theorem 5 yields the case of ordinary fluid lumpability. □

Clearly, as an OFL partition does not depend on the initial values, a perturbation of initial values is interesting only in the case of EFL.

We turn now to a characterisation of ε-OFL and ε-EFL. It is natural consider an ε-extension of semi-isomorphism to relate fluid atoms that are isomorphic up to an appropriate perturbation of their rates.

Definition 18 *(ε-semi-isomorphism).* Two fluid atoms P and Q are ε-semi-isomorphic for some $\varepsilon > 0$, if there is a bijection $\sigma : ds(P) \to ds(Q)$ which satisfies

$$\left| \sum_{P_i \xrightarrow{(\alpha,r)} P_j} r - \sum_{\sigma(P_i) \xrightarrow{(\alpha,r)} \sigma(P_j)} r \right| \leq \varepsilon$$

for all $P_i, P_j \in ds(P)$ and $\alpha \in \mathcal{A}$. Such σ is called ε-semi-isomorphism.

Analogously to EFL and OFL, the following characterises ε-lumpability with respect to ε-semi-isomorphism.

Theorem 10. *For any well-posed FEPA model M and norm $\|\cdot\|$, there exists a $C > 0$ such that if $\{\mathcal{P}^1, \ldots, \mathcal{P}^n\}$ is a $\|\xi - \zeta\|$-exactly/ordinarily fluid lumpable partition of $M(\xi)$, where $\xi, \zeta \in \mathbb{R}_{>0}^{|\nu(M)|}$, then:*

1) *Any two fluid atoms P_j^i, $P_{j'}^i$ of $M(\xi)$ are $C\|\xi - \zeta\|$-semi-isomorphic;*
2) *In the special case where for all $\alpha \in \mathcal{A}$ and $P, P' \in \mathcal{B}(M)$ there is at most one α-transition from P to P' and $\|\cdot\| = \|\cdot\|_\infty$, 1) holds for $C = 1$.*

Proof. As $\{\mathcal{P}^1, \ldots, \mathcal{P}^n\}$ is an OFL/EFL partition of $\mathcal{G}(M(\zeta))$, Theorems 2 and 6 assure that the fluid atoms P_j^i, $P_{j'}^i$ in $M(\zeta)$ are semi-isomorphic. Moreover, there exists a $C' > 0$ such that $\|\cdot\|_\infty \leq C'\|\cdot\|$. For any $\alpha \in \mathcal{A}$ and $P, P' \in \mathcal{B}(M)$, let $N_{(P,\alpha,P')}$ denote the number of α-transitions from P to P' and $N := \max\{N_{(P,\alpha,P')} \mid P, P' \in \mathcal{B}(M) \wedge \alpha \in \mathcal{A}\}$. The constant $C := NC'$ yields then the claim. □

For instance, the above theorem ensures that P_d, $P_{d'}$ are $\|\xi - \zeta\|_\infty$-semi-isomorphic in $Sys(\xi)$, cf. (2), for all $\xi \in \mathbb{R}_{>0}^{|\nu(Sys)|}$, if $\zeta = (r, s, \ldots, r, s, r, w)$.

5. Numerical evaluation

In this section we provide some numerical evidence of the aggregation error introduced by ε-EFL and ε-OFL. Let us consider the FEPA model (2) where the fluid atoms are given by

$$P_d \stackrel{\text{def}}{=} (\alpha, r_d).P'_d \qquad P'_d \stackrel{\text{def}}{=} (\beta, s).P_d \qquad Q \stackrel{\text{def}}{=} (\alpha, r).Q' \qquad Q' \stackrel{\text{def}}{=} (\gamma, w).Q\,. \tag{8}$$

We arbitrarily chose the rates of the independent actions, fixing $s = 0.5$ and $w = 15.0$, while we varied the values of r_d. With this choice, this model can be interpreted as a high-level description of a *multi-class* service system where one resource, modelled by Q, can be accessed by different classes of clients, P_d, each with its own service demand characterised by r_d.

Our intent is to approximate ODEs systems where P_i and P_j are aggregated for some $1 \leq i, j \leq D$. Thus, in order to obtain non-isomorphic fluid atoms, we made r_d dependent on $1 \leq d \leq D$, setting $r_d = 1.0 + (d-1)\Delta$. Here, Δ is a parameter that was varied between 0.0005 and 0.1000 at 0.005 steps in our tests. In this way, it is directly proportional to the intensity of the perturbation. For instance, in a model with $D = 12$ and $\Delta = 0.1000$, we have $r_{10}/r_1 = 2.1$, showing a non-negligible difference between the rate parameters of fluid atom P_1 and those of P_{10}. In order to enforce asymmetry also in the initial populations, we made the initial populations of P_d components dependent on d. Specifically, the initial population function was set as $V_{P_d}(0) = 200 + (d-1)$, $V_{P'_d}(0) = 0$, $V_Q(0) = 400$, and $V_{Q'}(0) = 0$; thus, the P_d fluid atoms have initial populations separated by a few percent. For evaluating both ε-EFL and ε-OFL, we considered a perturbed model where r_d in (8) was made independent of d and set equal to the average value in the original model, i.e.,

$$\tilde{r}_d = 1.0 + (\Delta/D)\sum_{d=1}^{D}(d-1).$$

In such a perturbed model, all P_d fluid atoms are now isomorphic.

