Fluid Aggregations for Markovian Process Algebra

Max Tschaikowski

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Max Tschaikowski

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Erstgutachter	Prof. Mirco Tribastone, Ph.D. Ludwig-Maximilians-Universität München Deutschland
Zweitgutachter	Prof. Jane Hillston, Ph.D. The University of Edinburgh United Kingdom
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Abstract

Quantitative analysis by means of discrete-state stochastic processes is hindered by the well-known phenomenon of state-space explosion, whereby the size of the state space may have an exponential growth with the number of objects in the model. When the stochastic process underlies a Markovian process algebra model, this problem may be alleviated by suitable notions of behavioural equivalence that induce *lumping* at the underlying continuous-time Markov chain, establishing an exact relation between a potentially much smaller aggregated chain and the original one. However, in the modelling of massively distributed computer systems, even aggregated chains may be still too large for efficient numerical analysis. Recently this problem has been addressed by *fluid* techniques, where the Markov chain is approximated by a system of ordinary differential equations (ODEs) whose size does *not* depend on the number of the objects in the model. The technique has been primarily applied in the case of massively replicated *sequential* processes with small local state space sizes. This thesis devises two different approaches that broaden the scope of applicability of efficient fluid approximations. *Fluid lumpability* applies in the case where objects are *composites* of simple objects, and aggregates the potentially massive, naively constructed ODE system into one whose size is independent from the number of composites in the model. Similarly to *quasi* and *near* lumpability, we introduce approximate *fluid lumpability* that covers ODE systems which can be aggregated after a small perturbation in the parameters. The technique of *spatial aggregation*, instead, applies to models whose objects perform a random walk on a two-dimensional lattice. Specifically, it is shown that the underlying ODE system, whose size is proportional to the number of the regions, converges to a system of partial differential equations of constant size as the number of regions goes to infinity. This allows for an efficient analysis of large-scale mobile models in continuous space like ad hoc networks and multi-agent systems.

Zusammenfassung

Die auf stochastischen Prozessen mit diskretem Zustandsraum basierende quantitative Analyse wird im Allgemeinen durch das Phänomen der Zustandsraumexplosion erschwert, da die Anzahl der Zustände in der Regel exponentiell abhängig von der Anzahl der Objekte im Modell ist. Wenn der stochastische Prozess durch eine Markowsche Prozessalgebra induziert wird und somit eine Markow-Kette in stetiger Zeit ist, kann dieses Problem mit Hilfe von Äquivalenzrelationen, welche ein *Lumping* der Markow-Kette ermöglichen, gemildert werden. Das Lumping erlaubt dabei, die ursprüngliche Markow-Kette mit einer potentiell deutlich kleineren, aggregierten Markow-Kette *exakt* in Beziehung zu bringen. Leider kommt es vor, dass beim Modellieren massiv verteilter Computersysteme selbst aggregierte Markow-Ketten für eine effiziente numerische Analyse zu groß sind. Dieses Problem wurde kürzlich mit Hilfe von *fluiden* Methoden analysiert. Die Idee ist dabei die Markow-Kette durch ein System von gewöhnlichen Differentialgleichungen (GDL) zu approximieren, dessen Größe *nicht* von der Anzahl der Objekte im Modell abhängt. Dies wurde im Fall der massiven Replikation von Prozessen mit kleinen lokalen Zustandsräumen erfolgreich getan. Diese Dissertation führt zwei unterschiedliche Methoden ein, welche den effektiven Anwendungsbereich der fluiden Approximation erweitern. So kann die *fluid lumpability* immer dann angewendet werden, wenn Objekte als *Kompositionen* einfacher Objekte dargestellt werden können und aggregiert das potentiell massive GDL System zu einem kleineren GDL System, dessen Größe unabhängig von der Anzahl der Kompositionen im Modell ist. Ähnlich zu *quasi* und *near* lumpability, betrachten wir die Methode der approximativen *fluid lumpability*, mit deren Hilfe GDL Systeme nach einer kleinen Veränderung der Parameter aggregiert werden können. Dagegen kann die Methode der *räumlichen Aggregation* auf Modelle angewendet werden, deren Objekte eine Irrfahrt auf einem zweidimensionalen Gitter vollführen. Hier zeigen wir, dass das betreffende GDL System, dessen Größe proportional zur Anzahl der Gitterpunkte ist, gegen ein System von partiellen Differentialgleichungen von konstanter Größe konvergiert, wenn das Gitter immer feinmaschiger wird. Dies erlaubt eine effiziente Analyse von umfangreichen mobilen Modellen in einem Kontinuum, etwa ad-hoc-Netzen und Multiagentensystemen.

Eidesstattliche Erklärung

Hiermit erkläre ich an Eidesstatt, dass die Dissertation von mir selbstständig, ohne unerlaubte Beihilfe angefertigt worden ist.

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Contents

Table of Notation

$q(i,j)$	transition rate from state a i into a state j
$\pi(i)$	steady state probability of a state i
$\mathcal{A}$	set of action types
$q_\alpha(i,j)$	transition rate from i into j arising from α-actions
P, Q, R, S	sequential PEPA component
G	PEPA model
$r_\alpha(G)$	α-apparent rate of a PEPA model G
$ds(G)$	derivative set of a PEPA model G
$dg(G)$	derivation graph of a PEPA model G
σ, ρ	bijection, semi-isomorphism
M	FPA model
$\mathcal{G}(M)$	set of fluid atoms of an FPA model M
$\mathcal{B}(M)$	set of sequential components of an FPA model M
V, W	population function
$v, \mathfrak{v}$	concentration function
$r_\alpha(M, v)$	fluid apparent rate of an FPA model M with respect to the concentration function v
$\mathcal{R}_\alpha(M, v, P)$	fluid component rate of a sequential component P of an FPA model M with respect to function v
$p_\alpha(\cdot,\cdot)$	derivative weighting function
$\dot{v}$	time derivative of the concentration function $t \mapsto v(t)$
$\overline{P}$	label partition of an FPA model
$\overline{P}^i$	element of a label partition $\overline{P}$
$\mathcal{P}$	tuple partition
$\vec{P}^i$	tuple (of labels)
$\mathfrak{P}$	partition of a tuple partition $\mathcal{P}$
$\sim_{\mathfrak{P}}$	label equivalence
$\stackrel{A}{=}$	an equality which follows from statement A
$\approx_{\mathfrak{P}}$	projected label equivalence
$\tilde{M}$	nested FPA model
$[\![\cdot]\!]_L^N$	replication operator of nested FPA models
$\tilde{G}(\tilde{M})$	labels of a nested FPA model $\tilde{M}$
$\mathcal{I}(\tilde{M})$	interpretation of a nested FPA model $\tilde{M}$
ξ, ζ	rate occurrences in an FPA model
$\mathcal{R}_K$	regular lattice on $[0;1]^2$ with step size $1/K$
Ω_K	boundary of $\mathcal{R}_K$
$\mathcal{S}(M)$	spatial version of an FPA model M
$\mu_K(P)$	migration rate of an agent P on $\mathcal{R}_K$
$\triangle, \triangle^d$	continuous and discrete Laplace operator
∂_z	partial derivative with respect to z
$\vec{\omega}$	PDE approximation of a spatial FPA model $\mathcal{S}(M)$

Chapter 1

Introduction

Markov processes have proven useful in the quantitative modelling of systems. In the case of discrete-state Markov chains, either in (homogeneous) discrete or in continuous time, the solution for transient and steady-state analysis is cast into a classical linear algebra problem for which a wide range of efficient numerical techniques exist [1]. Markov chain models are however intrinsically based on an interleaving semantics, which causes the infamous problem of state-space explosion: the state space size may grow exponentially with the number of elements of the system. A number of approaches to state-space reduction have been devised, including product-form solutions (e.g., [2]), decompositions (e.g., [3]), matrix analytics methods (e.g. [4]) and lumping techniques, where a (hopefully much smaller) chain may be defined which preserves the system's original stochastic behaviour, either exactly, as in the case of ordinary and exact lumpability (e.g., [5]), or in an approximate manner (e.g., *near* [5] and *quasi* lumpability [6]).

In this thesis we are concerned with continuous-time Markov chains (CTMCs) inferred by Markovian process algebra (e.g., [7, 8, 9]). In this context, lumpability has been at the basis of suitable notions of behavioural equivalence between processes which induce an aggregated Markov chain; in the literature, these relations are known as *strong equivalence* in PEPA [7, Chap. 8], *strong Markovian bisimilarity* in MTIPP [10] and EMPA [11] and *strong performance equivalence* in MPA [12]. Although, in general, lumping techniques require the availability of the full CTMC to be aggregated, exploiting results of congruence of such relations with respect to parallel composition has allowed for methods that are able to construct the lumped CTMC *on-the-fly*, i.e., directly without constructing the original CTMC first [13, 14]. Although these methods may not yield optimal lumping, they have proven successful in exploiting structural symmetries [15, 16]. For instance, distinct states which are syntactically equal up to a permutation, e.g., $P \mid Q$ and $Q \mid P$, can be lumped into the same macro-state of the aggregated CTMC. This typically reduces the computational complexity of the state-space size from exponential to polynomial in the number of sequential processes. In the case of massively distributed systems, however, a polynomial

growth may still lead to CTMCs which are hard to tackle from a numerical point of view [17].

To cope with these difficulties, more recent work has been carried out towards equipping stochastic process algebra with *fluid* semantics. The underlying mathematical object for the analysis is now a system of ordinary differential equations (ODEs) which gives an approximate time-course evolution of the *population* of processes exhibiting a particular local state. Especially in the case of large *population processes*, this approximation is very accurate but typically much more compact than the lumped CTMC, as it is independent of the actual population sizes but is only dependent on the number of local behaviours of the distinct sequential processes. The relationship between the CTMC and the fluid semantics has been studied in the context of PEPA [18], an extension called PEPA + Π, useful for the analysis of biochemical systems [19], Bio-PEPA [20], Cardelli's stochastic interacting processes [21], and stochastic Concurrent Constraint Programming [22]. In the context of queueing networks, [23, 24] derive limit solutions for steal and push strategies if the size of the network goes to infinity, whereas [25] shows an insensitivity result on the fluid level. Another instance of fluid approximation is [26], where a fluid model of a peer-to-peer network with many nodes is given. More generally, [27, 28] devise frameworks for interacting objects and identify conditions under which the underlying population based Markov chains converge to a fluid limit as the number of objects tends to infinity. Building on fluid semantics, it is possible to express rewards like energy consumption in terms of ODEs, rather than CTMCs. This allows for an efficient analysis and is studied in [29, 30]. In [31], instead, fluid semantics are used to derive the *stochastic* behaviour of a single object within a population of similar objects, allowing therefore for stochastic model checking.

Unfortunately, ODE models of realistic complex systems may still be too large for feasible analysis. During the last forty years this issue was tackled, in essence, by two different approaches. The first approach tries to *approximately* relate the original ODE system to a smaller one. For instance, [32] splits the original ODE system into a *fast* and a *slow* part, while [33, 34] identify parts of the ODE system which have a *negligible* impact on the overall trajectory. The method of proper orthogonal projection [35], instead, bounds the distance to the solution of an approximating ODE system of smaller size. The second approach, instead, is similar to the idea of stochastic lumping and tries to *exactly* relate the original ODE system to a smaller, *aggregated* one. To the best of our knowledge, this idea was first applied in the context of control theory [36] and adopted afterwards in economics [37], theoretical ecology [38] and biological chemistry [39]. The more recent work [40] can be seen as an extension of [36].

In this thesis, we study both exact and approximative aggregations in the context of the stochastic process algebra PEPA, the first process algebra to be equipped with a fluid semantics [18]. In particular, we consider a fluid framework of PEPA called Fluid Process Algebra (FPA), originating from Grouped PEPA [17].

Exact Fluid Lumpability It is well-known [41] that if the CTMC states within the same element of an exactly lumpable partition are initially equiprobable, then they will be equiprobable at all future time points. The analogous notion of *exact fluid lumpability*, cf. Chapter 3, is intuitively defined as a partition over the ODEs of a model whereby two ODEs belonging to the same partition element have indistinguishable solutions *if their initial conditions are the same*; an aggregated ODE model may be defined which only considers a representative ODE for each partition element. Similarly to stochastic lumpability, such partitions are called *exactly fluid lumpable*. Here, we want to stress that the aggregations induced by exact fluid lumpability can be used to *fully* recover the original ODE system. In contrast to this, aggregations stemming from [40] are usually not reversible, meaning that the original ODE system cannot be recovered from the aggregated one. Indeed, to the best of our knowledge, only this thesis and its precursor paper [42] propose such an aggregation.

As discussed above, aggregation may be induced by suitable behavioural relationships at the process algebra level. In PEPA, this may be accomplished by means of a strong equivalence relation over the states of a labelled transition system. The set of equivalence classes produced by such a relation represents the partition of the underlying lumped CTMC. Similarly, we define a notion of behavioural equivalence for FPA, called *projected label equivalence*, which induces an exactly fluid lumpable partition.

In PEPA, different strong equivalence relations may be merged to obtain possibly coarser partitions. More formally, the transitive closure of the union of several strong equivalence relations *always* induces an ordinarily lumpable partition [7]. An analogous result holds for FPA, where, under certain conditions, it is shown that the transitive closure of the union of several projected label equivalences induces an exactly fluid lumpable partition. This is important, since there exist exactly fluid lumpable partitions for which construction of at least two different projected equivalences are needed. At last, we show that the notion of projected label equivalence implies a form of stochastic equivalence, called *semi-isomorphism*. Informally, two graphs are semi-isomorphic if a suitable merging of transitions in both makes them isomorphic.

Nested FPA Models In Chapter 4 we introduce the class of *nested* FPA models and show how its elements can be aggregated using the notion of exact fluid lumpability.

A nested model is a model with a syntactic element that describes replicas of composite processes. To build on intuition, let us consider the sequential components C, T and U given by

$$\begin{array}{lll} C \stackrel{def}{=} (exec, r).\widehat{C} & T \stackrel{def}{=} (exec, r).\widehat{T} & U \stackrel{def}{=} (io, z).\widehat{U} \\ \widehat{C} \stackrel{def}{=} (reset, s).C & \widehat{T} \stackrel{def}{=} (io, s').T & \widehat{U} \stackrel{def}{=} (idle, z').U. \end{array}$$

Informally, C models a CPU which performs *exec*- and *reset*-actions in successive order. Similarly, T describes a thread and U a resource. In PEPA, a group of

N_C CPUs which are working independently from each other is expressed by the compact bracket notation

$$C[N_C] = \underbrace{C \parallel C \parallel \ldots \parallel C}_{N_C \text{ times}}, \tag{1.1}$$

where $\parallel$ is an abbreviation of $\underset{\emptyset}{\bowtie}$ which denotes a CSP-style parallel composition over an empty action set. Using this notation, a resource which is shared by a group of D machines $C[N_C] \underset{\{exec\}}{\bowtie} T[N_T]$ can be written as

$$\underbrace{\left(C[N_C] \underset{\{exec\}}{\bowtie} T[N_T]\right) \parallel \left(C[N_C] \underset{\{exec\}}{\bowtie} T[N_T]\right) \parallel \ldots \parallel \left(C[N_C] \underset{\{exec\}}{\bowtie} T[N_T]\right)}_{D \text{ times}} \underset{\{io\}}{\bowtie} U[N_U], \tag{1.2}$$

where $\underset{L}{\bowtie}$ models synchronisation. For instance, $\underset{\{exec\}}{\bowtie}$ incorporates the contention for the same core by more threads. It can be shown that (1.2) has an ODE system of size $D(2+2)+2$. Thanks to the notion of exact fluid lumpability, however, one can recover its solution by solving an aggregated ODE system of size $1 \cdot (2+2) + 2$, making the problem independent of the multiplicity D.

In FPA, a replication of a sequential PEPA processes $P[N_P]$ corresponds to the *fluid atom* P and an external *population function* V that maps sequential components to non-negative integers. For instance, together with $V(C) = N_C$ and $V(\widehat{C}) = 0$, the FPA process C would represent $C[N_C]$ in PEPA. This approach is similar to the notion of *reduced context* presented in [43] or to the *species-oriented* view of the system in Bio-PEPA [20]. Using this, (1.2) can be encoded by the FPA processes

$$\underbrace{\left(C \underset{\{exec\}}{\bowtie} T\right) \parallel \left(C \underset{\{exec\}}{\bowtie} T\right) \parallel \ldots \parallel \left(C \underset{\{exec\}}{\bowtie} T\right)}_{D \text{ times}} \underset{\{io\}}{\bowtie} U, \tag{1.3}$$

and a corresponding population function V.

Nested FPA models introduce the syntactic element $[\![M]\!]_L^D$, which stands for a cooperation of D replicas of a given nested FPA model M over the actions set L. For instance, (1.3) is abbreviated to

$$\left[\!\left[C \underset{\{exec\}}{\bowtie} T\right]\!\right]_{\emptyset}^{D} \underset{\{io\}}{\bowtie} U,$$

because the machines are modelled as being working independently from each other. Note that this *generalises* the notation given in (1.1) which applies only to sequential processes. The level of nesting can be arbitrary. Let us consider

$$\left[\!\left[\left[\!\left[C \underset{\{exec\}}{\bowtie} T\right]\!\right]_{\emptyset}^{D} \underset{\{io\}}{\bowtie} U\right]\!\right]_{\emptyset}^{D'} \underset{\{exec\}}{\bowtie} E, \tag{1.4}$$

where $E \overset{def}{=} (exec, x).\widehat{E}$ and $\widehat{E} \overset{def}{=} (think, x').E$. Intuitively, the above model considers a situation where D' applications, each made of D machines sharing a

common resource U, serve a group of users which are given by E. For instance, in the case of $D' = 2$ and $D = 2$, (1.4) abbreviates the FPA model

$$\Big(\big((C \underset{\{exec\}}{\bowtie} T) \parallel (C \underset{\{exec\}}{\bowtie} T) \underset{\{io\}}{\bowtie} U\big) \parallel \big((C \underset{\{exec\}}{\bowtie} T) \parallel (C \underset{\{exec\}}{\bowtie} T) \underset{\{io\}}{\bowtie} U\big)\Big) \underset{\{exec\}}{\bowtie} E,$$

which induces in turn (with a suitable population function) the PEPA model

$$\begin{aligned}\Big(&\big((C[N_C] \underset{\{exec\}}{\bowtie} T[N_T]) \parallel (C[N_C] \underset{\{exec\}}{\bowtie} T[N_T]) \underset{\{io\}}{\bowtie} U[N_U]\big) \parallel \\ &\big((C[N_C] \underset{\{exec\}}{\bowtie} T[N_T]) \parallel (C[N_C] \underset{\{exec\}}{\bowtie} T[N_T]) \underset{\{io\}}{\bowtie} U[N_U]\big)\Big) \underset{\{exec\}}{\bowtie} E[N_E].\end{aligned}$$

In general, the ODE system size of a nested FPA model will grow polynomially with the number of levels of nesting; in this example, the number of ODEs is $D'(D(2+2)+2)+2$, where the factors $2+2$ and 2 are due to the local state space sizes of the term's sequential components, i.e. C, T, U and E. Similarly to before, the notion of exact fluid lumpability allows us to solve the original ODE system by solving a system of size $1 \cdot (1 \cdot (2+2)+2)+2$. That is, the size of the aggregated ODE system is *independent* of the multiplicities D' and D. Indeed, it turns out that this applies for any nested FPA model.