Assessment of ε-EFL. We considered different values of D to numerically evaluate the impact of different initial conditions on the quality of the aggregation of ε-EFL. Specifically, we set $D = 3, 6, 9, 12$. Let us recall that (2) has $2D + 2$ ODEs. For each value of D and Δ, the model solution was compared against that of the perturbed model with the initial population function set as follows: $V^{\varepsilon}_{P_d}(0) = 200 + (1/D)\sum_{d=1}^{D}(d-1)$, $V^{\varepsilon}_{P'_d}(0) = 0$, $V^{\varepsilon}_{Q}(0) = 400$, and $V^{\varepsilon}_{Q'}(0) = 0$. In this way, the initial population of P_d fluid atoms is made independent from d and is set equal to the average initial population across d, similarly to what done for the perturbation on r_d. It follows that, in the perturbed model, $\{\{P_1, \ldots, P_D\}, \{Q\}\}$ is an exactly fluid lumpable partition. Hence, the original model and the perturbed one are related by ε-EFL. For instance, the latter has the following aggregated ODE system for $\rho = \min$:

$$\begin{aligned}
\dot{V}^{\varepsilon}_{P} &= -\frac{1}{D}\min\left(D\tilde{r}_d V^{\varepsilon}_{P}, rV^{\varepsilon}_{Q}\right) + sV^{\varepsilon}_{P'}\\
\dot{V}^{\varepsilon}_{P'} &= +\frac{1}{D}\min\left(D\tilde{r}_d V^{\varepsilon}_{P}, rV^{\varepsilon}_{Q}\right) - sV^{\varepsilon}_{P'}\\
\dot{V}^{\varepsilon}_{Q} &= -\frac{1}{D}\min\left(D\tilde{r}_d V^{\varepsilon}_{P}, rV^{\varepsilon}_{Q}\right) + wV^{\varepsilon}_{Q'}\\
\dot{V}^{\varepsilon}_{Q'} &= +\frac{1}{D}\min\left(D\tilde{r}_d V^{\varepsilon}_{P}, rV^{\varepsilon}_{Q}\right) - wV^{\varepsilon}_{Q}
\end{aligned}$$

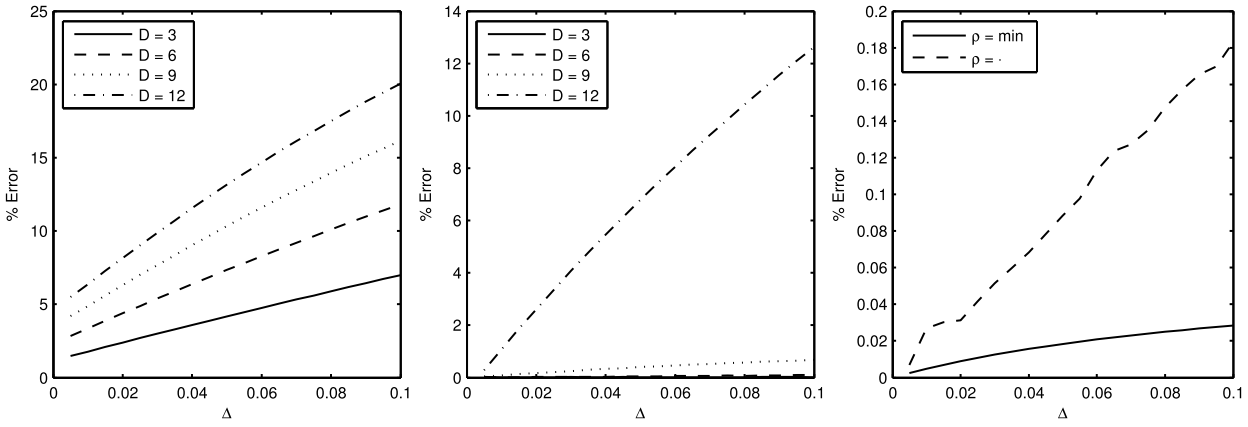
with initial conditions $V^{\varepsilon}_{P}(0) = V^{\varepsilon}_{P_1}(0) = \cdots = V^{\varepsilon}_{P_D}(0)$ and $V^{\varepsilon}_{P'}(0) = 0$. Hence, this implies that $V^{\varepsilon}_{P}(t) = V^{\varepsilon}_{P_1}(t) = \cdots = V^{\varepsilon}_{P_D}(t)$ and $V^{\varepsilon}_{P'}(t) = V^{\varepsilon}_{P'_1}(t) = \cdots = V^{\varepsilon}_{P'_D}(t)$ for all t. Both models were solved over the time interval [0; 100], so as to ensure convergence of the ODE solution to equilibrium for all parameterisations considered. Solutions were registered at 0.2 time steps. The approximation relative error for ε-EFL is as:

$$100 \times \max_{t\in\{0,0.02,\ldots,100\}} \max_{S\in\{P_1,\ldots,P_d,Q\}} \frac{|V_S(t) - V^{\varepsilon}_S(t)|}{V_S(0)},$$

where $V_S(t)$ is the solution of the original model and $V^{\varepsilon}_S(t)$ is the corresponding solution in the perturbed one. The absolute difference is normalised with respect to the total population of the fluid atom.

The results are presented in Figs. 1a and 1b, for $\rho = \min$ and $\rho = \cdot$, respectively. In both cases, we observe a linear growth of the error as a function of the perturbation Δ. For any fixed D, the case $\rho = \cdot$ yields more accurate aggregates than $\rho = \min$, with particularly small errors for $D = 3, 6, 9$. These tests show that even non-negligible perturbations (i.e., up to Δ ca 0.04) can produce acceptable errors (i.e., less than 10%) in practice.

Assessment of ε-OFL. Analogous tests were performed for the assessment of ε-OFL, since in the perturbed model $\{\{P_1, \ldots, P_D\}, \{Q\}\}$ is also an ordinarily fluid lumpable partition. For instance, using the construction in Theorem 4 and taking $\rho = \cdot$, the (approximately) aggregated ODE system is given by



(a) ε-EFL for $\rho = \min$ (b) ε-EFL for $\rho = \cdot$ (c) ε-OFL, for $D = 12$

Fig. 1. Numerical evaluation of ε-lumpability.

$$\dot{W}^{\varepsilon}_{P} = -r \cdot \tilde{r}_d W^{\varepsilon}_{P} W^{\varepsilon}_{Q} + s W^{\varepsilon}_{P'}$$
$$\dot{W}^{\varepsilon}_{P'} = +r \cdot \tilde{r}_d W^{\varepsilon}_{P} W^{\varepsilon}_{Q} - s W^{\varepsilon}_{P'}$$
$$\dot{W}^{\varepsilon}_{Q} = -r \cdot \tilde{r}_d W^{\varepsilon}_{P} W^{\varepsilon}_{Q} + w W^{\varepsilon}_{Q'}$$
$$\dot{W}^{\varepsilon}_{Q'} = +r \cdot \tilde{r}_d W^{\varepsilon}_{P} W^{\varepsilon}_{Q} - w W^{\varepsilon}_{Q}$$

with initial conditions $W^{\varepsilon}_{P}(0) = \sum_{d=1}^{D} W_{P_d}(0)$, $W^{\varepsilon}_{P'}(0) = 0$, $W^{\varepsilon}_{Q}(0) = V_Q(0)$, and $W^{\varepsilon}_{Q'}(0) = V'_Q(0) = 0$. As discussed, unlike ε-EFL, ε-OFL *does not* depend on the initial population function. This is why in our tests the initial conditions were not changed in the perturbed model. Furthermore, we analysed only the case $D = 12$, which yielded the worst accuracy in ε-EFL; the other cases showed the same errors (up to numerical precision of the ODE solver). A different error metric was used, to reflect the fact that OFL involves sums of ODE solutions of the unaggregated model. The approximation relative error is defined as:

$$100 \times \max_{t \in \{0, 0.02, \ldots, 100\}} \max\left\{ \frac{|\sum_{d=1}^{D} V_{P_d}(t) - W^{\varepsilon}_{P}(t)|}{\sum_{d=1}^{D} V_{P_d}(0)}, \frac{|V_Q(t) - W^{\varepsilon}_{Q}(t)|}{V_Q(0)} \right\}.$$

The numerical results are shown in Fig. 1c. Overall, both for $\rho = \min$ and $\rho = \cdot$, the ε-OFL appears to be much more robust, with negligible errors across all values of Δ.

6. Related work

The closest related work to this paper has been discussed in some detail in Section 1. The aim of this section, instead, is to put our contribution in a broader context regarding aggregations of differential equations. With respect to the two exact notions of aggregation herein developed, the symmetries captured by EFL are specific to process algebra to the best of our knowledge. Instead, OFL can be seen as a process-algebraic instance of the theory of ODE lumpability presented in [35]. In its generality, this theory concerns nonlinear and autonomous ODE systems which are aggregated by means of a constant matrix applied to the variables of the original ODE system. Therefore, this may yield aggregated ODE variables that are a linear combination of the original ones. In this paper, we use aggregation matrices that are induced by a partition on the original system, thus essentially considering sums of the original variables. Approximate aggregations of ODE systems have also been studied in a general setting. Some techniques require a-priori knowledge of the model behaviour. For instance, singular perturbation theory and quasi-equilibrium techniques allow for model reduction if the ODE variables can be partitioned in two blocks according to the relative speed at which they evolve (e.g., [36]). Approaches which do not require the knowledge of multiple time scales are instead reviewed by Antoulas in [37]. For nonlinear systems, some of these methods, for instance balanced truncation, typically require the availability of *measurements* from the original ODE system in order to identify its relevant dynamics [38]. In [39] a model order reduction approach is presented which provides a-priori error bounds, which therefore does not require solving the original model. However, the class of nonlinear functions supported, so-called kernel expansions, do not encompass those used in FEPA.