Ordinary Fluid Lumpability In contrast to exact lumpability, if a partition is ordinary lumpable, it holds that the probabilities of the CTMC states in the same partition element sum up to the probability of the underlying macro state in the lumped CTMC [5]. For the analogous notion of *ordinary fluid lumpability* introduced in [44] and discussed in Chapter 5 of the present thesis, the *sum of the ODE solutions* belonging to the same partition element are fully recovered from the solution of a (smaller) ODE system consisting of one single ODE for each partition element. That is, ordinary fluid lumpability can be seen as an analogy of ordinary stochastic lumpability in the domain of ODE systems. For instance, the ODE system belonging to the PEPA model

$$\big(T[N_1] \parallel \ldots \parallel T[N_D]\big) \underset{\{exec\}}{\bowtie} U[N_U], \tag{1.5}$$

is of size $D \cdot 2 + 2$ and can be related, thanks to the notion of ordinary fluid lumpability, to an aggregated ODE system of size $1 \cdot 2 + 2$. In contrast to the notion of exact fluid lumpability, the aggregated ODE system keeps track of the total number of threads in the system. That is, while it is possible to have different initial populations $N_1, \ldots N_D$, the ODEs of each single thread group cannot be recovered from the aggregated ODE system. Here, we want to point out that ODE aggregation induced by the notion of ordinary fluid lumpability may be seen as a special case of the aggregation technique [40]. However, since ordinary fluid lumpability is developed in the context of FPA, it is possible to show that it is a congruence with respect to parallel composition of FPA and implies, under certain assumptions, that the aggregated processes are semi-isomorphic.

Fluid ε-Lumpability In Chapter 6 we study approximate versions of ordinary and exact fluid lumpability, as a means to relaxing symmetry in the ODE systems. In essence, a partition is ordinary fluid ε-lumpable, if a small perturbation ε in the parameters of the ODE system makes the partition ordinary fluid lumpable. For instance, let us consider the variation

$$\left(T_1[N_1] \parallel \ldots \parallel T_D[N_D]\right) \underset{\{exec\}}{\bowtie} U[N_U]$$

of (1.5) where $T_d \stackrel{def}{=} (exec, r_d).\widehat{T}_d$, $\widehat{T}_d \stackrel{def}{=} (io, s').T_d$ and $r_d = r + \varepsilon_d$ for all $1 \leq d \leq D$. It can be shown that the underlying ODE system applies for ordinary fluid lumpability only if $r_1 = \ldots = r_D$. However, since the ODE system is, intuitively, almost fluid lumpable if $\varepsilon = \|(\varepsilon_1, \ldots, \varepsilon_D)\| \approx 0$, it is reasonable to ask how close the solution of the perturbed ODE system will be to the original one. By exploiting the fluid semantics of FPA, we derive in the case of ordinary fluid ε-lumpability a bound for the distance which is *linear* in ε. In the case of exact fluid lumpability, instead, it is not sufficient to consider only perturbations in the ODE parameters, because assumptions are also made on the initial conditions. Therefore, its approximate counterpart considers a perturbation ε in ODE parameters and a perturbation δ in initial conditions. Similarly to ordinary fluid ε-lumpability, we derive a bound which is *linear* in both ε and δ. Moreover, it is shown that exact and ordinary fluid ε-lumpability imply, under certain assumptions, the notion of ε-semi-isomorphism, a natural extension of semi-isomorphism which coincides with the latter when $\varepsilon = 0$.

Spatial Aggregation All the previous approaches consider aggregations of ODE systems that are themselves ODEs. Instead, in Chapter 7 we consider aggregations that lead to systems of partial differential equations (PDEs). This technique is motivated by FPA models that exhibit an explicit notion of space and mobility. Specifically, we study the case where the sequential processes of an FPA model perform a random walk on a two-dimensional lattice in the unit square. Typical situations of practical interest to which this would apply are, for instance, personal communication services [45]: there are many base stations (e.g., in a wide-area cellular network) and each base station can be modelled as a region, which can contain potentially many mobile nodes that may migrate across the lattice. Another interesting application would be the modelling of spread patterns of smartphone viruses [46].

In order to allow users from (1.4) to perform a random walk on a lattice, we define sequential components $E^{(x,y)}$ and $\widehat{E}^{(x,y)}$ for *each* region (x, y) on the lattice. This is done by lifting the definition of a "stationary" component to space by labelling it with the location where it is, and by adding the possibility of moving across locations. For example, since the stationary component E is given by $E \stackrel{def}{=} (exec, x).\widehat{E}$ and $\widehat{E} \stackrel{def}{=} (think, x').E$, we define

$$E^{(x,y)} \stackrel{def}{=} (exec^{(x,y)}, x).\widehat{E}^{(x,y)} + (\delta, \mu).E^{(x-\Delta s,y)} + \\ + (\delta, \mu).E^{(x+\Delta s,y)} + (\delta, \mu).E^{(x,y-\Delta s)} + (\delta, \mu).E^{(x,y+\Delta s)},$$

where Δs and δ denote the spatial step size and the diffusion action, respectively. Consequently, if $\Delta s = 1/K$ for some fixed lattice granularity $K \geq 1$, the number of sequential components needed will be of order $\mathcal{O}(K^2)$. Since this remains valid for an arbitrary FPA model whose sequential components are lifted to the spatial domain and each sequential component induces one ODE, even fluid approximation is numerically tedious in the case of a fine grained lattices. However, under the assumption that the migration speed across the lattice is invariant under K, it can be shown that the ODE systems converge, as $K \to \infty$, to a PDE system independent from the lattice granularity and only dependent on the number of local states of the original *stationary* sequential processes. This allows for an efficient analysis of large-scale mobile systems in, intuitively, *continuous* space.

After giving some underlying background work, the following chapters discuss the aforementioned results in detail.

Chapter 2

Preliminaries

After giving a brief overview of stochastic lumping, this chapter presents the background material on PEPA, its behavioural equivalences and fluid interpretation. Specifically, Section 2.1 discusses the notions of ordinary and exact (stochastic) lumpability, whereas Section 2.2 and Section 2.3 overview syntax and semantics of PEPA and its behavioural equivalences. Afterwards, the fluid semantics of PEPA are rigourously formulated in terms of a Fluid Process Algebra (FPA), cf. Section 2.4. The chapter is concluded by Section 2.5 where the new notion of *well-posedness* is introduced. This will prove to be useful in Chapter 3 and 5, where it will be shown that well-posedness implies a behavioural equivalence relation called semi-isomorphism.

2.1 Stochastic Lumpability

This exposition of lumpability is based on the results of [5, 41, 47, 48]. Using standard notation we will hereby denote the state space of the original CTMC by $\{1, \ldots, n\}$, the probability of being in state i at time t by $\pi_t(i)$, the steady state probability of state i by $\pi(i)$, and the transition rate from i to j by $q(i, j)$. Moreover we define

$$q(X, j) := \sum_{i \in X} q(i, j) \qquad \text{and} \qquad q(i, X) := \sum_{j \in X} q(i, j)$$

for a set $X \subseteq \{1, \ldots, n\}$.

Definition 1 (Ordinary and Exact Lumpability)**.** *Let a partition of the state space of the original CTMC be denoted by* $\chi = \{X_1, \ldots, X_N\}$.

- χ *is called* ordinarily lumpable *if*

$$\forall X_I, X_J \in \chi.\, \forall x_i, x_i' \in X_I.\, \big(q(x_i, X_J) = q(x_i', X_J)\big).$$

- χ *is called* exactly lumpable *if*

$$\forall X_I, X_J \in \chi.\, \forall x_j, x_j' \in X_J.\, \big(q(X_I, x_j) = q(X_I, x_j')\big).$$

Ordinarily and exactly lumpable partitions can be used to transform the original CTMC into a smaller (lumped) CTMC.

Theorem 1 (Ordinarily and Exactly Lumped CTMCs)**.** *It holds that:*

- *An ordinarily lumpable partition χ of the state space of the original CTMC $\{1, \ldots, n\}$ induces an ordinarily lumped CTMC with state space χ, initial distribution $\pi_0(X_I) := \sum_{x_i \in X_I} \pi_0(x_i)$ and transition rates*

$$q(X_I, X_J) := q(x_i, X_J),$$

  where $x_i \in X_I$ can be chosen arbitrarily.

- *An exactly lumpable partition χ of the state space of the original CTMC $\{1, \ldots, n\}$ induces an exactly lumped CTMC with state space χ, initial distribution $\pi_0(X_I) := \sum_{x_i \in X_I} \pi_0(x_i)$ and transition rates*

$$q(X_I, X_J) := \frac{|X_J|}{|X_I|} q(X_I, x_j),$$

  where $x_j \in X_J$ can be chosen arbitrarily.

The next two theorems relate the stochastic behaviour of the original CTMC to ordinarily, respectively exactly, lumped CTMCs.

Theorem 2. *The ordinarily lumped CTMC which arises from the original CTMC and an ordinarily lumpable partition χ on $\{1, \ldots, n\}$, satisfy for all initial distributions π_0 and $X_I \in \chi$,*

- *$\pi(X_I) = \sum_{x_i \in X_I} \pi(x_i)$ if the original CTMC is irreducible.*
- *$\pi_t(X_I) = \sum_{x_i \in X_I} \pi_t(x_i)$.*

In contrast to an ordinarily lumped CTMC, an exactly lumped CTMC completely determines the stochastic behaviour of the original CTMC, as stated in the following theorem.

Theorem 3. *The exactly lumped CTMC which arises from the original CTMC and an exactly lumpable partition χ on $\{1, \ldots, n\}$ satisfies*

- *$\pi(x_i) = \frac{1}{|X_I|} \pi(X_I)$ for all initial distributions π_0, $X_I \in \chi$ and $x_i \in X_I$ if the original CTMC is irreducible.*
- *$\pi_t(x_i) = \frac{1}{|X_I|} \pi_t(X_I)$ for all $X_I \in \chi$, $x_i \in X_I$ and $t \geq 0$, if π_0 is equidistributed on χ, i.e., $\pi_0(x_i) = \pi_0(x_i')$ for all $X_I \in \chi$ and $x_i, x_i' \in X_I$.*

2.2 Syntax and Semantics of PEPA

In this section we introduce PEPA [7]. Although the original PEPA incorporates hiding, we drop it for the sake of consistency with [42, 49]. Also, we drop the concept of passive rates, because it may lead to ODE systems with discontinuous right-hand sides [50]. Finally, since it is more convenient in fluid analysis to identify populations by constants rather than arbitrary process terms, and each PEPA process in its original formulation can be rewritten in such a way [13], the following non-standard definition of PEPA will be used.

Definition 2 (PEPA)**.** *Let $\mathcal{A}$ denote the set of all action types and $\mathcal{A}ct := \mathcal{A} \times \mathbb{R}_{>0}$ be the set of all* activities*. The syntax of a PEPA model is given by the grammar*

$$S ::= P \mid \sum_{i \in I} (\alpha_i, r_i).P_i, \qquad G ::= S \mid G \underset{L}{\bowtie} G,$$

where $(\alpha, r) \in \mathcal{A}ct$, $L \subseteq \mathcal{A}$ and $P \stackrel{\text{def}}{=} S$ denotes a constant*.*

The terms S introduce *sequential components*, with $\sum_{i \in I} (\alpha_i, r_i).P_i$ a choice between activities. The value r_i in activity (α_i, r_i) denotes a coefficient that contributes to determine the rate of the exponential distribution at which the activity is defined to occur. The terms G define *model components* and allow for synchronisation via shared action types in the set L. We use $G \parallel G$ whenever $L = \emptyset$. Also, for any $N \geq 1$, we let $P[N]$ abbreviate $(P \parallel \ldots \parallel P)$, where the constant P is present N times.

The notion of *apparent rate* is formally introduced in the following as a function which associates a nonnegative real number with a process term. Informally, it can be interpreted as the maximum rate at which a process can perform an action [51].

Definition 3 (Apparent Rate)**.** *The apparent rate of action α in a PEPA component P, denoted by $r_\alpha(P)$, is defined as follows:*

$$r_\alpha(P) = r_\alpha(S) \quad \text{if } P \stackrel{\text{def}}{=} S$$

$$r_\alpha\Big(\sum_{i \in I} (\alpha_i, r_i).P_i\Big) = \sum_{i \in I : \alpha_i = \alpha} r_i$$

$$r_\alpha(G_0 \underset{L}{\bowtie} G_1) = \begin{cases} r_\alpha(G_0) + r_\alpha(G_1) & , \ \alpha \notin L \\ \min(r_\alpha(G_0), r_\alpha(G_1)) & , \ \alpha \in L \end{cases}$$

Using the structured operational semantics of PEPA given in Figure 2.1, we write $G \xrightarrow{(\alpha, r)} G'$ whenever there is an α-transition with rate r from process G to process G'. We say that G' is a *derivative* of G. The set of all derivatives reachable from a process term is defined as follows.

Definition 4 (Derivative Set)**.** *The derivative set of a PEPA component G, denoted by $ds(G)$, is defined as the smallest set such that:*

$$\frac{}{\sum_{i\in I}(\alpha_i, r_i).P_i \xrightarrow{(\alpha_j, r_j)} P_j} \quad \text{where} \quad j \in I \qquad \frac{S \xrightarrow{(\alpha,r)} S'}{P \xrightarrow{(\alpha,r)} S'} \quad P \stackrel{def}{=} S$$

$$\frac{G_0 \xrightarrow{(\alpha,r_1)} G_0'}{G_0 \underset{L}{\bowtie} G_1 \xrightarrow{(\alpha,r_1)} G_0' \underset{L}{\bowtie} G_1} \alpha \notin L \qquad \frac{G_1 \xrightarrow{(\alpha,r_2)} G_1'}{G_0 \underset{L}{\bowtie} G_1 \xrightarrow{(\alpha,r_2)} G_0 \underset{L}{\bowtie} G_1'} \alpha \notin L$$

$$\frac{G_0 \xrightarrow{(\alpha,r_1)} G_0' \quad G_1 \xrightarrow{(\alpha,r_2)} G_1'}{G_0 \underset{L}{\bowtie} G_1 \xrightarrow{(\alpha,R)} G_0' \underset{L}{\bowtie} G_1'} \alpha \in L, \qquad R = \frac{r_1}{r_\alpha(G_0)} \frac{r_2}{r_\alpha(G_1)} r_\alpha(G_0 \underset{L}{\bowtie} G_1)$$

Figure 2.1: Structured operational semantics of PEPA.

- $G \in ds(G)$;
- *if* $G' \in ds(G)$ *and* $G' \xrightarrow{(\alpha,r)} G''$ *then* $G'' \in ds(G)$.

The derivative set forms the nodes of the *derivation graph*, which gives the overall behaviour of the process in terms of a transition system labelled with activities, formally defined as follows.

Definition 5 (Derivation Graph)**.** *The derivation graph* $dg(G)$ *of a PEPA component* G *has* $ds(G)$ *as the set of nodes. The multiset of transitions* $\mathcal{T} \subseteq ds(G) \times \mathcal{A}ct \times ds(G)$ *is such that*

$$G_0 \xrightarrow{(\alpha,r)} G_1 \Leftrightarrow (G_0, (\alpha, r), G_1) \in \mathcal{T},$$

with multiplicity equal to the number of distinct derivations of $G_0 \xrightarrow{(\alpha,r)} G_1$.

Let us demonstrate the above notions on an example. For instance, a CPU core and a thread could be modelled by means of the following two-state sequential components.

$$\begin{aligned} C &\stackrel{def}{=} (exec, r).\widehat{C} & \widehat{C} &\stackrel{def}{=} (reset, s).C \\ T &\stackrel{def}{=} (exec, r).\widehat{T} & \widehat{T} &\stackrel{def}{=} (io, s').T \end{aligned} \tag{2.1}$$

The CPU core cycles through the states C, where it is *executable* (as indicated by the *action type exec*) with rate r, and $\widehat{C}$, where it does a reset action which makes it available for a further execution. Thus, the derivative set of C is $ds(C) = \{C, \widehat{C}\}$. Similarly, a thread evolves through states T, where it wishes to execute on a CPU, and $\widehat{T}$, where it performs input/output bound operations

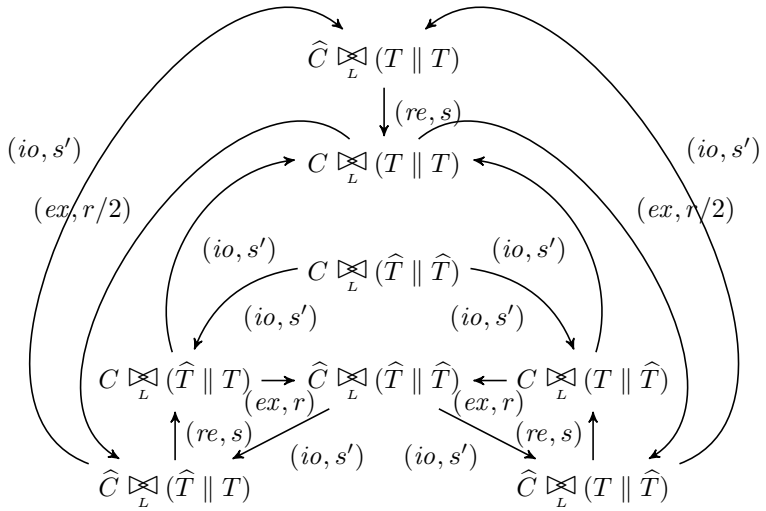

Figure 2.2: Derivation graph of (2.2) in the case of $N_C = 1$ and $N_T = 2$. $L := \{exec\}$; transition labels: *ex* stands for *exec* and *re* stands for *reset*.

(i.e., $ds(T) = \{T, \widehat{T}\}$). Building on that, one could model a machine with N_C cores and N_T threads using the process

$$Sys := C[N_C] \underset{\{exec\}}{\bowtie} T[N_T]. \tag{2.2}$$

Thus, in the situation where $N_C = 1$, $N_T = 2$ the system consists of one CPU and two threads. The derivation graph for such a case is shown in Figure 2.2.

A derivation graph is interpreted as a CTMC in a straightforward way, by ignoring self-loops and associating vertices with states and transitions with arcs; two distinct transitions between the same two states are merged into the same CTMC transition with a total rate equal to the sum of the two.

2.3 Behavioural Equivalences of PEPA

Before we turn to the fluid semantics, we discuss several notions of behavioural equivalence which will be used in the remainder of the thesis. The first is isomorphism and is given by a map between the derivative sets of two processes which induces a one-to-one correspondence, i.e. a *graph isomorphism*, between their derivation graphs.

Definition 6 (Isomorphism, cf. Definition 6.2.1 in [7])**.** *Two PEPA processes G and $\tilde{G}$ are isomorphic if there is a bijection $\sigma : ds(G) \to ds(\tilde{G})$ which satisfies,*

for all $G_i, G_j \in ds(G)$ *and* $(\alpha, r) \in \mathcal{A}ct$

$$\{|(\alpha, r) \mid (G_i, (\alpha, r), G_j) \in \mathcal{T}_G|\} = \{|(\alpha, r) \mid \big(\sigma(G_i), (\alpha, r), \sigma(G_j)\big) \in \mathcal{T}_{\tilde{G}}|\},$$

where $\mathcal{T}_G$ *and* $\mathcal{T}_{\tilde{G}}$ *denotes the multiset of transitions in* $dg(G)$ *and* $dg(\tilde{G})$*, respectively.*

For instance, in the case of

$$\begin{aligned} B &\stackrel{def}{=} (exec, r).\widehat{B} & B' &\stackrel{def}{=} (exec, r).\widehat{B}' \\ \widehat{B} &\stackrel{def}{=} (reset, s).B & \widehat{B}' &\stackrel{def}{=} (reset, s).B', \end{aligned}$$

the processes B and B' are isomorphic.