Concurrency theoretic notions of behavioural equivalence and ODE model order reduction have cross-fertilised already in the literature. Most notable is the work of Pappas and co-authors who have brought the ideas of simulation and bisimulation to the world of control theory and dynamical systems, e.g., [40–42]. However, these works do not consider a higher level language that maps onto ODE systems. Rather, the dynamical evolution of an ODE system is interpreted as a labelled transition system with an uncountable state space. Instead, in this paper the labelled transition system under consideration

is the finite—typically very small—discrete state space of a fluid atom which induces the differential equations. Our reasoning occurs at the process-algebra level, studying the behaviour of the fluid atoms, rather than directly the underlying ODE system. Moreover, the setting is different. While they deal with a state-space representation with an explicit output map, e.g., the matrix C in the linear dynamical system $\dot{x} = Ax + Bu$, $y = Cx$. By contrast, in this paper we work with a nonlinear system in the form $\dot{x} = A(x)$ (with A a nonlinear vector field).

7. Conclusion

This paper has studied the problem of performing aggregations of ODE systems induced by a process algebra model. We have defined a process algebra that uniformly treats two different dynamics of interaction. It allows to capture models of performance of computing systems, using the minimum-based semantics of the process algebra PEPA, as well as models of chemical reaction networks, implementing a product-based semantics that captures the law of mass action. We have extended previous work on exact fluid lumpability by introducing the alternative notion of ordinary fluid lumpability. This allows to reduce a model exactly, at the cost of losing track of the distinct state of the variables to be aggregated, only preserving their sums. We have studied approximate variants by allowing models with heterogeneous processes to be treated as homogeneous models by appropriate perturbations of rate parameters and the initial populations. Although the numerical results suggest that this aggregation can be robust in practice, tightening of the theoretical error bound is part of future work for increasing the a-priori confidence on the practical usefulness of these techniques.

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Appendix A

The following lemmas are used in the proofs of Theorems 2 and 6.

Lemma 1. *Fix a well-posed FEPA model M, one of its fluid atoms P^0, a $P' \in ds(P^0)$ and assume that $r_\alpha(P') > 0$. Then, $\mathcal{R}_\alpha(M, V, P') > 0$ for the population function*

$$V_P := \begin{cases} 1, & P \notin ds(P^0) \\ 1, & P \in ds(P^0) \wedge P = P' \\ 0, & P \in ds(P^0) \wedge P \neq P' \end{cases}$$

Proof. We prove this by structural induction on M.

- $M = P$: Since M has then only one fluid atom, i.e. $P^0 = P$, the claim follows with $r_\alpha(P') > 0$.
- $M = M_1 \parallel_L M_2$: We assume w.l.o.g. that $P^0 \in \mathcal{G}(M_1)$. Since the case $\alpha \notin L$ follows directly from the I.H., we focus on the case $\alpha \in L$. Let us denote by V_i the M_i-part of V. Since $\mathcal{R}_\alpha(M_1, V_1, P') > 0$ by I.H., we infer $r_\alpha(M_1, V_1) > 0$. Moreover, the well-posedness of M yields $r_\alpha(M_2, V_2) > 0$. (Note that well-posedness guarantees only the existence of some V_2' such that $r_\alpha(M_2, V_2') > 0$. However, this implies $r_\alpha(M_2, V_2) > 0$, since all populations of V_2 are positive.) This yields $\rho(r_\alpha(M_1, V_1), r_\alpha(M_2, V_2)) > 0$, implying $\mathcal{R}_\alpha(M, V, P') > 0$. □

Lemma 2. *Let M be a FEPA model, $P^0 \in \mathcal{G}(M)$, $P' \in ds(P^0)$ satisfying $r_\alpha(P') > 0$ and V a population function of M such that $r_\alpha(M, V) > 0$. Then, it holds that $r_\alpha(M, \widehat{V}) > 0$, where*

$$\widehat{V}_P = \begin{cases} 1, & P \in ds(P^0) \wedge P = P' \\ 0, & P \in ds(P^0) \wedge P \neq P' \\ V_P, & P \notin ds(P^0) \end{cases}$$

Proof. We prove the claim using structural induction.

- $M = P^0$: the claim follows with $r_\alpha(P') > 0$.
- $M = M_1 \parallel_L M_2$: We assume without loss of generality that $P^0 \in \mathcal{G}(M_1)$. Then, it holds that $r_\alpha(M_2, V) = r_\alpha(M_2, \widehat{V})$.
  - $\alpha \in L$: Note that $0 < r_\alpha(M_1 \parallel_L M_2, V) = \rho(r_\alpha(M_1, V), r_\alpha(M_2, V))$ implies $r_\alpha(M_1, V) > 0$ and $r_\alpha(M_2, V) > 0$. As $r_\alpha(M_1, \widehat{V}) > 0$ by I.H., it holds that $\rho(r_\alpha(M_1, \widehat{V}), r_\alpha(M_2, \widehat{V})) > 0$.
  - $\alpha \notin L$: As the claim is trivial in the case of $r_\alpha(M_2, V) > 0$, we may assume that $r_\alpha(M_2, V) = 0$. Then, $r_\alpha(M_1 \parallel_L M_2, \widehat{V}) = r_\alpha(M_1, \widehat{V})$ and the claim follows with the induction hypothesis. □

Lemma 3. *Let M be a FEPA model, $P^0 \in \mathcal{G}(M)$, $P' \in ds(P^0)$ satisfying $r_\alpha(P') > 0$ and V a population function of M such that $\mathcal{R}_\alpha(M, V, P') > 0$. Then, it holds that $\mathcal{R}_\alpha(M, \widehat{V}, P') > 0$, where*

$$\widehat{V}_P = \begin{cases} 1, & P \in ds(P^0) \wedge P = P' \\ 0, & P \in ds(P^0) \wedge P \neq P' \\ V_P, & P \notin ds(P^0) \end{cases}$$

Proof. We prove the claim using structural induction.

- $M = P^0$: The claim follows with $r_\alpha(P') > 0$.
- $M = M_1 \parallel_L M_2$: We assume without loss of generality that $P^0 \in \mathcal{G}(M_1)$. Then, it holds that $r_\alpha(M_2, V) = r_\alpha(M_2, \widehat{V})$.
  - $\alpha \in L$: The I.H., Lemma 2 and

$$0 < \mathcal{R}_\alpha\big(M, V, P'\big) = \frac{\mathcal{R}_\alpha(M_1, V, P')}{r_\alpha(M_1, V)} \rho\big(r_\alpha(M_1, V), r_\alpha(M_2, V)\big)$$

    imply then

$$0 < \frac{\mathcal{R}_\alpha(M_1, \widehat{V}, P')}{r_\alpha(M_1, \widehat{V})} \rho\big(r_\alpha(M_1, \widehat{V}), r_\alpha(M_2, \widehat{V})\big) = \mathcal{R}_\alpha\big(M, \widehat{V}, P'\big)$$

  - $\alpha \notin L$: It holds that $0 < \mathcal{R}_\alpha(M, V, P') = \mathcal{R}_\alpha(M_1, V, P')$ and $\mathcal{R}_\alpha(M, \widehat{V}, P') = \mathcal{R}_\alpha(M_1, \widehat{V}, P')$. Hence, the I.H. yields the claim. □

The statements below are used in the proof of Theorem 8.

Proposition 1. *Let us assume that $\rho = \min$. For a FEPA model $M \equiv M(\xi)$ and*

$$F_P(\xi, V) := \sum_{\alpha \in \mathcal{A}} \Bigg(\sum_{P' \in \mathcal{B}(M)} p_\alpha\big(P', P\big) \mathcal{R}_\alpha\big(M, V, P'\big) - \mathcal{R}_\alpha(M, V, P) \Bigg),$$

$F(\xi, \cdot)$ and $F(\cdot, V)$ are globally Lipschitz. Moreover, given that K_V denotes the Lipschitz constant of $F(\cdot, V)$ for some fixed V, it holds that $\sup_{\|V\| \leq c} K_V < \infty$ for all $c > 0$.

Proof. The first claim follows from Lemma B.1 in [43]. We show the second claim by exchanging the roles of parameters and variables in the proof of Lemma B.1. Specifically, one shows first that for each $Q \in \mathcal{B}(M)$ and $\alpha \in \mathcal{A}$ the set $\mathbb{R}_{>0}^{|\nu(M)|}$ can be covered by closed convex subsets $A_1, \ldots, A_I$ such that for a given $1 \leq \iota \leq I$, it holds that

$$\mathcal{R}_\alpha(M, V, Q) = V_Q\, r_\alpha(Q)(\xi) \prod_{n=1}^{D} \frac{b_n(\xi, V)}{a_n(\xi, V)}$$

for all $\xi \in A_\iota$, where $D \geq 1$ and $a_1, b_1, \ldots, a_n, b_n$ are apparent rates which satisfy

$$a_n(\xi, V) \geq b_n(\xi, V) \wedge a_n(\xi, V) \geq V_Q\, r_\alpha(Q)(\xi) \prod_{m=1}^{n-1} \frac{b_m(\xi, V)}{a_m(\xi, V)}$$

for all $1 \leq n \leq D$. As $r_\alpha(Q)(\xi) = \sum_{k \in S} \xi_k$ for some set $S \subseteq \{1, \ldots, |\nu(M)|\}$, the first equation rewrites to

$$\mathcal{R}_\alpha(M, V, Q) = V_Q \sum_{k \in S} \xi_k \prod_{n=1}^{D} \frac{b_n(\xi, V)}{a_n(\xi, V)}.$$