We introduce next a slightly weaker notion, called *semi-isomorphism*, which relates two processes with respect to their *merged derivation graphs* (cf. Definition 8), defined as the graphs obtained by replacing multiple equally-labelled transitions between two states with a single transition with the same action type and a rate which is the sum across all such transition rates.

Definition 7 (Semi-Isomorphism)**.** *Two PEPA processes* G *and* $\tilde{G}$ *are semi-isomorphic if there is a bijection* $\sigma : ds(G) \to ds(\tilde{G})$ *which satisfies* $\sum_{G_i \xrightarrow{(\alpha,r)} G_j} r = \sum_{\sigma(G_i) \xrightarrow{(\alpha,r)} \sigma(G_j)} r$ *for all* $G_i, G_j \in ds(G)$ *and* $\alpha \in \mathcal{A}$*. We shall call such a* σ *a semi-isomorphism.*

As an example, let us consider the processes

$$\begin{aligned} C &\stackrel{def}{=} (exec, r).\widehat{C} & C' &\stackrel{def}{=} (exec, r/2).\widehat{C}' + (exec, r/2).\widehat{C}' \\ \widehat{C} &\stackrel{def}{=} (reset, s).C & \widehat{C}' &\stackrel{def}{=} (reset, s).C'. \end{aligned} \tag{2.3}$$

Then, it can be shown that C is semi-isomorphic to C'. However, C and C' are not isomorphic because the number of transitions in their derivation graphs is different.

The notion of merged derivation graph given below relates isomorphism to semi-isomorphism.

Definition 8 (Merged Derivation Graph)**.** *The merged derivation graph* $dg_m(G)$ *of* G *arises from* $dg(G)$*, if, for all* $\alpha \in \mathcal{A}$*, all* α*-transitions between any two states whose rate-sum across all transitions is equal to* q *are replaced by a single transition* (α, q)*.*

Though easy to prove, due to its importance the following is stated as a theorem.

Theorem 4. *Let* $\sigma : ds(G) \to ds(\tilde{G})$ *be a semi-isomorphism between the PEPA processes* G *and* $\tilde{G}$*. Then it holds that* $dg_m(G)$ *and* $dg_m(\tilde{G})$ *stand in a one-to-one correspondence.*

Proof. We fix the unique $G' \in ds(G)$ which satisfies $\sigma(G') = \tilde{G}$. Since G' is in $dg(G)$, G' is also in $dg_m(G)$. Hence, $\sigma(G')$ is in $dg_m(\sigma(G))$ which implies, in turn, that $\sigma(G')$ is in $dg(\sigma(G))$. Since $\sigma(G)$ is obviously in $dg(\sigma(G'))$, we infer $dg(\sigma(G)) = dg(\sigma(G'))$. As this implies $dg_m(\sigma(G)) = dg_m(\tilde{G})$ and $dg_m(G)$ stands in an one-to-one correspondence to $dg_m(\sigma(G))$, this shows the claim. □

In general, it is easy to see that PEPA isomorphism induces semi-isomorphism and that the CTMCs of semi-isomorphic PEPA processes stand in a one-to-one correspondence. Next comes PEPA's version of bisimulation.

Definition 9 (Strong Bisimulation, cf. Definition 7.2.1 in [7])**.** *Let $\mathfrak{G}$ denote the set of all PEPA components. Then*

- *$R \subseteq \mathfrak{G} \times \mathfrak{G}$ is a strong bisimulation if $(G_0, G_1) \in R$ implies*
  - $\forall \alpha \in \mathcal{A}\big[r_\alpha(G_0) = r_\alpha(G_1)\big]$
  - $\forall a \in \mathcal{A}ct\Big[G_0 \xrightarrow{a} G_0' \Rightarrow \exists G_1' \in \mathfrak{G}\Big(G_1 \xrightarrow{a} G_1' \wedge (G_0', G_1') \in R\Big)\Big]$
  - $\forall a \in \mathcal{A}ct\Big[G_1 \xrightarrow{a} G_1' \Rightarrow \exists G_0' \in \mathfrak{G}\Big(G_0 \xrightarrow{a} G_0' \wedge (G_0', G_1') \in R\Big)\Big]$
- *$G_0, G_1 \in \mathfrak{G}$ are strongly bisimilar, if there exists a strong bisimulation $R \subseteq \mathfrak{G} \times \mathfrak{G}$ such that $(G_0, G_1) \in R$.*

Like strong bisimulation in CCS, cf. Chapter 4 in [52], strong bisimulation in PEPA relates processes whose behaviour cannot be distinguished by an external observer. We end the section with the notion of strong equivalence.

Definition 10 (Strong Equivalence, cf. Definition 8.2.1 in [7])**.** *Let $\mathfrak{G}$ denote the set of all PEPA components. Then*

- *An equivalence relation $R \subseteq \mathfrak{G}_0 \times \mathfrak{G}_0$, where $\mathfrak{G}_0 \subseteq \mathfrak{G}$, is a strong equivalence on $\mathfrak{G}_0$ if $(G_0, G_1) \in R$ implies*

$$\forall \alpha \in \mathcal{A}.\, \forall S \in \mathfrak{G}_0/R.\, \Big(q_\alpha(G_0, S) = q_\alpha(G_1, S)\Big),$$

  where $q_\alpha(G', S') := \displaystyle\sum_{\hat{G}' \in S'} \sum_{G' \xrightarrow{(\alpha, r)} \hat{G}'} r.$

- *Two PEPA components $G_0, G_1 \in \mathfrak{G}$ are strongly equivalent, if there is a strong equivalence R on $\mathfrak{G}$ such that $(G_0, G_1) \in R$.*

It can be shown that for any two strongly equivalent PEPA processes G_1 and G_2 there exist strong equivalences R_1 and R_2 on $ds(G_1)$ and $ds(G_2)$, respectively, such that $ds(G_i)/R_i$ is ordinarily lumpable, with $i = 1, 2$, and the corresponding lumped CTMCs are isomorphic, cf. Section 8.5 in [7].

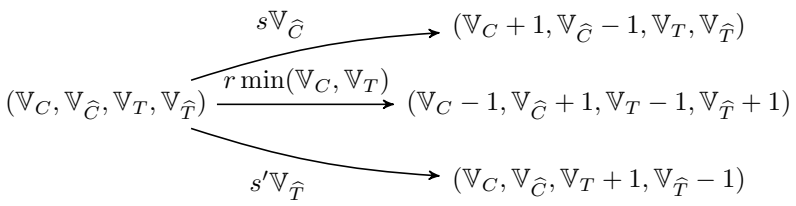

Figure 2.3: Generic state of the lumped CTMC defined in (2.4).

2.4 Fluid Process Algebra

In this section, we study the fluid semantics of PEPA. Let us start by recalling that the model *Sys* from (2.2) has $|ds(Sys)| = 2^{N_C+N_T}$ states. As a first step toward fluid analysis, we now consider a smaller CTMC which can be exactly related to the original one in the sense of ordinary lumpability, cf. Theorem 2. This lumped CTMC is a *population process*, i.e. it keeps track of the number of copies of each sequential component in the model. We will make use of the following preliminaries.

Definition 11. *Fix a PEPA model G.*
i) The set of sequential components of G, denoted by $\mathcal{B}(G)$, is defined as

$$\mathcal{B}(S) := ds(S), \qquad \mathcal{B}(G_0 \underset{L}{\bowtie} G_1) := \mathcal{B}(G_0) \cup \mathcal{B}(G_1).$$

ii) For any $P \in \mathcal{B}(G)$, the number of occurrences of P in a PEPA process $G' \in ds(G)$ is denoted by $\mathcal{C}(G', P)$.

Note that $\mathcal{B}(G)$ is not a multiset. Rather, any sequential component which is a subprocess of some $G' \in ds(G)$, must be an element of $\mathcal{B}(G)$.

Let $Sys(t)$ denote the CTMC induced by *Sys*. Then, the stochastic process

$$\mathbb{V}(t) = (\mathbb{V}_C(t), \mathbb{V}_{\widehat{C}}(t), \mathbb{V}_T(t), \mathbb{V}_{\widehat{T}}(t)), \quad \text{with} \quad \mathbb{V}_P(t) := \mathcal{C}(Sys(t), P), \tag{2.4}$$

where $P \in \mathcal{B}(Sys) = \{C, \widehat{C}, T, \widehat{T}\}$ and $t \geq 0$, can be shown to be the lumped CTMC of $Sys(t)$. (A proof is given in Appendix A.1.) The lumped CTMC has $(N_C+1)(N_T+1)$ states and is fully characterised by its generic state in Fig. 2.3. By assuming that the initial populations scale with N, i.e. $N_C = v_c(0)N$ and $N_T = v_T(0)N$ for some $v_T(0), v_C(0) > 0$, we can consider the scaled version of the lumped CTMC $\frac{1}{N}\mathbb{V}(t)$. Note that the rates in Figure 2.3 can be expressed in terms of concentrations, e.g. $\frac{1}{N}\left(r \min(\mathbb{V}_C, \mathbb{V}_T)\right) = r \min(\frac{\mathbb{V}_C}{N}, \frac{\mathbb{V}_T}{N})$, $\frac{1}{N}\left(s\mathbb{V}_{\widehat{C}}\right) = s\frac{\mathbb{V}_{\widehat{C}}}{N}$ and $\frac{1}{N}\left(s'\mathbb{V}_{\widehat{T}}\right) = s'\frac{\mathbb{V}_{\widehat{T}}}{N}$. Since the generic state $(\frac{1}{N}\mathbb{V}_C, \frac{1}{N}\mathbb{V}_{\widehat{C}}, \frac{1}{N}\mathbb{V}_T, \frac{1}{N}\mathbb{V}_{\widehat{T}})$ makes jumps of order $1/N$, e.g. the synchronisation leads to a change in the state with a vector $(-\frac{1}{N}, +\frac{1}{N}, -\frac{1}{N}, +\frac{1}{N})$, this motivates to approximate the scaled CTMC in the case of large N by the ODE system

$$\begin{aligned} \dot{v}_C &= -r \min(v_C, v_T) + s v_{\widehat{C}} & \dot{v}_{\widehat{C}} &= +r \min(v_C, v_T) - s v_{\widehat{C}} \\ \dot{v}_T &= -r \min(v_C, v_T) + s' v_{\widehat{T}} & \dot{v}_{\widehat{T}} &= +r \min(v_C, v_T) - s' v_{\widehat{T}} \end{aligned} \tag{2.5}$$

subjected to the initial condition for the *concentrations*

$$v_C(0) = (1/N)N_C \qquad v_{\widehat{C}}(0) = (1/N)N_{\widehat{C}}$$
$$v_T(0) = (1/N)N_T \qquad v_{\widehat{T}}(0) = (1/N)N_{\widehat{T}}$$

The above discussion suggests that fluid approximation is the limit of a *sequence* of CTMCs indexed by N.

Instead of working with PEPA, we find it more convenient to introduce a new process algebra called Fluid Process Algebra (FPA). Each FPA process is a generator of a *sequence of PEPA models*, indexed by the parameter N, such that larger N lead to larger initial populations of sequential processes. This allows us to state the convergence to a system of ODEs as $N \to \infty$.

Definition 12 (FPA Model)**.** *An FPA model M is given by the grammar*

$$M ::= M \underset{L}{\bowtie} M \mid P,$$

where $L \subseteq \mathcal{A}$ and P is a PEPA constant. Without loss of generality, for any distinct constants in M, P and P', we require that $ds(P) \cap ds(P') = \emptyset$, where equality between processes is intended to be syntactical equality.

The following is needed to define the sequence of generated PEPA models.

Definition 13. *Let M be an FPA model. Then:*

1. *The set of* labels *or* fluid atoms *of M, denoted by $\mathcal{G}(M)$, is given by*

$$\mathcal{G}(P) := \{P\}, \qquad \mathcal{G}(M_0 \underset{L}{\bowtie} M_1) := \mathcal{G}(M_0) \cup \mathcal{G}(M_1).$$

2. *The set of sequential components of M, $\mathcal{B}(M)$, is given by*

$$\mathcal{B}(P) := ds(P), \qquad \mathcal{B}(M_0 \underset{L}{\bowtie} M_1) := \mathcal{B}(M_0) \cup \mathcal{B}(M_1).$$

3. *A function $v : X \to \mathbb{R}_{\geq 0}$ with $\mathcal{B}(M) \subseteq X$ is a concentration function of M.*

4. *A function $V : X \to \mathbb{N}_0$ with $\mathcal{B}(M) \subseteq X$ is a population function of M.*

5. *For a population function V of M, the underlying PEPA model M_V is inductively given as follows.*

   - *If $M = P$: Using $V_P := V(P)$ for all $P \in domain(V)$, we define*

     $$P_V := P_1[V_{P_1}] \parallel P_2[V_{P_2}] \parallel \ldots \parallel P_n[V_{P_n}], \quad \text{for } ds(P) = \{P_1, \ldots, P_n\}.$$

   - *If $M = M^0 \underset{L}{\bowtie} M^1$: We define then $M_V := M^0_V \underset{L}{\bowtie} M^1_V$.*

For instance, let us fix the FPA model

$$\mathcal{M} := C \underset{\{exec\}}{\bowtie} T, \tag{2.6}$$

where C and T are as in (2.1), and the population function $V(0)$ of $\mathcal{M}$ such that

$$V(0)_C = N_C, \qquad V(0)_{\widehat{C}} = 0, \qquad V(0)_T = N_T, \qquad V(0)_{\widehat{T}} = 0.$$

Then, the lumped CTMC of $\mathcal{M}_{V(0)}$ corresponds to the lumped CTMC of *Sys*.

We now turn to the general case, starting with the definition of the lumped CTMC $\mathbb{V}(t)$. For an arbitrary FPA model M and a population function $V(0)$ of M, let $G(t)$ denote the CTMC induced by $M_{V(0)}$. Then, the population process

$$\mathbb{V}(t) = (\mathbb{V}(t)_P)_{P \in \mathcal{B}(M)}, \qquad \text{with} \quad \mathbb{V}(t)_P = \mathcal{C}(G(t), P),$$

is a CTMC which is related in the sense of ordinary lumpability to $G(t)$, cf. Appendix A.1. The next definitions are needed to define the underlying ODE system of an FPA model M and are similar to those in [17, 42].

Definition 14 (Fluid Apparent Rate)**.** *For an FPA model M, $\alpha \in \mathcal{A}$ and a concentration function v, the* fluid apparent rate *is given as follows.*

$$r_\alpha(M_0 \underset{L}{\bowtie} M_1, v) := \begin{cases} r_\alpha(M_0, v) + r_\alpha(M_1, v) & , \ \alpha \notin L \\ \min(r_\alpha(M_0, v), r_\alpha(M_1, v)) & , \ \alpha \in L \end{cases}$$
$$r_\alpha(P, v) := \sum_{P' \in ds(P)} v_{P'} r_\alpha(P'),$$

where $r_\alpha(P')$ denotes the apparent rate according to Definition 3.

Definition 15 (Fluid Component Rate)**.** *Let M be an FPA model, $\alpha \in \mathcal{A}$ and v be a concentration function. The* fluid component rate *of $P' \in \mathcal{B}(M)$ is given by*

- Synchronised cooperation: *if $P' \in \mathcal{G}(M_i)$, $i = 0, 1$, and $\alpha \in L$ then*

$$\mathcal{R}_\alpha(M_0 \underset{L}{\bowtie} M_1, v, P') := \frac{\mathcal{R}_\alpha(M_i, v, P')}{r_\alpha(M_i, v)} r_\alpha(M_0 \underset{L}{\bowtie} M_1, v).$$

- Unsynchronised cooperation: *if $P' \in \mathcal{G}(M_i)$, $i = 0, 1$, and $\alpha \notin L$ then*

$$\mathcal{R}_\alpha(M_0 \underset{L}{\bowtie} M_1, v, P') := \mathcal{R}_\alpha(M_i, v, P').$$

- Fluid atom: *then it holds that $M = P$ and*

$$\mathcal{R}_\alpha(P, v, P') := v_{P'} r_\alpha(P').$$

Before defining the underlying ODE system of an FPA model M using the notion of fluid component rate, we connect the latter to the CTMC $G(t)$ using Theorem 2.15 from [17]. For this, let us first introduce the *derivative weighting function*

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

Informally, $p_\alpha(P, P')$ refers to the probability that P becomes P' after performing an α action. Then, according to the aforementioned theorem, it holds that the sum of the α-transitions rates of $G(t)$ which increase the number of P's in the model is

$$\sum_{P' \in \mathcal{B}(M) \setminus \{P\}} p_\alpha(P', P) \mathcal{R}_\alpha(M, \mathbb{V}(t), P'),$$

while the sum of the α-transitions rates of $G(t)$ which decrease the number of P's is

$$\sum_{P' \in \mathcal{B}(M) \setminus \{P\}} p_\alpha(P, P') \mathcal{R}_\alpha(M, \mathbb{V}(t), P),$$

where $\alpha \in \mathcal{A}$ and $P \in \mathcal{B}(M)$. Intuitively, this allows us to calculate the net change of $\mathbb{V}_P(t)$ due to all α-transitions as the difference

$$\begin{aligned}
&\sum_{P' \in \mathcal{B}(M) \setminus \{P\}} p_\alpha(P', P) \mathcal{R}_\alpha(M, \mathbb{V}(t), P') - \sum_{P' \in \mathcal{B}(M) \setminus \{P\}} p_\alpha(P, P') \mathcal{R}_\alpha(M, \mathbb{V}(t), P) \\
&\quad = \sum_{P' \in \mathcal{B}(M)} p_\alpha(P', P) \mathcal{R}_\alpha(M, \mathbb{V}(t), P') - \sum_{P' \in \mathcal{B}(M)} p_\alpha(P, P') \mathcal{R}_\alpha(M, \mathbb{V}(t), P) \\
&\quad = \sum_{P' \in \mathcal{B}(M)} p_\alpha(P', P) \mathcal{R}_\alpha(M, \mathbb{V}(t), P') - \mathcal{R}_\alpha(M, \mathbb{V}(t), P),
\end{aligned}$$

where the last equation follows by $\sum_{P' \in \mathcal{B}(M)} p_\alpha(P, P') = 1$. This motivates the following definition.

Definition 16. *Throughout the thesis, we adopt Newton's dot notation for derivatives with respect to time, i.e. $\dot{x}$ refers to $\frac{d}{dt}x$. The ODE system of an FPA model M, $\dot{v} = F(M, v)$, is defined, in components, by*

$$\dot{v}_P = \sum_{\alpha \in \mathcal{A}} \Big(\Big(\sum_{P' \in \mathcal{B}(M)} p_\alpha(P', P) \mathcal{R}_\alpha(M, v, P') \Big) - \mathcal{R}_\alpha(M, v, P) \Big), \text{ with } P \in \mathcal{B}(M).$$

We are now in a position to formally state the convergence result of the fluid approximation.