From the definition of $F_P(\cdot, V)$ it becomes evident that we have to consider also $p_\alpha(Q, P)(\xi)\mathcal{R}_\alpha(M, V, Q)$, where $Q \in \mathcal{B}(M)$. Noting that

$$r_\alpha(Q)(\xi) \geq p_\alpha(Q, P)(\xi) r_\alpha(Q)(\xi) = \sum_{Q \xrightarrow{(\alpha, \xi_i)} P} \xi_i = \sum_{k \in S'} \xi_k$$

for some set $S' \subseteq \{1, \ldots, |\nu(M)|\}$, we infer

$$p_\alpha(Q, P)(\xi)\mathcal{R}_\alpha(M, V, Q) = V_Q \sum_{k \in S'} \xi_k \prod_{n=1}^{D} \frac{b_n(\xi, V)}{a_n(\xi, V)}$$

and

$$a_n(\xi, V) \geq V_Q\, r_\alpha(Q)(\xi) \prod_{m=1}^{n-1} \frac{b_m(\xi, V)}{a_m(\xi, V)} \geq V_Q \sum_{k\in S'} \xi_k \prod_{m=1}^{n-1} \frac{b_m(\xi, V)}{a_m(\xi, V)}$$

for all $1 \leq n \leq D$, meaning that both $p_\alpha(Q, P)(\xi)\mathcal{R}_\alpha(M, V, Q)$ and $\mathcal{R}_\alpha(M, V, Q)$ belong to the same class of functions.

Clearly, the function $f(\xi, V) := V_Q \sum_{k\in S} \xi_k \prod_{n=1}^{D} \frac{b_n(\xi,V)}{a_n(\xi,V)}$ is continuous in all $\xi \in A_\iota$. Moreover, each $\mathrm{int}(A_\iota)$ may be assumed to be nonempty: if $\xi \in A_i$ and $\mathrm{int}(A_i) = \emptyset$, there exists a sequence $(\xi^n)_n$ in $\mathbb{R}_{>0}^{|\nu(M)|} \setminus A_i \subseteq \bigcup_{\iota\neq i} A_\iota$ which converges to ξ. As $\bigcup_{\iota\neq i} A_\iota$ is closed, it follows that $\xi \in \bigcup_{\iota\neq i} A_\iota$, meaning that $\bigcup_{\iota\neq i} A_\iota$ covers already $\mathbb{R}_{>0}^{|\nu(M)|}$. Thus, A_ι can be disregarded.

Now, for each partial derivative $\partial_{\xi_j} f(\cdot, V)$ we give a bound on $\mathrm{int}(A_\iota)$ which depends only on M and V. For this, let us fix some $\xi \in \mathrm{int}(A_\iota)$. Then it holds that

$$\partial_{\xi_j} f(\xi, V) = \begin{cases} V_Q\, c_j \prod_{n=1}^{D} \frac{b_n(\xi,V)}{a_n(\xi,V)} + (V_Q \sum_{k\in S} \xi_k)\partial_{\xi_j} \prod_{n=1}^{D} \frac{b_n(\xi,V)}{a_n(\xi,V)}, & j \in S \\ (V_Q \sum_{k\in S} \xi_k)\partial_{\xi_j} \prod_{n=1}^{D} \frac{b_n(\xi,V)}{a_n(\xi,V)}, & j \notin S \end{cases}$$

Using $F[n](\xi, V) := \prod_{m=1}^{n} \frac{b_m(\xi,V)}{a_m(\xi,V)}$ for $0 \leq n \leq D$ we infer

$$\partial_{\xi_j} F[n] = \frac{F[n-1]}{a_n}\partial_{\xi_j} b_n - \frac{F[n]}{a_n}\partial_{\xi_j} a_n + \frac{b_n}{a_n}\partial_{\xi_j} F[n-1].$$

Thus, the above inequalities yield

$$\left|\partial_{\xi_j} F[n](\xi, V)\left(V_Q \sum_{k\in S} \xi_k\right)\right| \leq \left|\partial_{\xi_j} b_n(\xi, V)\right| + \left|\partial_{\xi_j} a_n(\xi, V)\right| + \left|\partial_{\xi_j} F[n-1](\xi, V)\left(V_Q \sum_{k\in S} \xi_k\right)\right|$$

and we conclude

$$\left|\partial_{\xi_j} f(\xi, V)\right| \leq \sum_{n=1}^{D} \left|\partial_{\xi_j} b_n(\xi, V)\right| + \sum_{n=1}^{D} \left|\partial_{\xi_j} a_n(\xi, V)\right| \leq C\|V\|_\infty$$

for some $C > 0$ which depends on j and $Q \in \mathcal{B}(M)$. One proceeds then similarly to the proof of Lemma B.1 from [43]. □

Proposition 2. *Let us assume that $\rho = \cdot$. Then, for a FEPA model M and*

$$F_P(\xi, V) := \sum_{\alpha\in\mathcal{A}} \left(\sum_{P'\in\mathcal{B}(M)} p_\alpha(P', P)\mathcal{R}_\alpha(M, V, P') - \mathcal{R}_\alpha(M, V, P) \right),$$

it holds that $F(\cdot,\cdot)$ is locally Lipschitz.