Theorem 5. *Let us fix an FPA model M and an initial concentration function $v(0) : \mathcal{B}(M) \to \mathbb{R}_{\geq 0}$. Then, $\dot{v} = F(M, v)$ subject to $v(0)$ has a unique solution v in $\mathbb{R}^{|\mathcal{B}(M)|}$ whose time domain contains $[0; \infty)$. Moreover, define $V^N(0)$ to be the population function*

$$\big(V^N(0)\big)_P = \lfloor N v(0)_P \rfloor, \qquad \text{with} \quad P \in \mathcal{B}(M),$$

and let $\mathbb{V}^N(t)$ *denote the lumped CTMC induced by* $M_{V^N(0)}$*. Then, for all* $T > 0$*,*

$$\lim_{N\to\infty} \mathbb{P}\left\{ \sup_{0\le t\le T} \left\| \frac{1}{N}\mathbb{V}^N(t) - v(t) \right\| > \varepsilon \right\} = 0, \qquad \forall \varepsilon > 0.$$

Proof. The proof is routine, by modern standards, and is a combination of Theorem 2.11 from [53], Theorem 2.15 from [17] and Lemma B.1 from [54]. It can be found in Appendix A.1. □

For instance, the above theorem ensures that $(\frac{1}{N}\mathbb{V}^N(t))_{t\ge 0}$ from (2.4) converges in probability to the solution of the ODE (2.5) as $N \to \infty$, provided that

$$\mathbb{V}^N(0) = (\mathbb{V}^N_C(0), \mathbb{V}^N_{\hat{C}}(0), \mathbb{V}^N_T(0), \mathbb{V}^N_{\hat{T}}(0)) = (\lfloor N v_C(0) \rfloor, 0, \lfloor N v_T(0) \rfloor, 0).$$

2.5 Well-Posedness

This section introduces the notion of well-posedness, which will be shown later to be a necessary condition to imply semi-isomorphism in the context of fluid lumpability. Moreover, it is shown that for any FPA model M there exists a well-posed model $\Theta(M)$ with an ODE system which is, after a renaming of variables, equal to the one induced by M. We start with the definition of well-posedness.

Definition 17 (Well-Posedness)**.** *An FPA model* M *is well-posed if for all occurrences* $M_1 \underset{L}{\bowtie} M_2$ *in* M *it holds* $\exists v_1.\big(r_\alpha(M_1, v_1) > 0\big) \wedge \exists v_2.\big(r_\alpha(M_2, v_2) > 0\big)$ *for all* $\alpha \in L$*.*

In essence, a model is well-posed whenever any synchronised action may be performed by both operands, for some concentration function. In order to build intuition on such a restriction, it is useful to consider a sample model which is not well-posed, that is, ill-posed. The model is defined as

$$IP := P_1 \underset{\{\alpha,\delta_1,\delta_2\}}{\bowtie} Q_1, \tag{2.7}$$

with

$$\begin{aligned} P_1 &\stackrel{def}{=} (\alpha, r).P_2 + (\delta_3, u).P_2 & Q_1 &\stackrel{def}{=} (\delta_1, u).Q_2 \\ P_2 &\stackrel{def}{=} (\delta_2, u).P_1 & Q_2 &\stackrel{def}{=} (\alpha, r).Q_1 + (\delta_3, u).Q_1 \end{aligned} \tag{2.8}$$

The model is ill-posed with respect to action types δ_1 and δ_2. For δ_1, it is clear that there exists no concentration function v such that $r_{\delta_1}(P_1, v) \neq 0$, whereas $r_{\delta_1}(Q_1, v) = u v_{Q_1}$; a similar observation holds for δ_2. Clearly, the presence of ill-posedness may be a symptom of potential problems in the model description, since synchronising a process which can perform a certain action α with another model which cannot is not meaningful.

Since well-posedness is only concerned with action types belonging to cooperation sets, IP could be transformed into a well-posed model by *removing* δ_1

and δ_2 from its only cooperation set and considering only $\bowtie_{\{\alpha\}}$. However, just this change would give rise to a completely different behaviour, because now δ_1- and δ_2-activities may be observed. Let us now *stop* the occurrence of such action by replacing the strictly positive rate u with 0. Formally, we are considering an extension of PEPA/FPA. However, this is harmless because all the definitions, statements and proofs defined herein carry over straightforwardly. Intuitively, this is because zero-transitions disappear in the underlying mathematical object for the analysis: in the case of a CTMC, such transitions would correspond to zero-entries in the generator matrix, whereas in the fluid semantics zero-rates for unsynchronised actions provide symbolic component rates and apparent rates that always evaluate to zero. Thus, let us consider the as-transformed *well-posed* model

$$\hat{IP} := \hat{P}_1 \underset{\{\alpha\}}{\bowtie} \hat{Q}_1$$

with

$$\hat{P}_1 \stackrel{def}{=} (\alpha, r).\hat{P}_2 + (\delta_3, u).\hat{P}_2 \qquad \hat{P}_2 \stackrel{def}{=} (\delta_2, 0).\hat{P}_1$$
$$\hat{Q}_1 \stackrel{def}{=} (\delta_1, 0).\hat{Q}_2 \qquad \hat{Q}_2 \stackrel{def}{=} (\alpha, r).\hat{Q}_1 + (\delta_3, u).\hat{Q}_1$$

and denote the fluid approximation of IP and $\hat{IP}$ by v and $\mathfrak{v}$, respectively. It is easy to see that IP and $\hat{IP}$ yield, after a renaming of variables, the same ODE systems. Indeed, it holds that $v_T(t) = \mathfrak{v}_{\hat{T}}(t)$ for all $T \in \mathcal{B}(IP)$ and $t > 0$, if the same holds at $t = 0$.

To sum up, by removing blocked actions from cooperation sets and stopping them in the sequential components, we transformed an ill-posed model into a well-posed model in such a way that the underlying ODE systems are equal up to a renaming of variables. In particular, the transformation of M into $\Theta(M)$ happens by modifying only the sequential components and cooperation sets of the former, meaning that the global structure of M is not affected. Thus, we may study the well-posed model $\hat{IP}$, instead of the ill-posed one IP for the purposes of fluid analysis.

The remainder of this section provides concepts and results for carrying out this transformation in general. Definition 18 performs the transformation of an FPA model by introducing zero-transitions.

Definition 18 (Stop Function)**.** *Let M be an FPA model and $\alpha \in \mathcal{A}$. The stop function is given by*

$$st(M_0 \underset{L}{\bowtie} M_1, \alpha) := st(M_0, \alpha) \underset{L}{\bowtie} st(M_1, \alpha)$$
$$st(S, \alpha) := st'(S, \alpha)$$

where $st'(S, \alpha)$ arises from S by setting the rates of all α transitions to 0, i.e.

$$st'\Big(\sum_{i\in I}(\alpha_i, r_i).P_i, \alpha\Big) := \sum_{i\in I:\alpha_i\neq\alpha}(\alpha_i, r_i).st'(P_i, \alpha) + \sum_{i\in I:\alpha_i=\alpha}(\alpha_i, 0).st'(P_i, \alpha)$$
$$st'(P, \alpha) := P^{\diamondsuit} \quad \textit{and} \quad P^{\diamondsuit} \stackrel{\text{def}}{=} st'(S, \alpha), \quad \textit{if} \quad P \stackrel{\text{def}}{=} S$$

For instance, applying st to P_1 from (2.8) using δ_2, $st(P_1, \delta_2)$, yields $P_1^\diamondsuit$ where $P_1^\diamondsuit \stackrel{def}{=} (\alpha, r).P_2^\diamondsuit + (\delta_3, u).P_2^\diamondsuit$ and $P_2^\diamondsuit \stackrel{def}{=} (\delta_2, 0).P_1^\diamondsuit$. A further application with respect to δ_3 would yield $st(P_1^\diamondsuit, \delta_3) = P_1^{\diamondsuit\diamondsuit}$ where $P_1^{\diamondsuit\diamondsuit} \stackrel{def}{=} (\alpha, r).P_2^{\diamondsuit\diamondsuit} + (\delta_3, 0).P_2^{\diamondsuit\diamondsuit}$ and $P_2^{\diamondsuit\diamondsuit} \stackrel{def}{=} (\delta_2, 0).P_1^{\diamondsuit\diamondsuit}$. That is, the *stop* function transforms the constants by appending the FPA label under which the PEPA component is placed at each application. However, the function does not add or remove constants. Therefore, there is a bijection between the constants of a model M and those of $st(M, \alpha)$, for any α. In what follows, $\diamondsuit(P)$ denotes the unique counterpart of P in a model M subjected to the stop function. This notion is formalised in the next proposition which is the key ingredient of our transformation.

Proposition 1. *Let M_0 and M_1 be two well-posed FPA models such that $\exists v.(r_\delta(M_0, v) \neq 0)$ and $\forall v.(r_\delta(M_1, v) = 0)$ for some $\delta \in L \subseteq \mathcal{A}$. Together with*

$$\diamondsuit(P) = \begin{cases} P & , \ P \in \mathcal{B}(st(M_0, \delta) \underset{L\setminus\{\delta\}}{\bowtie} M_1) \\ \diamondsuit(P^\diamondsuit) & , \ \textit{otherwise} \end{cases}$$

where $P \in \mathcal{B}(M_0 \underset{L}{\bowtie} M_1)$, the following can be shown.

- *For all $\alpha \in \mathcal{A}$, $P \in \mathcal{B}(M_0 \underset{L}{\bowtie} M_1)$ and concentration functions v of $M_0 \underset{L}{\bowtie} M_1$ it holds that*

$$r_\alpha(M_0 \underset{L}{\bowtie} M_1, v) = r_\alpha(st(M_0, \delta) \underset{L\setminus\{\delta\}}{\bowtie} M_1, \mathfrak{v})$$
$$\mathcal{R}_\alpha(M_0 \underset{L}{\bowtie} M_1, v, P) = \mathcal{R}_\alpha(st(M_0, \delta) \underset{L\setminus\{\delta\}}{\bowtie} M_1, \mathfrak{v}, \diamondsuit(P)),$$

  where $\mathfrak{v}_{\diamondsuit(P)} := v_P$ for all $P \in \mathcal{B}(M_0 \underset{L}{\bowtie} M_1)$. That is, by stopping and removing the δ-action, the fluid rates of $M_0 \underset{L}{\bowtie} M_1$ can be expressed by those of $st(M_0, \delta) \underset{L\setminus\{\delta\}}{\bowtie} M_1$.

- *The ODE systems underlying $M_0 \underset{L}{\bowtie} M_1$ and $st(M_0, \delta) \underset{L\setminus\{\delta\}}{\bowtie} M_1$ are equal up to a renaming of variables. Thus, if $v(0)$ is the initial concentration function of $M_0 \underset{L}{\bowtie} M_1$ and $\mathfrak{v}_{\diamondsuit(P)}(0) := v_P(0)$ for all $P \in \mathcal{B}(M_0 \underset{L}{\bowtie} M_1)$, then it holds that $\mathfrak{v}_{\diamondsuit(P)}(t) = v_P(t)$ for all $P \in \mathcal{B}(M_0 \underset{L}{\bowtie} M_1)$ and $t \geq 0$, if v and $\mathfrak{v}$ are the fluid approximation of $M_0 \underset{L}{\bowtie} M_1$ and $st(M_0, \delta) \underset{L\setminus\{\delta\}}{\bowtie} M_1$, respectively.*

Proof. We prove the statements separately.

- If $\alpha = \delta$, we note that the definition of st implies $r_\delta(st(M_0, \delta), \mathfrak{v}) = 0$ and that $r_\delta(M_1, \mathfrak{v}) = 0$ due to the assumption $\forall v.(r_\delta(M_1, v) = 0)$. The case $\alpha \neq \delta$ follows by showing that for all FPA models M, concentration functions v of M and $\alpha \in \mathcal{A} \setminus \{\delta\}$ it holds

$$r_\alpha(M, v) = r_\alpha(st(M, \delta), \mathfrak{v}),$$
$$\mathcal{R}_\alpha(M, v, P) = \mathcal{R}_\alpha(st(M, \delta), \mathfrak{v}, \diamondsuit(P)), \quad \forall P \in \mathcal{B}(M),$$

where $\mathfrak{v}_{\diamondsuit(P)} := v_P$ for all $P \in \mathcal{B}(M)$. The proof is by means of structural induction and is straightforward.

- Let us fix an arbitrary $P \in \mathcal{B}(M_0 \underset{L}{\bowtie} M_1)$. Using the abbreviation $S := \mathcal{B}\big(M_0 \underset{L}{\bowtie} M_1\big)$, the first half implies

$$\sum_{\alpha\in\mathcal{A}} \Big(\sum_{\widetilde{P}\in S} p_\alpha(\widetilde{P}, P)\mathcal{R}_\alpha(M_0 \underset{L}{\bowtie} M_1, v, \widetilde{P}) - \mathcal{R}_\alpha(M_0 \underset{L}{\bowtie} M_1, v, P)\Big) =$$
$$= \sum_{\alpha\in\mathcal{A}} \Big(\sum_{\widetilde{P}\in S} p_\alpha(\diamondsuit(\widetilde{P}), \diamondsuit(P))\mathcal{R}_\alpha(st(M_0,\delta) \underset{L\setminus\{\delta\}}{\bowtie} M_1, \mathfrak{v}, \diamondsuit(\widetilde{P})) - \mathcal{R}_\alpha(st(M_0,\delta) \underset{L\setminus\{\delta\}}{\bowtie} M_1, \mathfrak{v}, \diamondsuit(P))\Big),$$

where $\mathfrak{v}_{\diamondsuit(P)} := v_P$ for all $P \in \mathcal{B}(M_0 \underset{L}{\bowtie} M_1)$, and Definition 16 yields the claim.

□

Let us use the above proposition to transform the ill-posed model IP from (2.7). As fluid atoms are always well-posed, the proposition asserts that the fluid approximation of IP is exactly related to that of $st(P_1, \delta_2) \underset{\{\alpha,\delta_1\}}{\bowtie} Q_1 = P_1^\diamondsuit \underset{\{\alpha,\delta_1\}}{\bowtie} Q_1$. A further application of the proposition shows that the fluid approximation of $P_1^\diamondsuit \underset{\{\alpha,\delta_1\}}{\bowtie} Q_1$ is related in an exact way to that of $WP := P_1^\diamondsuit \underset{\{\alpha\}}{\bowtie} st(Q_1, \delta_1) = P_1^\diamondsuit \underset{\{\alpha\}}{\bowtie} Q_1^\diamondsuit$. Thus, the fluid approximation of the ill-posed model IP is related in an exact way to that of a well-posed model WP.

Proposition 1 can be used to transform more complex models. Consider, for instance, the model $IP \underset{\{\alpha,\delta_3\}}{\bowtie} R_1$, where IP cooperates with a fluid atom given by $R_1 \stackrel{def}{=} (\alpha, r).R_2$ and $R_2 \stackrel{def}{=} (\beta, s).R_1$. Note that in this model the ill-posedness arises not only from δ_1 and δ_2, but also from δ_3. Fortunately, Proposition 1 applies for compositional reasoning. To see this, we need the following auxiliary result which states, informally, that if the models M^i and $\tilde{M}^i$ have the same fluid rates, where $i = 1, 2$, then so do also the compositions $M^1 \underset{L}{\bowtie} M^2$ and $\tilde{M}^1 \underset{L}{\bowtie} \tilde{M}^2$.

Lemma 1. *For a given FPA model M^i, where $i = 1, 2$, assume that there exist an FPA model $\tilde{M}^i$ and a bijection $\sigma^i : \mathcal{B}(M^i) \to \mathcal{B}(\tilde{M}^i)$ such that for all concentration functions v^i of M^i, $\alpha \in \mathcal{A}$ and $P \in \mathcal{B}(M^i)$ it holds that $r_\alpha(M^i, v^i) = r_\alpha(\tilde{M}^i, \mathfrak{v}^i)$ and $\mathcal{R}_\alpha(M^i, v^i, P) = \mathcal{R}_\alpha(\tilde{M}^i, \mathfrak{v}^i, \sigma^i(P))$ with $\mathfrak{v}^i_{\sigma^i(Q)} := v^i_Q$ for all $Q \in \mathcal{B}(M^i)$. Then, for any cooperation set L and $\mathfrak{v}_{\sigma(Q)} := v_Q$, where*

$$v_P := \begin{cases} v^1_P & , \ P \in \mathcal{B}(M^1) \\ v^2_P & , \ P \in \mathcal{B}(M^2) \end{cases} \qquad \sigma(P) := \begin{cases} \sigma^1(P) & , \ P \in \mathcal{B}(M^1) \\ \sigma^2(P) & , \ P \in \mathcal{B}(M^2) \end{cases}$$

it holds that

$$r_\alpha(M^1 \underset{L}{\bowtie} M^2, v) = r_\alpha(\tilde{M}^1 \underset{L}{\bowtie} \tilde{M}^2, \mathfrak{v})$$
$$\mathcal{R}_\alpha(M^1 \underset{L}{\bowtie} M^2, v, P) = \mathcal{R}_\alpha(\tilde{M}^1 \underset{L}{\bowtie} \tilde{M}^2, \mathfrak{v}, \sigma(P)), \quad \forall P \in \mathcal{B}(M^1 \underset{L}{\bowtie} M^2)$$

Proof. A straightforward application of Definition 14 and 15 yields the claim. □

For instance, to derive the well-posed transform of $IP \underset{\{\alpha,\delta_3\}}{\bowtie} R_1$, we first transform IP into WP. In the second step, we observe that the ODE systems of $IP \underset{\{\alpha,\delta_3\}}{\bowtie} R_1$ and $WP \underset{\{\alpha,\delta_3\}}{\bowtie} R_1$ are equal up to renaming. We do so by noting that the first half of Proposition 1 implies the assumptions of Lemma 1 in the case of $M^1 := IP$, $\tilde{M}^1 := WP$ and $M^2 := \tilde{M}^2 := R_1$. At last, we apply in the third step Proposition 1 to the well-posed models WP and R_1. This shows that the ODE system of $WP \underset{\{\alpha,\delta_3\}}{\bowtie} R_1$ is equal up to renaming to that of $st(WP, \delta_3) \underset{\{\alpha\}}{\bowtie} R_1 = (P_1^{\diamond\diamond} \underset{\{\alpha\}}{\bowtie} Q_1^{\diamond\diamond}) \underset{\{\alpha\}}{\bowtie} R_1$, where

$$P_1^{\diamond\diamond} \overset{def}{=} (\alpha, r).P_2^{\diamond\diamond} + (\delta_3, 0).P_2^{\diamond\diamond} \qquad P_2^{\diamond\diamond} \overset{def}{=} (\delta_2, 0).P_1^{\diamond\diamond}$$
$$Q_1^{\diamond\diamond} \overset{def}{=} (\delta_1, 0).Q_2^{\diamond\diamond} \qquad Q_2^{\diamond\diamond} \overset{def}{=} (\alpha, r).Q_1^{\diamond\diamond} + (\delta_3, 0).Q_1^{\diamond\diamond}$$

The algorithm discussed in the above example is generalised in the next definition.

Definition 19. *Let us fix an FPA model M. The well-posed transformation $\Theta(M)$ of M is given by*

$$\Theta(P) := P, \qquad \Theta(M_0 \underset{L}{\bowtie} M_1) := \Theta_0\big(\Theta(M_0) \underset{L}{\bowtie} \Theta(M_1)\big),$$

where Θ_0 transforms a not necessarily well-posed cooperation $M_0 \underset{L}{\bowtie} M_1$ of two well-posed models M_0 and M_1 into a well-posed cooperation $\Theta_0(M_0 \underset{L}{\bowtie} M_1)$ by means of the following case distinction.

- *$M_0 \underset{L}{\bowtie} M_1$ is well-posed: we set then $\Theta_0(M_0 \underset{L}{\bowtie} M_1) := M_0 \underset{L}{\bowtie} M_1$.*
- *$M_0 \underset{L}{\bowtie} M_1$ is not well-posed: let us fix* all *actions $\eta_1, \ldots, \eta_k \in L$ such that $\forall v.(r_{\eta_n}(M_0, v) = 0 \wedge r_{\eta_n}(M_1, v) = 0)$, where $1 \leq n \leq k$, and* all *actions $\delta_1, \ldots, \delta_m \in L$ such that $\exists v(r_{\delta_n}(M_{i_n}, v) \neq 0)$ and $\forall v.(r_{\delta_n}(M_{i'_n}, v) = 0)$ for some $i_n \in \{0, 1\}$ and $i'_n := 1 - i_n$, where $1 \leq n \leq m$. Then, we first remove all η_n- and δ_n-actions from L and stop afterwards each δ_n-action present in M_0 and M_1. More formally, we set $\Theta_0(M_0 \underset{L}{\bowtie} M_1) := M_0^m \underset{L \setminus \{\eta_1, \ldots, \eta_k, \delta_1, \ldots, \delta_m\}}{\bowtie} M_1^m$, where $M_j^0 := M_j$ and*

$$M_j^n := \begin{cases} st(M_j^{n-1}, \delta_n) & , \ \exists v.(r_{\delta_n}(M_j^{n-1}, v) \neq 0) \\ M_j^{n-1} & , \ otherwise \end{cases}$$

for $j = 0, 1$ and $1 \leq n \leq m$.

Similarly to Proposition 1, $\diamondsuit(P) \in \mathcal{B}(\Theta(M))$ refers to the unique counterpart of $P \in \mathcal{B}(M)$ and is given as follows.

Definition 20. *For a given FPA model M and $P \in \mathcal{B}(M)$, define $\diamondsuit(P) \equiv \diamondsuit(P, M)$ by*

$$\diamondsuit(P, M) = \begin{cases} P & , \ P \in \mathcal{B}(\Theta(M)) \\ \diamondsuit(P^{\diamondsuit}, M) & , \ \textit{otherwise} \end{cases}$$

We are now in a position to state the main result of this section.

Theorem 6. *The ODE systems underlying an FPA model M and its well-posed transformation $\Theta(M)$ are equal up to a renaming of variables. Specifically, if $v(0)$ is the initial concentration function of M and $\mathfrak{v}_{\diamondsuit(P)}(0) := v_P(0)$ for all $P \in \mathcal{B}(M)$, then it holds $\mathfrak{v}_{\diamondsuit(P)}(t) = v_P(t)$ for all $P \in \mathcal{B}(M)$ and $t \geq 0$, where v and $\mathfrak{v}$ denote the fluid approximation of M and $\Theta(M)$, respectively.*

Proof. We show the following three properties which readily imply the claim.

1) $r_\alpha(M, v) = r_\alpha(\Theta(M), \mathfrak{v})$ for all $\alpha \in \mathcal{A}$.

2) $\mathcal{R}_\alpha(M, v, P) = \mathcal{R}_\alpha(\Theta(M), \mathfrak{v}, \diamondsuit(P))$ for all $\alpha \in \mathcal{A}$ and $P \in \mathcal{B}(M)$.

3) The ODE systems of M and $\Theta(M)$ are equal up to a renaming of variables.

The proof is by means of structural induction on M.

- $M = P$: In the case where M is a fluid atom, the claim trivially holds since $\Theta(M)$ is syntactically equivalent to M.
- $M = M_0 \underset{L}{\bowtie} M_1$: The induction hypothesis ensures that 1) - 3) hold for $\Theta(M_0)$ and $\Theta(M_1)$. Using Lemma 1, we infer that 1) and 2) apply also for $M_0 \underset{L}{\bowtie} M_1$. By making a case distinction on the value of $p_\alpha(\diamondsuit(\widetilde{P}), \diamondsuit(P))$, where $P, \tilde{P} \in \mathcal{B}(M)$ are arbitrary but fixed, we next show that

$$\begin{aligned} p_\alpha(\widetilde{P}, P)\mathcal{R}_\alpha(M_0 \underset{L}{\bowtie} M_1, v, \widetilde{P}) = \\ = p_\alpha(\diamondsuit(\widetilde{P}), \diamondsuit(P))\mathcal{R}_\alpha(\Theta(M_0) \underset{L}{\bowtie} \Theta(M_1), \mathfrak{v}, \diamondsuit(\widetilde{P})) \end{aligned} \quad (2.9)$$

  Let us assume without loss of generality that there exists a $Q \in \mathcal{G}(M)$ such that $P, \widetilde{P} \in ds(Q)$.

  a) $p_\alpha(\diamondsuit(\widetilde{P}), \diamondsuit(P)) > 0$: Definition 19 implies that the α-action was not stopped in the fluid atom Q, meaning that $p_\alpha(\diamondsuit(\widetilde{P}), \diamondsuit(P)) = p_\alpha(\widetilde{P}, P)$. This and the fact that $M_0 \underset{L}{\bowtie} M_1$ satisfies 2) shows (2.9).

  b) $p_\alpha(\diamondsuit(\widetilde{P}), \diamondsuit(P)) = 0$ and $p_\alpha(\widetilde{P}, P) = 0$: trivial.

  c) $p_\alpha(\diamondsuit(\widetilde{P}), \diamondsuit(P)) = 0$ and $p_\alpha(\widetilde{P}, P) > 0$: Definition 19 implies that the α-action was stopped in the fluid atom Q, hence $r_\alpha(\diamondsuit(\widetilde{P})) = 0$. This yields $0 = \mathcal{R}_\alpha(\Theta(M_0) \underset{L}{\bowtie} \Theta(M_1), \mathfrak{v}, \diamondsuit(\widetilde{P})) = \mathcal{R}_\alpha(M_0 \underset{L}{\bowtie} M_1, v, \widetilde{P})$, where the last equality follows by 2), which readily implies (2.9).

Using 2) and (2.9) we infer

$$\begin{aligned}
&\sum_{\alpha\in\mathcal{A}}\Big(\sum_{\widetilde{P}\in\mathcal{B}(M)} p_\alpha(\widetilde{P},P)\mathcal{R}_\alpha(M_0 \underset{L}{\bowtie} M_1,v,\widetilde{P}) - \mathcal{R}_\alpha(M_0 \underset{L}{\bowtie} M_1,v,P)\Big)\\
&=\sum_{\alpha\in\mathcal{A}}\Big(\sum_{\widetilde{P}\in\mathcal{B}(M)} p_\alpha(\diamondsuit(\widetilde{P}),\diamondsuit(P))\mathcal{R}_\alpha(\Theta(M_0) \underset{L}{\bowtie} \Theta(M_1),\mathfrak{v},\diamondsuit(\widetilde{P}))\\
&\qquad\qquad - \mathcal{R}_\alpha(\Theta(M_0) \underset{L}{\bowtie} \Theta(M_1),\mathfrak{v},\diamondsuit(P))\Big),
\end{aligned}$$

which shows that the ODE systems of $M_0 \underset{L}{\bowtie} M_1$ and $\Theta(M_0) \underset{L}{\bowtie} \Theta(M_1)$ are equal up to a renaming of variables. Since Proposition 1 ensures that $\Theta(M_0) \underset{L}{\bowtie} \Theta(M_1)$ and $\Theta_0(\Theta(M_0) \underset{L}{\bowtie} \Theta(M_1))$ satisfy 1) - 3), this yields the claim.

□

Chapter 3

Exact Fluid Lumpability

This chapter discusses the theory of exact fluid lumpability which was introduced in [42] and extended in [49]. The idea behind exact fluid lumpability is to partition the set of fluid atoms of an FPA model M in such a way that the fluid atoms belonging to the same block have, intuitively, the same ODE trajectories. Notice that a necessary condition is that any two fluid atoms within the same block must have the same initial condition. Such a partitioning allows one to relate the solution of the original ODE system to that of a smaller, lumped ODE system with the ODEs of only one label for each element of the partition. Thereby, the name of *exactly fluid lumpable partitions* stems from the parallel with the theory of exact lumpability for Markov chains, where a partition over the state space has to satisfy the requirement that states within the same block must have the same initial probability, cf. Theorem 3 in Section 2.1.

The chapter is organised as follows. We start by introducing in Section 3.1 a motivating example which suggests that the theory is particularly convenient in practice to exploit symmetries in large-scale models with replicated behaviour. After defining exact fluid lumpability in Section 3.2, we introduce in Section 3.3 a notion of behavioural equivalence, called *label equivalence*, which induces exactly fluid lumpable partitions. We continue with Section 3.3.2 by studying the relationship between label equivalence and PEPA's behavioural equivalences from Section 2.3. Specifically, it is shown that well-posedness implies semi-isomorphism. Using this result, we infer in Section 3.3.3 that well-posedness allows for a merging of different label equivalences, thereby yielding coarser ODE partitions.

3.1 Motivating Example

Let us consider the variation $C \underset{\{exec\}}{\bowtie} C' \underset{\{exec\}}{\bowtie} T$ of (2.6), where C, T and C' are as in (2.1) and (2.3), that is

$$C \stackrel{def}{=} (exec, r).\widehat{C}, \quad C' \stackrel{def}{=} (exec, r/2).\widehat{C}' + (exec, r/2).\widehat{C}', \quad T \stackrel{def}{=} (exec, r).\widehat{T},$$
$$\widehat{C} \stackrel{def}{=} (reset, s).C, \quad \widehat{C}' \stackrel{def}{=} (reset, s).C', \quad \widehat{T} \stackrel{def}{=} (io, s').T.$$

In the following, we study the FPA process which arises by composing D copies of $C \underset{\{exec\}}{\bowtie} C' \underset{\{exec\}}{\bowtie} T$ with U, where

$$U \stackrel{def}{=} (io, z).\widehat{U}, \qquad \widehat{U} \stackrel{def}{=} (idle, z').U.$$

This may be interpreted as a collection of D different environments serving client requests whose overall frequency is modulated by an external process U (where, intuitively, the smaller the rate z the larger the probability that the clients are not issuing a request, thus the less utilised the system will be). The corresponding FPA process is then

$$Sys' := \Big(\big(C_1 \underset{\{exec\}}{\bowtie} C_1' \underset{\{exec\}}{\bowtie} T_1 \big) \underset{\emptyset}{\bowtie} \ldots \underset{\emptyset}{\bowtie} \big(C_D \underset{\{exec\}}{\bowtie} C_D' \underset{\{exec\}}{\bowtie} T_D \big) \Big) \underset{\{io\}}{\bowtie} U, \quad (3.1)$$

where, for all $1 \leq d \leq D$,

$$C_d \stackrel{def}{=} (exec, r).\widehat{C}_d, \quad C_d' \stackrel{def}{=} (exec, r/2).\widehat{C}_d' + (exec, r/2).\widehat{C}_d', \quad T_d \stackrel{def}{=} (exec, r).\widehat{T}_d,$$
$$\widehat{C}_d \stackrel{def}{=} (reset, s).C_d, \quad \widehat{C}_d' \stackrel{def}{=} (reset, s).C_d', \quad \widehat{T}_d \stackrel{def}{=} (io, s').T_d.$$

These define distinct copies of C, C' and T. The usage of subscripts enforces the technical requirement that $ds(P_1) \cap ds(P_2) = \emptyset$ for any two labels $P_1, P_2 \in \mathcal{G}(Sys')$, cf. Definition 12. In the following, we fix the initial concentrations

$$\begin{array}{lll} v_{C_d}(0) = \mathfrak{c}_C & v_{C_d'}(0) = \mathfrak{c}_C & v_{T_d}(0) = \mathfrak{c}_T \\ v_{\widehat{C}_d}(0) = 0 & v_{\widehat{C}_d'}(0) = 0 & v_{\widehat{T}_d}(0) = 0 \\ v_U(0) = \mathfrak{c}_U & v_{\widehat{U}}(0) = 0 & \end{array} \quad (3.2)$$

where $1 \leq d \leq D$. For instance, in the case of $D = 2$, the above concentrations yield the sequence of PEPA processes

$$\Big(\big(C_1[\lfloor \mathfrak{c}_C N \rfloor] \underset{\{exec\}}{\bowtie} C_1'[\lfloor \mathfrak{c}_C N \rfloor] \underset{\{exec\}}{\bowtie} T_1[\lfloor \mathfrak{c}_T N \rfloor] \big) \underset{\emptyset}{\bowtie} \big(C_2[\lfloor \mathfrak{c}_C N \rfloor] \underset{\{exec\}}{\bowtie} C_2'[\lfloor \mathfrak{c}_C N \rfloor] \underset{\{exec\}}{\bowtie} T_2[\lfloor \mathfrak{c}_T N \rfloor] \big) \Big) \underset{\{io\}}{\bowtie} U[\lfloor \mathfrak{c}_U N \rfloor],$$

where $N \geq 1$ denotes the scaling parameter from Theorem 5. At this point, it is reasonable to ask in which sense the above model differs from

$$\Big(C_1[\lfloor \mathfrak{c}_C 2N \rfloor] \underset{\{exec\}}{\bowtie} C_1'[\lfloor \mathfrak{c}_C 2N \rfloor] \underset{\{exec\}}{\bowtie} T_1[\lfloor \mathfrak{c}_T 2N \rfloor] \Big) \underset{\{io\}}{\bowtie} U[\lfloor \mathfrak{c}_U N \rfloor].$$

Intuitively, the first model considers a distributed computer architecture with two identical subsystems, while the second one has a single subsystem of doubled

size. This question is studied in detail in Section 4.3 where it is shown that such models share a common fluid approximation but are in general not isomorphic, not strongly bisimilar and not strongly equivalent. Recalling that the underlying stochastic processes are indistinguishable from the fluid model if N tends to infinity, this implies, intuitively, that the "stochastic difference" between both models vanishes as $N \to \infty$.

Returning back to our discussion, we observe that each $C_d \underset{\{exec\}}{\bowtie} C'_d \underset{\{exec\}}{\bowtie} T_d$, with $1 \leq d \leq D$, contributes $|ds(C_d)| + |ds(C'_d)| + |ds(T_d)| = 6$ ODEs. Hence, the size of the fluid approximation of Sys' is $6D + |ds(U)| = 6D + 2$ and the underlying ODE system is

$$\begin{aligned}
\dot{v}_{C_d} &= -r \min\left(v_{C_d}, v_{C'_d}, v_{T_d}\right) + s v_{\widehat{C}_d} & \dot{v}_{\widehat{C}_d} &= -\dot{v}_{C_d} \\
\dot{v}_{C'_d} &= -r \min\left(v_{C_d}, v_{C'_d}, v_{T_d}\right) + s v_{\widehat{C}'_d} & \dot{v}_{\widehat{C}'_d} &= -\dot{v}_{C'_d} \\
\dot{v}_{T_d} &= -r \min\left(v_{C_d}, v_{C'_d}, v_{T_d}\right) + & \dot{v}_{\widehat{T}_d} &= -\dot{v}_{T_d} \\
&\quad + \frac{s' v_{\widehat{T}_d}}{s' \sum_{d'=1}^{D} v_{\widehat{T}_{d'}}} \min\left(s' \sum_{d'=1}^{D} v_{\widehat{T}_{d'}}, z v_U\right) & & \\
\dot{v}_U &= -\min\left(s' \sum_{d'=1}^{D} v_{\widehat{T}_{d'}}, z v_U\right) + z' v_{\widehat{U}} & \dot{v}_{\widehat{U}} &= -\dot{v}_U
\end{aligned} \tag{3.3}$$

for all $1 \leq d \leq D$. When D is large, ODE analysis may become problematic from a computational viewpoint.

We now exploit two basic intuitions. The first one is that the FPA triples $C_d \underset{\{exec\}}{\bowtie} C'_d \underset{\{exec\}}{\bowtie} T_d$ are all similar to each other, in two ways: (i) the fluid atoms describe the same sequential behaviour; and (ii) they operate in a similar context: each triple is independent of each other, but they are all synchronised with the same fluid atom U. Therefore, it is reasonable to assume that, on average, all triples behave in the same way. This fact yields a potential candidate for aggregation. Overall, this intuition leads to making the assumption that the ODE solution satisfies the equalities

$$\begin{aligned}
v_{C_1}(t) &= v_{C_d}(t), & v_{\widehat{C}_1}(t) &= v_{\widehat{C}_d}(t), \\
v_{C'_1}(t) &= v_{C'_d}(t), & v_{\widehat{C}'_1}(t) &= v_{\widehat{C}'_d}(t), \\
v_{T_1}(t) &= v_{T_d}(t), & v_{\widehat{T}_1}(t) &= v_{\widehat{T}_d}(t),
\end{aligned} \tag{3.4}$$

for all $1 \leq d \leq D$ and $t \geq 0$.

The other intuition that can be exploited is that, although C and C' are syntactically different, their behaviour is essentially the same because the total rate from C to $\widehat{C}$ for action *exec* is the same as that for the transition from C' to $\widehat{C}'$. Thus, it is reasonable to also assume that the trajectories of the concentrations of C-components and C'-components are indistinguishable. Formally, this leads to claiming the following:

$$v_{C_d}(t) = v_{C'_d}(t) \qquad v_{\widehat{C}_d}(t) = v_{\widehat{C}'_d}(t) \tag{3.5}$$

for all $1 \leq d \leq D$ and $t \geq 0$.

Although these can be written as

$$\begin{aligned} v_{C_1}(t) &= v_{C_d}(t) & v_{\widehat{C}_1}(t) &= v_{\widehat{C}_d}(t) \\ v_{C_1}(t) &= v_{C'_d}(t) & v_{\widehat{C}_1}(t) &= v_{\widehat{C}'_d}(t) \\ v_{T_1}(t) &= v_{T_d}(t) & v_{\widehat{T}_1}(t) &= v_{\widehat{T}_d}(t) \end{aligned} \tag{3.6}$$

for all $1 \leq d \leq D$ and $t \geq 0$, we prefer to state them as two separate groups of equations because (3.4) and (3.5) will be shown to be inferred from two relations, called *projected label equivalences* (cf. Definition 24), directly arising from two distinct label equivalences on $\mathcal{G}(Sys')$; Equation (3.6) is instead induced by the transitive closure of the union of such relations, which will yield a coarser partition but does not arise from a label equivalence.

If those assumptions hold, the underlying ODE systems admit a simple exact reduction. Simplifying (3.3) for a fixed d, say $d = 1$, and using (3.6) allow us to rewrite the fractions and summations in the right-hand sides in a way that is independent of labels different from C_1, T_1 and U:

$$\begin{aligned} \dot{v}_{C_1} &= -r \min\left(v_{C_1}, v_{T_1}\right) + s v_{\widehat{C}_1} & \dot{v}_{\widehat{C}_1} &= -\dot{v}_{C_1} \\ \dot{v}_{T_1} &= -r \min\left(v_{C_1}, v_{T_1}\right) + (1/D) \min\left(s' D \cdot v_{\widehat{T}_1}, z v_U\right) & \dot{v}_{\widehat{T}_1} &= -\dot{v}_{T_1} \\ \dot{v}_U &= -\min\left(s' D \cdot v_{\widehat{T}_1}, z v_U\right) + z' v_{\widehat{U}} & \dot{v}_{\widehat{U}} &= -\dot{v}_U \end{aligned} \tag{3.7}$$

By using the initial concentrations (3.2) of (3.3) and assuming that both ODE systems have a unique solution, through (3.6) we can exactly relate the solution of (3.3), which has $(2+2+2)D+2$ equations, to that of (3.7), which has only $(2+2)+2$ equations, thus making the problem independent of D.

3.2 Definitions

The ideas presented in the previous section are now generalised for any FPA model. Each formal definition will be accompanied by a simple application to our motivating example.

We begin with the notion of exact fluid lumpability.