Proof. As in Proposition 1, using structural induction one shows that there exists a $\mathcal{D}(M) \geq 1$ such that for each $Q \in \mathcal{B}(M)$ and $\alpha \in \mathcal{A}$ it holds that

$$\mathcal{R}_\alpha(M(\xi), V, Q) = V_Q\, r_\alpha(Q)(\xi) \prod_{n=1}^{D} a_n(\xi, V)$$

for some $1 \leq D \leq \mathcal{D}(M)$ and apparent rate functions $a_1, \ldots, a_n$. Since $r_\alpha(Q)(\xi) = \sum_{k\in S} \xi_k$ for some set $S \subseteq \{1, \ldots, |\nu(M)|\}$ and

$$p_\alpha(Q, P)(\xi) r_\alpha(Q)(\xi) = \sum_{Q \xrightarrow{(\alpha,\xi_i)} P} \xi_i = \sum_{k\in S'} \xi_k$$

for some set $S' \subseteq \{1, \ldots, |\nu(M)|\}$, this yields

$$\mathcal{R}_\alpha(M(\xi), V, Q) = V_Q \sum_{k\in S} \xi_k \prod_{n=1}^{D} a_n(\xi, V)$$

and

$$p_\alpha(Q, P)(\xi)\mathcal{R}_\alpha(M(\xi), V, Q) = V_Q \sum_{k\in S'} \xi_k \prod_{n=1}^{D} a_n(\xi, V).$$

Obviously, $F(\cdot,\cdot)$ is partially continuously differentiable and the proof is complete. □