Definition 21 (Exact Fluid Lumpability)**.** *Let $\overline{P} = \{\overline{P}^1, \ldots, \overline{P}^n\}$, where $\overline{P}^i = \{P^i_j \mid 1 \leq j \leq k_i\}$, be a partition of the label set of an FPA model M. The partition is called exactly fluid lumpable if there exist bijections*

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

where $\sigma_{P^i_1} \equiv id_{ds(P^i_1)}$, such that for all initial concentrations $v(0)$ which satisfy

$$v_P(0) = v_{\sigma_{P^i_j}(P)}(0), \qquad \forall 1 \leq i \leq n.\ \forall P \in ds(P^i_1).\ \forall 1 \leq j \leq k_i$$

the same holds for all $t \geq 0$ *in the corresponding ODE solution* v*, i.e.*

$$v_P(t) = v_{\sigma_{P_j^i}(P)}(t), \qquad \forall 1 \leq i \leq n.\, \forall P \in ds(P_1^i).\, \forall 1 \leq j \leq k_i.\, \forall t \geq 0.$$

We shall say that $\sigma_\bullet$ *establishes the exact fluid lumpability of* $\overline{P}$ *and that* $\overline{P}^i$*, where* $1 \leq i \leq n$*,* is related to P_1^i.

Informally, for each element $\overline{P}^i = \{P_j^i \mid 1 \leq j \leq k_i\}$ of an exactly fluid lumpable partition $\overline{P}$, we identify a representative P_1^i which is associated to any other element of $\overline{P}^i$, P_j^i, by means of a bijection $\sigma_{P_j^i} : ds(P_1^i) \to ds(P_j^i)$ such that the following holds: if, for $t = 0$ and all $1 \leq i \leq n$ and $1 \leq j \leq k_i$, the concentrations of $ds(P_j^i)$ are given by that of $ds(P_1^i)$ by means of $\sigma_{P_j^i}$, the same holds true for any $t > 0$.

Remark 1. *One could also consider bijections from* $ds(P_j^i)$ *to* $ds(P_1^i)$ *in the above definition. However, due to technical reasons and matter of taste, we prefer to use the present formulation.*

For instance, assumption (3.6) holds if

$$\left\{\overline{P}^1, \overline{P}^2, \overline{P}^3\right\} = \left\{\{C_1, C_1', \ldots, C_D, C_D'\}, \{T_1, \ldots, T_D\}, \{U\}\right\} \tag{3.8}$$

is an exactly fluid lumpable partition which is established by the family

$$\sigma_P(Q) := \begin{cases} C_d & , \exists 1 \leq d \leq D.\, (P = C_d) \wedge Q = C_1 \\ \widehat{C}_d & , \exists 1 \leq d \leq D.\, (P = C_d) \wedge Q = \widehat{C}_1 \\ C_d' & , \exists 1 \leq d \leq D.\, (P = C_d') \wedge Q = C_1 \\ \widehat{C}_d' & , \exists 1 \leq d \leq D.\, (P = C_d') \wedge Q = \widehat{C}_1 \\ T_d & , \exists 1 \leq d \leq D.\, (P = T_d) \wedge Q = T_1 \\ \widehat{T}_d & , \exists 1 \leq d \leq D.\, (P = T_d) \wedge Q = \widehat{T}_1 \end{cases} \tag{3.9}$$

Remark 2. *Fox a fixed FPA model* M*, assume that* $\overline{P} = \{\overline{P}^1, \ldots, \overline{P}^n\}$*, where* $\overline{P}^i = \{P_j^i \mid 1 \leq j \leq k_i\}$*, is an exactly fluid lumpable partition of* $\mathcal{G}(M)$ *which is established by the bijections*

$$\sigma_{P_j^i} : ds(P_1^i) \to ds(P_j^i), \qquad 1 \leq i \leq n,\ 1 \leq j \leq k_i.$$

Then, for arbitrary $1 \leq j_i \leq k_i$*, where* $1 \leq i \leq n$*, the bijections*

$$\rho_{P_j^i} := \sigma_{P_j^i} \circ \sigma_{P_{j_i}^i}^{-1} : ds(P_{j_i}^i) \to ds(P_j^i), \qquad 1 \leq i \leq n,\ 1 \leq j \leq k_i,$$

establish also the exactly fluid lumpability of $\overline{P}$*. That is, the notion of exactly fluid lumpability does not depend on the choice of the representatives.*

Let us fix an FPA model M and assume that $\overline{P} = \{\overline{P}^1, \ldots, \overline{P}^n\}$ is exactly fluid lumpable. Next, we define the underlying lumped ODE system. The latter should relate all ODE traces of $\mathcal{B}(M)$ to that of the ODE model which considers only the states of the lumped concentrations, i.e. $\mathcal{B}^{\text{lump}}(M) := \bigcup_{i=1}^{n} ds(P_1^i)$. Thus, let us fix an arbitrary $P \in \mathcal{B}^{\text{lump}}(M)$ and write its ODE:

$$\dot{v}_P = \sum_{\alpha \in \mathcal{A}} \Big(\sum_{P'} p_\alpha(P', P) \mathcal{R}_\alpha(M, v, P') - \mathcal{R}_\alpha(M, v, P) \Big)$$

Then, any concentration $v_{\tilde{P}}(t)$ on the right-hand-side of the ODE can be expressed by lumped concentrations, as there are unique $1 \leq i \leq n$ and $1 \leq j \leq k_i$ such that $\tilde{P} \in ds(P_j^i)$ and $v_{\tilde{P}}(t) = v_{\sigma_{P_j^i}^{-1}(\tilde{P})}(t)$ with $\sigma_{P_j^i}^{-1}(\tilde{P}) \in ds(P_1^i)$.

This shows that the ODE $\dot{v}_P$ can be expressed in terms of $\{v_Q \mid Q \in \mathcal{B}^{\text{lump}}(M)\}$. The next definition formalises this.

Definition 22 (Exactly Lumped Fluid Model)**.** *Let $\overline{P} = \{\overline{P}^1, \ldots, \overline{P}^n\}$ be an exactly fluid lumpable partition of $\mathcal{G}(M)$ which is established by $\sigma_\bullet$. Moreover, let D_P^{lump}, where $P \in \mathcal{B}^{lump}(M)$, denote the equation which arises from*

$$\sum_{\alpha \in \mathcal{A}} \Big(\sum_{P'} p_\alpha(P', P) \mathcal{R}_\alpha(M, v, P') - \mathcal{R}_\alpha(M, v, P) \Big)$$

by replacing all $v_{\tilde{P}}(t)$, where $\tilde{P} \in ds(P_j^i)$ for some $1 \leq i \leq n$ and $1 \leq j \leq k_i$, with $v_{\sigma_{P_j^i}^{-1}(\tilde{P})}(t)$. The exactly lumped fluid model *of M with respect to $\sigma_\bullet$ and $v(0)$ is the solution of the lumped ODE system $\dot{v}_P = D_P^{lump}$, $P \in \mathcal{B}^{lump}(M)$, subjected to the initial value $v(0)_{|\mathcal{B}^{lump}(M)}$.*

For instance, if the family of bijections (3.9) establish the exactly lumpable partition (3.8), we infer that the exactly lumped fluid model of our motivating example (3.1) with respect to such a partition is (3.7).

Recall that we assumed that both the original and the lumped ODE system have a unique solution. To see this, note that a restriction of a Lipschitz function is again Lipschitz and that the original ODE system is Lipschitz [54].

3.3 Construction of Exactly Fluid Lumpable Partitions

Section 3.3.1 discusses two related equivalences for the construction of exactly fluid lumpable partitions. The first, *label equivalence* is used to construct a *projected label equivalence*, and relates *tuples* of labels. If two tuples, say $(P_1, \ldots, P_n)$ and $(P'_1, \ldots, P'_n)$ are related, then this implies that the fluid atoms P_i and P'_i, $1 \leq i \leq n$, have the same fluid approximation. This makes P_i and P'_i *projected label equivalent*, implying that the two labels belong to the same block of an exactly fluid lumpable partition. Section 3.3.2 studies the stochastic

relationship between PEPA components that are related by a projected label equivalence. In addition to being of interest per se, this study will be instrumental for proving that the transitive closure of the union of several projected label equivalences induces an exactly fluid lumpable partition, as done in Section 3.3.3, for the class of *well-posed* models.

3.3.1 Label Equivalence and Projected Label Equivalence

Definition 23 (Label Equivalence)**.** *Let M be an FPA 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 $1 \leq i \leq N$ and $1 \leq k \leq K_i$ with $P = P^i_k$. Further, let $\mathfrak{P} = \{\mathfrak{p}_1, \ldots, \mathfrak{p}_n\}$ denote a partition of $\mathcal{P}$. $\vec{P}^i$ and $\vec{P}^j$ are said to be* label equivalent*, written $\vec{P}^i \sim_{\mathfrak{P}} \vec{P}^j$, if $\vec{P}^i, \vec{P}^j \in \mathfrak{p}_l$ for some $1 \leq l \leq n$, $K_i = K_j$ and there exist bijections $\sigma_k : ds(P^i_k) \to ds(P^j_k)$, where $1 \leq k \leq K_i$, such that for all concentration functions v of M and*

$$v^\sigma_P := \begin{cases} v_{\sigma_k(P)} & , \exists 1 \leq k \leq K_i.\ (P \in ds(P^i_k)) \\ v_{\sigma_k^{-1}(P)} & , \exists 1 \leq k \leq K_i.\ (P \in ds(P^j_k)) \\ v_P & , \textit{otherwise} \end{cases}$$

it holds that

i) The component rates, cf. Definition 15, satisfy:

a) The α-component rate out of each $P \in ds(P^i_k)$ with respect to v is equal to the α-component rate out of $\sigma_k(P) \in ds(P^j_k)$ with respect to v^σ,

$$\mathcal{R}_\alpha(M, v, P) = \mathcal{R}_\alpha(M, v^\sigma, \sigma_k(P))$$

b) The sum of α-component rates into each $P \in ds(P^i_k)$ with respect to v is equal to the sum of the α-component rates into $\sigma_k(P) \in ds(P^j_k)$ with respect to v^σ,

$$\sum_{P'} p_\alpha(P', P)\mathcal{R}_\alpha(M, v, P') = \sum_{P'} p_\alpha(P', \sigma_k(P))\mathcal{R}_\alpha(M, v^\sigma, P')$$

c) For all $P \in ds(P^l_k)$ such that $P^l_k \notin \vec{P}^i, \vec{P}^j$ it holds $\mathcal{R}_\alpha(M, v, P) = \mathcal{R}_\alpha(M, v^\sigma, P)$

ii) The apparent rates, cf. Definition 14, satisfy: $r_\alpha(M, v) = r_\alpha(M, v^\sigma)$.

Informally, two tuples $\vec{P}^i, \vec{P}^j$ are label equivalent if the component and apparent rates respect an exchange of fluid atom concentrations within the tuples. Hence, label equivalence especially applies to symmetries within the model under study. For instance, let us fix the subprocess of (3.1)

$$Sys := \big(C_1 \underset{\{exec\}}{\bowtie} C'_1 \underset{\{exec\}}{\bowtie} T_1\big) \underset{\emptyset}{\bowtie} \ldots \underset{\emptyset}{\bowtie} \big(C_D \underset{\{exec\}}{\bowtie} C'_D \underset{\{exec\}}{\bowtie} T_D\big),$$

the tuple partition $\mathcal{P}_1 := \{(C_1, C_1', T_1), \ldots, (C_D, C_D', T_D)\}$ of $\mathcal{G}(Sys)$, and two arbitrary $1 \leq i, j \leq D$. Given the bijections

$$\begin{aligned}
&\sigma_1^{(C_i,C_i',T_i),(C_j,C_j',T_j)} : ds(C_i) \to ds(C_j), \quad C_i \mapsto C_j,\ \widehat{C}_i \mapsto \widehat{C}_j \\
&\sigma_2^{(C_i,C_i',T_i),(C_j,C_j',T_j)} : ds(C_i') \to ds(C_j'), \quad C_i' \mapsto C_j',\ \widehat{C}_i' \mapsto \widehat{C}_j' \\
&\sigma_3^{(C_i,C_i',T_i),(C_j,C_j',T_j)} : ds(T_i) \to ds(T_j), \quad T_i \mapsto T_j,\ \widehat{T}_i \mapsto \widehat{T}_j,
\end{aligned} \tag{3.10}$$

v^σ is obtained from v by essentially swapping the concentration functions related to the (syntactically) same components under two different labels i.e., by exchanging v_{C_i} with v_{C_j}, $v_{\widehat{C}_i}$ with $v_{\widehat{C}_j}$, $v_{C_i'}$ with $v_{C_j'}$, $v_{\widehat{C}_i'}$ with $v_{\widehat{C}_j'}$, v_{T_i} with v_{T_j} and $v_{\widehat{T}_i}$ with $v_{\widehat{T}_j}$. It holds that, for any action type $\alpha \in \mathcal{A}$, the (symbolic) α-apparent rate is invariant under such an exchange of concentrations and the α-component rates into and out of C_i are equal to the corresponding α-component rates of C_j. The former can be inferred from

$$r_\alpha(C_d \underset{\{exec\}}{\bowtie} C_d' \underset{\{exec\}}{\bowtie} T_d, v^\sigma) = \begin{cases} r_\alpha(C_j \underset{\{exec\}}{\bowtie} C_j' \underset{\{exec\}}{\bowtie} T_j, v) & ,\ d = i \\ r_\alpha(C_i \underset{\{exec\}}{\bowtie} C_i' \underset{\{exec\}}{\bowtie} T_i, v) & ,\ d = j \\ r_\alpha(C_d \underset{\{exec\}}{\bowtie} C_d' \underset{\{exec\}}{\bowtie} T_d, v) & ,\ d \notin \{i, j\} \end{cases}$$

and

$$r_\alpha(Sys, v) = \sum_{d=1}^{D} r_\alpha(C_d \underset{\{exec\}}{\bowtie} C_d' \underset{\{exec\}}{\bowtie} T_d, v),$$

while the latter follows by

$$\begin{aligned}
\mathcal{R}_\alpha(Sys, v, C_i) &= \mathcal{R}_\alpha(C_i \underset{\{exec\}}{\bowtie} C_i' \underset{\{exec\}}{\bowtie} T_i, v, C_i) \\
&= \frac{\mathcal{R}_\alpha(C_i, v, C_i)}{r_\alpha(C_i, v)} r_\alpha(C_i \underset{\{exec\}}{\bowtie} C_i' \underset{\{exec\}}{\bowtie} T_i, v) \\
&= \frac{\mathcal{R}_\alpha(C_j, v^\sigma, C_j)}{r_\alpha(C_j, v^\sigma)} r_\alpha(C_j \underset{\{exec\}}{\bowtie} C_j' \underset{\{exec\}}{\bowtie} T_j, v^\sigma) \\
&= \mathcal{R}_\alpha(Sys, v^\sigma, C_j)
\end{aligned}$$

and

$$\begin{aligned}
\mathcal{R}_\alpha(Sys, v, C_d) &= \mathcal{R}_\alpha(C_d \underset{\{exec\}}{\bowtie} C_d' \underset{\{exec\}}{\bowtie} T_d, v, C_d) \\
&= \frac{\mathcal{R}_\alpha(C_d, v, C_d)}{r_\alpha(C_d, v)} r_\alpha(C_d \underset{\{exec\}}{\bowtie} C_d' \underset{\{exec\}}{\bowtie} T_d, v) \\
&= \frac{\mathcal{R}_\alpha(C_d, v^\sigma, C_d)}{r_\alpha(C_d, v^\sigma)} r_\alpha(C_d \underset{\{exec\}}{\bowtie} C_d' \underset{\{exec\}}{\bowtie} T_d, v^\sigma) \\
&= \mathcal{R}_\alpha(Sys, v^\sigma, C_d)
\end{aligned}$$

with $d \notin \{i, j\}$. Note that the above equalities are meant to hold *for all* concentration functions v of Sys. That is, an algorithm which establishes exact

fluid lumpability has to perform a *symbolic* checking in the style of a computer algebra system. Since similar equalities hold for all aforementioned label pairs, one infers that $(C_i, C_i', T_i) \sim_{\{\mathcal{P}_1\}} (C_j, C_j', T_j)$, for any $1 \leq i, j \leq D$.

Remark 3. *We wish to point out that the above notion of label equivalence generalises the original one presented in [42] in that only tuples from the same $\mathfrak{p} \in \mathfrak{P}$, rather than from the entire $\mathcal{P}$, are compared. That is, $\sim_{\mathcal{P}}$ in the sense of Definition 12 from [42] is recovered by $\sim_{\mathfrak{P}}$ if $\mathfrak{P} := \{\mathcal{P}\}$. This additional degree of freedom is crucial for the fluid lumping of nested FPA models discussed in Chapter 4.*

The next theorem relates the fluid trajectories of label equivalent tuples.

Theorem 7. *Let M be an FPA model with fluid approximation v, $\mathcal{P}$ be a tuple partition on $\mathcal{G}(M)$ and $\mathfrak{P}$ be a partition of $\mathcal{P}$. Then, $\vec{P}^i \sim_{\mathfrak{P}} \vec{P}^j$ implies that*

$$\forall P \in \mathcal{B}(M).\, \Big(v_P(0) = v_P^\sigma(0)\Big) \quad \Rightarrow \quad \forall P \in \mathcal{B}(M).\, \forall t \geq 0.\, \Big(v_P(t) = v_P^\sigma(t)\Big),$$

where v^σ is as in Definition 23.

Proof. Since $v(0) = v^\sigma(0)$ and the solution is unique, it suffices to show that v^σ is a solution. For this, we fix an arbitrary $P \in \mathcal{B}(M)$ and distinguish the following three cases. First, if $P \in ds(P_k^l)$ such that $P_k^l \notin \vec{P}^i, \vec{P}^j$, then

$$\begin{aligned}\dot{v}_P^\sigma = \dot{v}_P &= \sum_{\alpha \in \mathcal{A}} \Big(\sum_{P'} p_\alpha(P', P) \mathcal{R}_\alpha(M, v, P') - \mathcal{R}_\alpha(M, v, P) \Big) \\ &\overset{\text{i)}}{=} \sum_{\alpha \in \mathcal{A}} \Big(\sum_{P'} p_\alpha(P', P) \mathcal{R}_\alpha(M, v^\sigma, P') - \mathcal{R}_\alpha(M, v^\sigma, P) \Big).\end{aligned}$$

Second, if $P \in ds(P_k^i)$, then

$$\begin{aligned}\dot{v}_{\sigma_k(P)}^\sigma = \dot{v}_P &= \sum_{\alpha \in \mathcal{A}} \Big(\sum_{P'} p_\alpha(P', P) \mathcal{R}_\alpha(M, v, P') - \mathcal{R}_\alpha(M, v, P) \Big) \\ &\overset{\text{i)}}{=} \sum_{\alpha \in \mathcal{A}} \Big(\sum_{P'} p_\alpha(P', \sigma_k(P)) \mathcal{R}_\alpha(M, v^\sigma, P') - \mathcal{R}_\alpha(M, v^\sigma, \sigma_k(P)) \Big).\end{aligned}$$

Third, if $P \in ds(P_k^j)$, then

$$\begin{aligned}\dot{v}_{\sigma_k^{-1}(P)}^\sigma = \dot{v}_P &= \sum_{\alpha \in \mathcal{A}} \Big(\sum_{P'} p_\alpha(P', P) \mathcal{R}_\alpha(M, v, P') - \mathcal{R}_\alpha(M, v, P) \Big) \\ &= \sum_{\alpha \in \mathcal{A}} \Big(\sum_{P'} p_\alpha(P', P) \mathcal{R}_\alpha(M, (v^\sigma)^\sigma, P') - \mathcal{R}_\alpha(M, (v^\sigma)^\sigma, P) \Big) \\ &\overset{\text{i)}}{=} \sum_{\alpha \in \mathcal{A}} \Big(\sum_{P'} p_\alpha(P', \sigma_k^{-1}(P)) \mathcal{R}_\alpha(M, v^\sigma, P') - \mathcal{R}_\alpha(M, v^\sigma, \sigma_k^{-1}(P)) \Big).\end{aligned}$$

□

For instance, $(C_i, C_i', T_i) \sim_{\{\mathcal{P}_1\}} (C_j, C_j', T_j)$ and Theorem 7 show that

$$v_{C_i}(0) = v_{C_j}(0) \qquad v_{C_i'}(0) = v_{C_j'}(0) \qquad v_{T_i}(0) = v_{T_j}(0)$$
$$v_{\widehat{C}_i}(0) = v_{\widehat{C}_j}(0) \qquad v_{\widehat{C}_i'}(0) = v_{\widehat{C}_j'}(0) \qquad v_{\widehat{T}_i}(0) = v_{\widehat{T}_j}(0)$$

implies

$$v_{C_i}(t) = v_{C_j}(t) \qquad v_{C_i'}(t) = v_{C_j'}(t) \qquad v_{T_i}(t) = v_{T_j}(t)$$
$$v_{\widehat{C}_i}(t) = v_{\widehat{C}_j}(t) \qquad v_{\widehat{C}_i'}(t) = v_{\widehat{C}_j'}(t) \qquad v_{\widehat{T}_i}(t) = v_{\widehat{T}_j}(t)$$

for all $t \geq 0$, where v denotes the fluid approximation of *Sys* with respect to a given $v(0)$.

This example also illustrates that, in general, one has to consider relations between *tuples* of labels, rather than just labels. For clarification, let us assume that our tuple partition of $\mathcal{G}(Sys)$ consists only of trivial tuples, i.e. $\mathcal{P}_2 := \{(P) \mid P \in \mathcal{G}(Sys)\}$. Then, for instance, the bijection

$$\sigma_1^{(C_i),(C_j)} : ds(C_i) \to ds(C_j), \quad C_i \mapsto C_j,\ \widehat{C}_i \mapsto \widehat{C}_j$$

where $1 \leq i < j \leq D$, does not establish $(C_i) \sim_{\{\mathcal{P}_2\}} (C_j)$. This is because the fluid atoms C_i' and C_j' or the fluid atoms T_i and T_j may have different initial concentrations. This problem does not manifest itself if we use the tuple partition $\mathcal{P}_1$, where the concentrations of larger processes, rather than that of single fluid atoms, are exchanged.

The next theorem states that label equivalence is a congruence with respect to the parallel composition of FPA.

Theorem 8 (Label Equivalence is a Congruence)**.** *Fix an FPA model M, a tuple partition $\mathcal{P}$ on $\mathcal{G}(M)$ and a partition $\mathfrak{P}$ of $\mathcal{P}$. Then the following holds:*

- *$\sim_{\mathfrak{P}}$ is an equivalence relation on $\mathcal{P}$.*
- *Fix an action set L, an FPA model M^0, a tuple partition $\mathcal{P}^0$ on $\mathcal{G}(M^0)$ and a partition $\mathfrak{P}^+$ of $\mathcal{P} \cup \mathcal{P}^0$. Then, $\vec{P}^i \sim_{\mathfrak{P}} \vec{P}^j$ in M implies $\vec{P}^i \sim_{\mathfrak{P}^+} \vec{P}^j$ in $M \underset{L}{\bowtie} M_0$, given that $\vec{P}^i, \vec{P}^j \in \mathfrak{p}$ for some $\mathfrak{p} \in \mathfrak{P}^+$.*

Proof. To increase the readability of the current section, we briefly sketch the proof strategy. A rigorous proof of this result is provided in Appendix A.2.

1. Reflexivity and symmetry are trivial. For the transitivity of $\sim_{\mathfrak{P}}$ we assume that

   $$\sigma_k^i : ds(P_k^i) \to ds(P_k^j), \quad \sigma_k^j : ds(P_k^j) \to ds(P_k^\nu), \quad 1 \leq k \leq K$$

   establish $\vec{P}^i \sim_{\mathfrak{P}} \vec{P}^j$, $\vec{P}^j \sim_{\mathfrak{P}} \vec{P}^\nu$, respectively. One can show then that

   $$(\sigma^j \circ \sigma^i)_k : ds(P_k^i) \to ds(P_k^\nu), P \mapsto \sigma^j(\sigma^i(P)), \quad 1 \leq k \leq K$$

   establishes $\vec{P}^i \sim_{\mathfrak{P}} \vec{P}^\nu$.

2. Let us fix some $P \in \mathcal{B}(M \underset{L}{\bowtie} M_0)$ and assume that $\vec{P}^i \sim_{\mathfrak{P}} \vec{P}^j$ is established by $\sigma_k^i : ds(P_k^i) \to ds(P_k^j)$, where $1 \leq k \leq K$. Since the case $\alpha \notin L$ is straightforward, we assume $\alpha \in L$ and make the following case distinction:

   - Case $P \in \mathcal{B}(M)$: Observing

     $$\mathcal{R}_\alpha(M \underset{L}{\bowtie} M_0, v, P) = \frac{\mathcal{R}_\alpha(M, v, P)}{r_\alpha(M, v)} \min(r_\alpha(M, v), r_\alpha(M_0, v)),$$

     $r_\alpha(M, v) = r_\alpha(M, v^\sigma)$ and $r_\alpha(M_0, v) = r_\alpha(M_0, v^\sigma)$ yields the claim. Let us remark that the last equality holds because σ_k, where $1 \leq k \leq K$, exchange concentrations in M and not M_0.
   - Case $P \in \mathcal{B}(M_0)$: Observing

     $$\mathcal{R}_\alpha(M \underset{L}{\bowtie} M_0, v, P) = \frac{\mathcal{R}_\alpha(M_0, v, P)}{r_\alpha(M_0, v)} \min(r_\alpha(M, v), r_\alpha(M_0, v)),$$

     $r_\alpha(M, v) = r_\alpha(M, v^\sigma)$, $r_\alpha(M_0, v) = r_\alpha(M_0, v^\sigma)$ and $\mathcal{R}_\alpha(M_0, v, P) = \mathcal{R}_\alpha(M_0, v^\sigma, P)$ yields the claim. Similarly to the previous case, the last two equalities hold because σ_k, where $1 \leq k \leq K$, exchange concentrations in M and not M_0.

□

As usual, the congruence property is useful for compositional reasoning. For instance, let us consider Sys' defined in (3.1) and fix the tuple partition

$$\mathcal{P}_1' := \mathcal{P}_1 \cup \mathcal{P}_0 = \{(C_1, C_1', T_1), \ldots, (C_D, C_D', T_D), (U)\} \tag{3.11}$$

of $\mathcal{G}(Sys')$, where $\mathcal{P}_0 := \{(U)\}$ is obviously the only possible tuple partition of $\mathcal{G}(U)$. Theorem 8 implies $(C_i, C_i', T_i) \sim_{\{\mathcal{P}_1'\}} (C_j, C_j', T_j)$, which yields

$$\mathcal{P}_1' / \sim_{\{\mathcal{P}_1'\}} = \big\{\{(C_1, C_1', T_1), \ldots, (C_D, C_D', T_D)\}, \{(U)\}\big\},$$

as $1 \leq i, j \leq D$ were chosen arbitrarily. This and Theorem 7 show then that

$$\big\{\{C_1, \ldots, C_D\}, \{C_1', \ldots, C_D'\}, \{T_1, \ldots, T_D\}, \{U\}\big\} \tag{3.12}$$

is an exactly fluid lumpable partition. Crucially, the following defines projected label equivalence, a relation which can be directly obtained (projected) from a label equivalence in order to relate labels, and not tuples of labels. According to Theorem 9, this immediately yields an exactly fluid lumpable partition.

Definition 24 (Projected Label Equivalence)**.** *Fix an FPA model M, a tuple partition $\mathcal{P}$ on $\mathcal{G}(M)$ and a partition $\mathfrak{P}$ of $\mathcal{P}$. The labels $P_1, P_2 \in \mathcal{G}(M)$ are projected label equivalent, $P_1 \approx_{\mathfrak{P}} P_2$, if $\vec{P}^i \sim_{\mathfrak{P}} \vec{P}^j$ and $k_i = k_j$ in the unique assignment $P_1 = P_{k_i}^i$, $P_2 = P_{k_j}^j$.*

For instance, the relation $(C_1, C_1', T_1) \sim_{\{\mathcal{P}_1'\}} (C_2, C_2', T_2)$ implies $C_1 \approx_{\{\mathcal{P}_1'\}} C_2$, $C_1' \approx_{\{\mathcal{P}_1'\}} C_2'$ and $T_1 \approx_{\{\mathcal{P}_1'\}} T_2$.

Theorem 9. *Fix an FPA model M, a tuple partition $\mathcal{P}$ on $\mathcal{G}(M)$ and a partition $\mathfrak{P}$ of $\mathcal{P}$. The relation $\approx_{\mathfrak{P}}$ is then an equivalence relation on $\mathcal{G}(M)$ and $\mathcal{G}(M)/\approx_{\mathfrak{P}}$ is an exactly fluid lumpable partition.*

Proof. Theorem 8 shows that $\approx_{\mathfrak{P}}$ defines an equivalence relation on $\mathcal{G}(M)$ and Theorem 7 implies that $\mathcal{G}(M)/\approx_{\mathfrak{P}}$ is an exactly fluid lumpable partition. □

Note that $\{\mathcal{P}_1'\}$ induces the exactly fluid lumpable partition (3.12) via $\approx_{\{\mathcal{P}_1'\}}$, which demonstrates the assumption (3.4) for our running example. Intuitively, this partition relates all fluid atoms expressed with the same sequential component, C, C', and T, if they are initialised with the same conditions. However, in general, for the same model there might be more tuple partitions which allow for a simplification: The partition

$$\mathcal{P}_2' := \mathcal{P}_2 \cup \mathcal{P}_0 = \{(P) \mid P \in \mathcal{G}(Sys')\}, \tag{3.13}$$

the family of bijections

$$\sigma_1^{(C_i),(C_i')} : ds(C_i) \to ds(C_i'), \quad C_i \mapsto C_i',\ \widehat{C}_i \mapsto \widehat{C}_i' \tag{3.14}$$

and Theorem 8 yield $(C_i) \sim_{\{\mathcal{P}_2'\}} (C_i')$ for all $1 \leq i \leq D$. As these are the only nontrivial relations on $\mathcal{P}_2'$, we get $\mathcal{P}_2'/\sim_{\{\mathcal{P}_2'\}} = \big\{\{(U)\}, \{(C_1),(C_1')\}, \{(T_1)\}, \ldots$ $\ldots, \{(C_D),(C_D')\}, \{(T_D)\}\big\}$. This shows, in turn, that $\{\mathcal{P}_2'\}$ induces the exactly fluid lumpable partition

$$\mathcal{G}(Sys')/\approx_{\{\mathcal{P}_2'\}} = \big\{\{C_1, C_1'\}, \{T_1\}, \ldots, \{C_D, C_D'\}, \{T_D\}, \{U\}\big\}. \tag{3.15}$$

Such a partition, instead, relates fluid atoms exhibiting distinct sequential components, C and C', and demonstrates the assumption (3.5) of the running example

$$v_{C_d}(t) = v_{C_d'}(t), \quad v_{\widehat{C}_d}(t) = v_{\widehat{C}_d'}(t), \qquad \forall.\ 1 \leq d \leq D \forall.\ t \geq 0.$$

Before being in a position to derive assumption (3.6), i.e.

$$\begin{aligned} v_{C_1}(t) &= v_{C_d}(t) & v_{\widehat{C}_1}(t) &= v_{\widehat{C}_d}(t) \\ v_{C_1}(t) &= v_{C_d'}(t) & v_{\widehat{C}_1}(t) &= v_{\widehat{C}_d'}(t) \\ v_{T_1}(t) &= v_{T_d}(t) & v_{\widehat{T}_1}(t) &= v_{\widehat{T}_d}(t) \end{aligned}$$

for all $1 \leq d \leq D$ and $t \geq 0$, we have to establish a relation between the notions of label equivalence and semi-isomorphism.

3.3.2 Exact Fluid Lumpability and Semi-Isomorphism

Let M denote a *well-posed* FPA model, $\mathcal{P}$ a tuple partition on $\mathcal{G}(M)$ and $\mathfrak{P}$ a partition of $\mathcal{P}$. Given that $\sigma_k : ds(P_k^i) \to ds(P_k^j)$, where $1 \leq k \leq K$, establish $\vec{P}^i \sim_{\mathfrak{P}} \vec{P}^j$ for some $\vec{P}^i, \vec{P}^j \in \mathcal{P}$, we show next that each σ_k is a semi-isomorphism. To build on intuition, we start with a sketch of the proof strategy used to achieve this result, which is formally stated as Theorem 10.

Since we need to show

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

for all $P', P'' \in ds(P_k^i)$ and $\alpha \in \mathcal{A}$, the idea is essentially to start with

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

from requirement i) of Definition 23 and set

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

Since this yields

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

and requirement i) of Definition 23 asserts $\mathcal{R}_\alpha(M, v, P') = \mathcal{R}_\alpha(M, v^\sigma, \sigma_k(P'))$, one can infer $p_\alpha(P', P'') = p_\alpha(\sigma_k(P'), \sigma_k(P''))$ in the case of $\mathcal{R}_\alpha(M, v, P') > 0$, which is always satisfied, by Lemma 3, if M is well-posed. Then, using the well-posedness of M it is also possible to show that $r_\alpha(P') = r_\alpha(\sigma_k(P'))$, if $r_\alpha(P') > 0$, cf. Lemma 4, 5 and 6, which readily yields then the claim if $r_\alpha(P') > 0$. The proof of the case $r_\alpha(P') = 0$ relies essentially on requirement i) of Definition 23 and on the fact that $r_\alpha(P') = 0$ implies $\mathcal{R}_\alpha(M, v, P') = 0$.

The remainder of this section formalises these ideas.

Lemma 2. *Fix an FPA model M. Then, for all $\alpha \in \mathcal{A}$, $P \in \mathcal{B}(M)$ and concentration functions v of M it holds that $\mathcal{R}_\alpha(M, v, P) \leq r_\alpha(M, v)$.*

Proof. Straightforward induction on M. □

Lemma 3. *Fix a well-posed FPA model M, one of its fluid atoms P_k, a $P' \in ds(P_k)$ and assume that $r_\alpha(P') > 0$. Then $\mathcal{R}_\alpha(M, v, P') > 0$ for the concentration function*

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

Proof. We prove this by structural induction on M.

- $M = P_0$: Since M has then only one fluid atom, i.e. $P_0 = P_k$, the claim follows by $r_\alpha(P') > 0$.

- $M = M_1 \underset{L}{\bowtie} M_2$: We assume without loss of generality that $P_k \in \mathcal{G}(M_1)$. 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., Lemma 2 yields $r_\alpha(M_1, v_1) > 0$. 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 concentrations of v_2 are positive.) This yields then $\min(r_\alpha(M_1, v_1), r_\alpha(M_2, v_2)) > 0$, implying $\mathcal{R}_\alpha(M, v, P') > 0$.

□

The next three lemmas show that $r_\alpha(P') = r_\alpha(\sigma_k(P'))$, if $r_\alpha(P') > 0$.

Lemma 4. *Fix a well-posed FPA model M and one of its fluid atoms P_k. Then there exist a $\delta > 0$ and a set of concentrations $\{w_P \mid P \in \mathcal{B}(M) \wedge P \notin ds(P_k)\}$ where*

$$w_E = w_{E'}, \quad \forall Q \in \mathcal{G}(M), Q \neq P_k.\, \forall E, E' \in ds(Q),$$

such that $r_\alpha(M, v) = r_\alpha(P_k, v)$ for all concentrations v of M which satisfy

$$\forall P \in \mathcal{B}(M).\, \big(P \notin ds(P_k) \Rightarrow v_P = w_P \ \wedge \ P \in ds(P_k) \Rightarrow v_P \leq \delta\big).$$

That is, the apparent rate of M is determined by its fluid atom P_k, if the concentrations of $\mathcal{B}(P_k)$ are sufficiently smaller than those of $\mathcal{B}(M) \setminus \mathcal{B}(P_k)$.

Proof. We prove this by structural induction on M.

- $M = P_0$: Since M has then only one fluid atom, i.e. $P_0 = P_k$, the claim is trivial.

- $M = M_1 \underset{L}{\bowtie} M_2$: We assume without loss of generality that $P_k \in \mathcal{G}(M_1)$, fix using the I.H. a $\delta' > 0$ and a set of concentrations $\{w'_P \mid P \in \mathcal{B}(M_1) \wedge P \notin ds(P_k)\}$ such that $r_\alpha(M_1, v_1) = r_\alpha(P_k, v_1)$ for all v_1 which satisfy

$$\forall P \in \mathcal{B}(M_1).\, \big(P \notin ds(P_k) \Rightarrow (v_1)_P = w'_P \ \wedge \ P \in ds(P_k) \Rightarrow (v_1)_P \leq \delta'\big) \tag{3.16}$$

  and make the following case distinction on α.

  - $\alpha \notin L$: The definitions $\delta := \delta'$ and

$$w_P := \begin{cases} w'_P & , \ P \in \mathcal{B}(M_1) \wedge P \notin ds(P_k) \\ 0 & , \ P \in \mathcal{B}(M_2) \end{cases}$$

    show then the claim.

  - $\alpha \in L$: Since M is well-posed, it holds that $r_\alpha(M_2, v_2) > 0$, where $(v_2)_P = 1$ for all $P \in \mathcal{B}(M_2)$. Hence, there is a $\delta'' > 0$ such that

$$r_\alpha(M_1, \delta'' v_1) = \delta'' r_\alpha(M_1, v_1) = \delta'' r_\alpha(P_k, v_1) \leq r_\alpha(M_2, v_2)$$

for all v_1 which satisfy (3.16). Together with $r_\alpha(M_1, v_1) = r_\alpha(P_k, v_1)$ $\Leftrightarrow \delta'' r_\alpha(M_1, v_1) = \delta'' r_\alpha(P_k, v_1) \Leftrightarrow r_\alpha(M_1, \delta'' v_1) = r_\alpha(P_k, \delta'' v_1)$ we infer then

$$r_\alpha(M_1 \underset{L}{\bowtie} M_2, (\delta'' v_1, v_2)) = r_\alpha(M_1, \delta'' v_1) = r_\alpha(P_k, \delta'' v_1)$$

for all such v_1. From this we conclude that $\delta := \delta' \delta''$ and

$$w_P := \begin{cases} \delta'' w'_P & , \ P \in \mathcal{B}(M_1) \wedge P \notin ds(P_k) \\ (v_2)_P & , \ P \in \mathcal{B}(M_2) \end{cases}$$

show the claim.

□

Lemma 5. *Fix an FPA model M, one of its fluid atoms P_k, a $P' \in ds(P_k)$ and assume that there are $\hat{c}, \delta > 0$ and a set of concentrations $\{w_P \mid P \in \mathcal{B}(M) \wedge P \notin ds(P_k)\}$ such that $r_\alpha(M, v^\eta) = \hat{c}\eta$ for all $0 \leq \eta \leq \delta$, where*

$$v_P^\eta := \begin{cases} w_P & , \ P \in \mathcal{B}(M) \wedge P \notin ds(P_k) \\ \eta & , \ P = P' \\ 0 & , \ P \in ds(P_k) \wedge P \neq P' \end{cases}$$

Then it holds that $\hat{c} = r_\alpha(P')$.