References

[1] R. Milner, Communication and Concurrency, Prentice–Hall, Inc., Upper Saddle River, NJ, USA, 1989.
[2] H. Hermanns, M. Rettelbach, Syntax, semantics, equivalences, and axioms for MTIPP, in: Proceedings of Process Algebra and Probabilistic Methods, Erlangen, 1994, pp. 71–87.
[3] J. Hillston, A Compositional Approach to Performance Modelling, Cambridge University Press, New York, NY, USA, 1996.
[4] P. Buchholz, Exact and ordinary lumpability in finite Markov chains, J. Appl. Probab. 31 (1) (1994) 59–75.
[5] M. Bernardo, A survey of Markovian behavioral equivalences, in: M. Bernardo, J. Hillston (Eds.), Formal Methods for Performance Evaluation, in: Lect. Notes Comput. Sci., vol. 4486, Springer, Berlin, Heidelberg, 2007, pp. 180–219.
[6] C.-C. Jou, S. Smolka, Equivalences, congruences, and complete axiomatizations for probabilistic processes, in: CONCUR, in: Lect. Notes Comput. Sci., vol. 458, 1990, pp. 367–383.
[7] J. Desharnais, R. Jagadeesan, V. Gupta, P. Panangaden, The metric analogue of weak bisimulation for probabilistic processes, in: LICS, 2002, pp. 413–422.
[8] F. van Breugel, J. Worrell, Towards quantitative verification of probabilistic transition systems, in: ICALP, in: Lect. Notes Comput. Sci., vol. 2076, Springer, 2001, pp. 421–432.
[9] A. Di Pierro, C. Hankin, H. Wiklicky, Quantitative relations and approximate process equivalences, in: CONCUR, 2003, pp. 498–512.
[10] A. Aldini, M. Bravetti, R. Gorrieri, A process-algebraic approach for the analysis of probabilistic noninterference, J. Comput. Secur. 12 (2) (2004) 191–245.
[11] V. Gupta, R. Jagadeesan, P. Panangaden, Approximate reasoning for real-time probabilistic processes, Log. Methods Comput. Sci. 2 (1) (2014).
[12] J. Hillston, Fluid flow approximation of PEPA models, in: Proceedings of Quantitative Evaluation of Systems, IEEE Computer Society Press, 2005, pp. 33–43.
[13] M. Kwiatkowski, I. Stark, The continuous pi-calculus: a process algebra for biochemical modelling, in: Proceedings of Computational Methods in Systems Biology, in: Lect. Notes Comput. Sci., vol. 5307, 2008, pp. 103–122.
[14] L. Cardelli, On process rate semantics, Theor. Comput. Sci. 391 (2008) 190–215.
[15] F. Ciocchetta, J. Hillston, Bio-PEPA: a framework for the modelling and analysis of biological systems, Theor. Comput. Sci. 410 (33–34) (2009) 3065–3084.
[16] R.A. Hayden, J.T. Bradley, A fluid analysis framework for a Markovian process algebra, Theor. Comput. Sci. 411 (22–24) (2010) 2260–2297.
[17] M. Tribastone, S. Gilmore, J. Hillston, Scalable differential analysis of process algebra models, IEEE Trans. Softw. Eng. 38 (1) (2012) 205–219.
[18] M. Tschaikowski, M. Tribastone, Tackling continuous state-space explosion in a Markovian process algebra, Theor. Comput. Sci. 517 (2014) 1–33.
[19] M. Aoki, Control of large-scale dynamic systems by aggregation, IEEE Trans. Autom. Control 13 (3) (1968) 246–253.
[20] Y. Iwase, S.A. Levin, V. Andreasen, Aggregation in model ecosystems I: perfect aggregation, Ecol. Model. 37 (1987).
[21] M.S. Okino, M.L. Mavrovouniotis, Simplification of mathematical models of chemical reaction systems, Chem. Rev. 2 (98) (1998) 391–408.
[22] M. Tschaikowski, M. Tribastone, Exact fluid lumpability for Markovian process algebra, in: CONCUR, in: Lect. Notes Comput. Sci., vol. 7545, 2012, pp. 380–394.
[23] M. Tschaikowski, M. Tribastone, Exact fluid lumpability in Markovian process algebra, Theor. Comput. Sci. 538 (2014) 140–166.
[24] V. Danos, J. Feret, W. Fontana, R. Harmer, J. Krivine, Abstracting the differential semantics of rule-based models: exact and automated model reduction, in: LICS, 2010, pp. 362–381.
[25] V. Danos, C. Laneve, Formal molecular biology, Theor. Comput. Sci. 325 (1) (2004) 69–110.
[26] J.R. Faeder, M.L. Blinov, W.S. Hlavacek, Rule-Based Modeling of Biochemical Systems with BioNetGen, Methods Mol. Biol., vol. 500, 2009, pp. 113–167.
[27] M. Tribastone, A fluid model for layered queueing networks, IEEE Trans. Softw. Eng. 39 (6) (2013) 744–756.
[28] V. Galpin, Continuous approximation of PEPA models and Petri nets, Int. J. Comput. Aided Eng. Technol. 2 (2010) 324–339.
[29] R.K. Watson, On an epidemic in a stratified population, J. Appl. Probab. 9 (3) (1972) 659–666.
[30] P. Wang, M.C. González, C.A. Hidalgo, A.-L. Barabási, Understanding the spreading patterns of mobile phone viruses, Science 324 (5930) (2009) 1071–1076.
[31] G. Iacobelli, M. Tribastone, Lumpability of fluid models with heterogeneous agent types, in: DSN, 2013, pp. 1–11.
[32] M. Tschaikowski, M. Tribastone, Extended differential aggregations in process algebra for performance and biology, in: Twelfth International Workshop on Quantitative Aspects of Programming Languages and Systems (QAPL), 2014.
[33] Rocco De Nicola, Diego Latella, Michele Loreti, A uniform definition of stochastic process calculi, ACM Comput. Surv. 46 (1) (2013) 5.
[34] P. Buchholz, Markovian process algebra: composition and equivalence, in: Proc. 2nd PAPM Workshop, Erlangen, Germany, 1994.
[35] J. Toth, G. Li, H. Rabitz, A.S. Tomlin, The effect of lumping and expanding on kinetic differential equations, SIAM J. Appl. Math. 57 (6) (1997) 1531–1556.
[36] F. Verhulst, Methods and Applications of Singular Perturbations: Boundary Layers and Multiple Timescale Dynamics, Texts Appl. Math., vol. 50, Springer, New York, 2005.
[37] A. Antoulas, Approximation of Large-Scale Dynamical Systems, Advances in Design and Control, SIAM, 2005.
[38] S. Lall, J.E. Marsden, S. Glavaški, A subspace approach to balanced truncation for model reduction of nonlinear control systems, Int. J. Robust Nonlinear Control 12 (6) (2002) 519–535.
[39] D. Wirtz, B. Haasdonk, Efficient a-posteriori error estimation for nonlinear kernel-based reduced systems, Syst. Control Lett. 61 (1) (2012) 203–211, http://dx.doi.org/10.1016/j.sysconle.2011.10.012.
[40] G.J. Pappas, Bisimilar linear systems, Automatica 39 (12) (2003) 2035–2047.
[41] A. Girard, G. Pappas, Approximate bisimulations for nonlinear dynamical systems, in: 44th IEEE Conference on Decision and Control, 2005, pp. 684–689.
[42] G. Pappas, G. Lafferriere, Hierarchies of stabilizability preserving linear systems, in: Proceedings of the 40th IEEE Conference on Decision and Control, vol. 3, 2001, pp. 2081–2086.
[43] R.A. Hayden, A. Stefanek, J.T. Bradley, Fluid computation of passage-time distributions in large Markov models, Theor. Comput. Sci. 413 (1) (2012) 106–141.