Proof. We prove this by structural induction on M.

- $M = P_0$: Since M has then only one fluid atom, i.e. $P_0 = P_k$, the claim is trivial.
- $M = M_1 \underset{L}{\bowtie} M_2$: We assume without loss of generality that $P_k \in \mathcal{G}(M_1)$, denote by v_i^η the M_i-part of v^η and observe that v_2^η does not depend on η. This and the assumption yield $r_\alpha(M_1, v_1^\eta) \leq r_\alpha(M_2, v_2^\eta)$ for some $0 < \delta' \leq \delta$ and all $0 \leq \eta \leq \delta'$ in the case of $\alpha \in L$ and $r_\alpha(M_2, v_2^\eta) = 0$ in the case of $\alpha \notin L$. Thus, $r_\alpha(M_1, v_1^\eta) = r_\alpha(M, v^\eta) = \hat{c}\eta$ for all $0 \leq \eta \leq \delta'$ and the I.H. yields the claim.

□

Lemma 6. *Fix a well-posed FPA model M, a tuple partition $\mathcal{P} = (\vec{P}^1, \ldots, \vec{P}^N)$ on $\mathcal{G}(M)$, $P_k^i \in \vec{P}^i$, $P' \in ds(P_k^i)$ and assume that $\vec{P}^i \sim_{\mathfrak{P}} \vec{P}^j$, where $\mathfrak{P}$ denotes some partition of $\mathcal{P}$, is established by σ_l, $1 \leq l \leq K_i$. Then $r_\alpha(P') = r_\alpha(\sigma_k(P'))$, if $r_\alpha(P') > 0$.*

Proof. We note that $r_\alpha(M, v) = r_\alpha(P') v_{P'}$, if v satisfies the assumption of Lemma 4 and $v_P = 0$ for all $P \in ds(P_k^i) \setminus \{P'\}$. This and $\vec{P}^i \sim_{\mathfrak{P}} \vec{P}^j$ yield

$$r_\alpha(M, v^\sigma) = r_\alpha(M, v) = r_\alpha(P') v_{P'}.$$

Since $v_{P'}$ can be chosen from $[0; \delta]$ and $v_{P'} = v^\sigma_{\sigma_k(P')}$, Lemma 5 implies $r_\alpha(P') = r_\alpha(\sigma_k(P'))$ in the case of $r_\alpha(P') > 0$. □

We can now establish the connection between label equivalence and semi-isomorphism.

Theorem 10. *Fix a well-posed FPA model M, a tuple partition $\mathcal{P} = \{\vec{P}^1, \ldots \ldots, \vec{P}^N\}$ on $\mathcal{G}(M)$ and assume that $\vec{P}^i \sim_{\mathfrak{P}} \vec{P}^j$ for some given partition $\mathfrak{P}$ of $\mathcal{P}$. Then, P^i_k is semi-isomorphic to P^j_k for all $1 \leq k \leq K_i$.*

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

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

and assume first that $r_\alpha(P') > 0$. Property i) of Definition 23 yields then

$$\sum_{P \in ds(P^i_k)} p_\alpha(P, P'') \mathcal{R}_\alpha(M, v, P) = \sum_{P \in ds(P^i_k)} p_\alpha(\sigma_k(P), \sigma_k(P'')) \mathcal{R}_\alpha(M, v^\sigma, \sigma_k(P))$$

which implies (together with the definition of v)

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

Since property i) also implies $\mathcal{R}_\alpha(M, v, P') = \mathcal{R}_\alpha(M, v^\sigma, \sigma_k(P'))$ and Lemma 3 induces $\mathcal{R}_\alpha(M, v, P') > 0$, we infer $p_\alpha(P', P'') = p_\alpha(\sigma_k(P'), \sigma_k(P''))$. This and Lemma 6 show then the desired equality

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

Let us assume now $r_\alpha(P') = 0$. Our goal is to show that $r_\alpha(\sigma_k(P')) = 0$. For this we observe that $r_\alpha(P') = 0$ implies $\mathcal{R}_\alpha(M, v, P') = 0$. This and property i) of Definition 23 yield then $\mathcal{R}_\alpha(M, v^\sigma, \sigma_k(P')) = 0$. Hence, the contraposition of Lemma 3 shows that $r_\alpha(\sigma_k(P')) = 0$. (Note that v^σ plays the role of v in the aforementioned Lemma, as we are considering P^j_k and not P^i_k.) □

The previous theorem states an implication of semi-isomorphism for projected label equivalence in the case of well-posedness. We end this section by discussing that if the model is ill-posed, in general label equivalence does not imply any of the stochastic notions of behavioural equivalence for PEPA.

To see this, let us consider again the ill-posed model (2.7). Given the tuple partition $\mathcal{P} = \{(P_1), (Q_1)\}$, one can show then that $(P_1) \sim_{\{\mathcal{P}\}} (Q_1)$, essentially because P_2 is hindered in performing the δ_2 and Q_1 is hindered in performing the δ_1 action. Because of this, we conclude that label equivalence implies none of the behavioural equivalences of Section 2.3, since each of those relations

- Set $\approx_i := \approx_{\mathfrak{P}_i}$, $\approx := (\approx_1 \cup \ldots \cup \approx_m)^*$ and fix for each $1 \leq \nu \leq n$ some $P^1_\nu \in E_\nu$, where $\mathcal{G}(M)/\approx = \{E_1, \ldots, E_n\}$.
- Let us fix some arbitrary $1 \leq \nu \leq n$ and $P \in E_\nu$. Since $\approx$ is the transitive closure of $\approx_1 \cup \ldots \cup \approx_m$, there must exist a sequence $Q_1, \ldots, Q_K$ such that $Q_1 = P^1_\nu, Q_K = P$ and $Q_k \approx_{i_k} Q_{k+1}$ with $i_k \in \{1, \ldots, m\}$ for all $1 \leq k \leq K-1$. Note that the definition of $\approx_{i_k}$ implies the existence of tuples $\vec{P}'_{i_k}, \vec{P}''_{i_k} \in \mathcal{P}_{i_k}$ which witness $Q_k \approx_{i_k} Q_{k+1}$. Thus, we can extract a bijection $\rho_k : ds(Q_k) \to ds(Q_{k+1})$ from the family of bijections which establishes $\vec{P}'_{i_k} \sim_{\mathfrak{P}_{i_k}} \vec{P}''_{i_k}$. Since each ρ_k is a semi-isomorphism by Theorem 10 and a composition of semi-isomorphisms is again a semi-isomorphism, we can fix a semi-isomorphism $\rho_P : ds(P^1_\nu) \to ds(P)$ and define $\Sigma_\nu := \{\rho_P \mid P \in E_\nu\}$. Specifically, we set $\rho_{P^1_\nu} := \mathrm{id}_{ds(P^1_\nu)}$.

Figure 3.1: Construction of the bijection family used in Theorem 11.

distinguishes between the types of action performed by a process, and, clearly, P_2 performs a δ_2 activity whereas Q_1 does not.

On the other hand, even isomorphism between fluid atoms is in general not *sufficient* for establishing a projected label equivalence between them. To see this, let us consider the model $(C_1 \underset{\{exec\}}{\bowtie} T_1) \underset{\emptyset}{\bowtie} C_2$, where C_1, C_2 and T_1 are as in (3.1), and take the tuple partition $\mathcal{P} = \{(C_1), (C_2), (T_1)\}$. Then it does not hold that $(C_1) \sim_{\{\mathcal{P}\}} (C_2)$, as C_1 is in a context where it is synchronised with T_1, whereas C_2 progresses independently. Using similar ideas, one can easily construct counterexamples for tuples of length greater than one.

3.3.3 Merging of Exactly Fluid Lumpable Partitions

Let us return to our running example Sys' given in (3.1) and the corresponding tuple partitions $\mathcal{P}'_1$, $\mathcal{P}'_2$ defined in (3.11) and (3.13), respectively. Specifically, recall that $\mathcal{G}(Sys')/\approx_{\mathcal{P}'_1}$ establishes assumption (3.4), while $\mathcal{G}(Sys')/\approx_{\mathcal{P}'_2}$ yields assumption (3.5). However, neither of these tuple partitions allows us to derive (3.6), that is, (3.4) and (3.5) at the same time. We remark again that the partition (3.8) would be obtained by $\mathcal{G}(Sys')/(\approx_{\{\mathcal{P}'_1\}} \cup \approx_{\{\mathcal{P}'_2\}})^*$, where * denotes the transitive closure. Crucially, one cannot find a tuple partition $\mathcal{P}$ of $\mathcal{G}(Sys')$ and a partition $\mathfrak{P}$ of $\mathcal{P}$ such that $\mathcal{G}(Sys')/\approx_{\{\mathcal{P}\}} = \mathcal{G}(Sys')/(\approx_{\{\mathcal{P}'_1\}} \cup \approx_{\{\mathcal{P}'_2\}})^*$, i.e. a combination of several projected label equivalences cannot be expressed as a projected label equivalence in general.

Fortunately, Theorem 10 can be used to prove the following crucial theorem, which states that, in the case of well-posedness, the transitive closure of the union of projected label equivalences induces an exactly fluid lumpable partition. We wish to point out that the proof of the following result is constructive, as Figure 3.1 illustrates how to construct the bijections which establish the stated result.

Theorem 11. *Fix a well-posed FPA model M, tuple partitions $\mathcal{P}_1, \ldots, \mathcal{P}_m$ of $\mathcal{G}(M)$ and let $\mathfrak{P}_i$ denote the partition of $\mathcal{P}_i$, where $1 \leq i \leq m$. A set of bijections $\Sigma_1 \cup \ldots \cup \Sigma_n$ as in Figure 3.1 establishes the exact fluid lumpability of $\mathcal{G}(M)/(\approx_{\mathfrak{P}_1} \cup \ldots \cup \approx_{\mathfrak{P}_m})^*$. Specifically, Σ_ν relates E_ν to P_ν^1, with $1 \leq \nu \leq n$.*

Proof. We have to show that Σ_ν relates E_ν to P_ν^1, where $1 \leq \nu \leq n$. For this, we fix for each $P \in \mathcal{G}(M)$ the unique $1 \leq \nu \leq n$ such that $P \in E_\nu$ and denote by ρ_P the unique semi-isomorphism $\sigma : ds(P_\nu^1) \to ds(P)$ in Σ_ν. Further, we choose for each $1 \leq i \leq m$ and $1 \leq l \leq l_i$, where $\mathcal{G}(M)/\approx_i = \{E_1^i, \ldots, E_{l_i}^i\}$, some $P_l^i \in E_l^i$ and define $\xi_P^i := \rho_P \circ \rho_{P_l^i}^{-1}$ for all $P \in E_l^i$. Since Remark 2, Theorem 10 and the definition of $\approx_i$ imply that there is a family of semi-isomorphisms $\sigma_\bullet^i$ which relates E_l^i to P_l^i for all $1 \leq l \leq l_i$ and $\xi_\bullet^i$ is also a family of semi-isomorphisms, $\xi_\bullet^i$ relates E_l^i to P_l^i for all $1 \leq l \leq l_i$.

Let us now fix some $1 \leq \nu \leq n$ and $Q \in E_\nu \setminus \{P_\nu^1\}$. As $E_\nu \in \mathcal{G}(M)/\approx$, there is a sequence of pairwise different $Q_1, \ldots, Q_K$ such that $Q_1 = P_\nu^1, Q_K = Q$ and $Q_k \approx_{i_k} Q_{k+1}$ with $i_k \in \{1, \ldots, m\}$ for all $1 \leq k \leq K-1$. Notice that $Q_1, \ldots, Q_K \in E_\nu$ and that there is a unique $1 \leq l \leq l_{i_k}$ such that $Q_k, Q_{k+1} \in E_l^{i_k}$ for all $1 \leq k \leq K-1$. Consequently, for all $R \in ds(P_\nu^1)$ and $1 \leq k \leq K-1$, it holds that

- $P_l^{i_k} \neq Q_k, Q_{k+1}$: $v_{\rho_{Q_k}(R)} = v_{(\xi_{Q_k}^{i_k})^{-1}(\rho_{Q_k}(R))} = v_{\rho_{P_l^{i_k}}(R)}$ and $v_{\rho_{Q_{k+1}}(R)} = = v_{(\xi_{Q_{k+1}}^{i_k})^{-1}(\rho_{Q_{k+1}}(R))} = v_{\rho_{P_l^{i_k}}(R)}$
- $P_l^{i_k} = Q_k$: $v_{\rho_{Q_{k+1}}(R)} = v_{(\xi_{Q_{k+1}}^{i_k})^{-1}(\rho_{Q_{k+1}}(R))} = v_{\rho_{Q_k}(R)}$
- $P_l^{i_k} = Q_{k+1}$: $v_{\rho_{Q_k}(R)} = v_{(\xi_{Q_k}^{i_k})^{-1}(\rho_{Q_k}(R))} = v_{\rho_{Q_{k+1}}(R)}$

Since this holds for all $1 \leq k \leq K-1$, we infer that

$$v_R = v_{\rho_{Q_1}(R)} = v_{\rho_{Q_2}(R)} = \ldots = v_{\rho_{Q_K}(R)} = v_{\rho_Q(R)}$$

for all $R \in ds(P_\nu^1)$. That is, Σ_ν relates E_ν to P_ν^1, where $1 \leq \nu \leq n$. □

3.4 Related Work

As an exact form of aggregation, to the best of our knowledge the only related technique to exact fluid lumpability is [36], its various applications [37, 38, 39] and the extension [40]. A specialised version of this aggregation that allows for compositional reasoning in the context of FPA is studied in Chapter 5. Chapter 4, instead, discusses an application of exact fluid lumpability. It is fair to say that, in contrast to exact fluid lumpability, aggregations induced by [40] usually do not allow one to *fully* recover the original ODE solution from the aggregated one. For instance, let us consider the well-known susceptible-infected-recovered ODE model [55]

$$\dot{S} = -\beta SI, \qquad \dot{I} = -\gamma I + \beta SI, \qquad \dot{R} = \gamma I, \tag{3.17}$$

where β and γ refer to the average infection and recovery rate, respectively. Watson considered in [56] a generalisation of it in which the species may be classified into K subtypes. Specifically, the author studied the ODE model

$$\begin{aligned}\dot{S}_k &= -S_k \sum_{l=1}^{K} \beta_{k,l} I_l \\ \dot{I}_k &= -\gamma_k I_k + S_k \sum_{l=1}^{K} \beta_{k,l} I_l \\ \dot{R}_k &= \gamma_k I_k, \end{aligned} \tag{3.18}$$

where $1 \leq k \leq K$. Let us consider the case where the infection and recovery rates of all subtypes are equal, i.e. $\beta \equiv \beta_{k,l}$ and $\gamma \equiv \gamma_k$. Then, the above ODE system can be rewritten into

$$\begin{aligned}\sum_{k=1}^{K} \dot{S}_k &= -\beta \sum_{k=1}^{K} S_k \cdot \sum_{l=1}^{K} I_l \\ \sum_{k=1}^{K} \dot{I}_k &= -\gamma \sum_{k=1}^{K} I_k + \beta \sum_{k=1}^{K} S_k \cdot \sum_{l=1}^{K} I_l \\ \sum_{k=1}^{K} \dot{R}_k &= \gamma \sum_{k=1}^{K} I_k. \end{aligned}$$

This implies that the ODE system (3.18) of size $3K$ can be aggregated to (3.17) using the relation

$$S = \sum_{k=1}^{K} S_k, \qquad I = \sum_{k=1}^{K} I_k, \qquad R = \sum_{k=1}^{K} R_k.$$

The above aggregation can be expressed in terms of [40]. Note, however, that the original ODE system (3.18) cannot be recovered from the aggregated one (3.17), essentially because summation is not bijective.

Chapter 4

Fluid Lumpability of Nested FPA Models

This chapter starts with a conservative extension of FPA by a syntactic element that describes replicas of composite processes, cf. Section 4.1. We convey those ideas using a motivating example which highlights the fact that nested models can be used to model distributed computer systems. Note, however, that repetition patterns arise also in other fields. For instance, in the context of biological systems [57], the cells of an organism could be expressed by composite processes, in order to increase the level of detail. By exploiting the new syntactic element of FPA, we show in Section 4.2 that the notion of exact fluid lumpability can be used to aggregate the ODE systems underlying nested models to ODE systems which do not depend on the number of replications. In Section 4.3 we discuss, among other related work, [58] where the notion of nested models was introduced and which can be seen as a predecessor of the theory presented in this chapter. In [58], one aggregates ODE system by performing a model-to-model simplification, that is one identifies the aggregated ODE system of the original nested model as the fluid approximation of another, *simplified* nested model. Unfortunately, since it can be shown that there are nested models whose aggregated ODE systems do not arise from a model-to-model simplification, [58] applies only to a subclass of nested models. Here, we overcome this problem using the notion of exact fluid lumpability.

4.1 Motivating Example

Let us fix the family of sequential processes

$$\begin{aligned} &C^{\vec{i}} \stackrel{def}{=} (exec, r).\widehat{C}^{\vec{i}}, \qquad T^{\vec{i}} \stackrel{def}{=} (exec, r).\widehat{T}^{\vec{i}}, \qquad U^{\vec{i}} \stackrel{def}{=} (io, z).\widehat{U}^{\vec{i}}, \\ &\widehat{C}^{\vec{i}} \stackrel{def}{=} (reset, s).C^{\vec{i}}, \qquad \widehat{T}^{\vec{i}} \stackrel{def}{=} (io, s').T^{\vec{i}}, \qquad \widehat{U}^{\vec{i}} \stackrel{def}{=} (idle, z').U^{\vec{i}}, \end{aligned} \tag{4.1}$$

where $\vec{i} \in \mathbb{N}^{<\omega}$, which replicate, in essence, CPUs, threads and resources from the running example (3.1). Then, an application in which two independent machines share an external resource may be described by the FPA model

$$Sys_0 := (C^1 \underset{\{exec\}}{\bowtie} T^1) \underset{\emptyset}{\bowtie} (C^2 \underset{\{exec\}}{\bowtie} T^2) \underset{\{io\}}{\bowtie} U^1.$$

Note that the superscript of a label identifies the position within the model. For instance, the label C^1 refers to a group of CPUs which belong to the *first* machine. Using the tuple partition $\mathcal{P} := \{(C^1, T^1), (C^2, T^2), (U^1)\}$, we infer $\mathcal{P} \;/\; \sim_{\{\mathcal{P}\}} = \big\{\{(C^1, T^1), (C^2, T^2)\}, \{(U^1)\}\big\}$, which implies in turn the exact fluid lumpability of $\big\{\{C^1, C^2\}, \{T^1, T^2\}, \{U^1\}\big\}$.

Let us elaborate on the above example by considering two independent applications which serve a pool of users given by $E = (exec, r).\widehat{E}$ and $\widehat{E} = (io, s').E$:

$$\begin{aligned} Sys := \Big(\Big[\Big(C^{1,1} \underset{\{exec\}}{\bowtie} T^{1,1} \Big) \underset{\emptyset}{\bowtie} \Big(C^{2,1} \underset{\{exec\}}{\bowtie} T^{2,1} \Big) \underset{\{io\}}{\bowtie} U^{1,1} \Big] \underset{\emptyset}{\bowtie} \\ \Big[\Big(C^{1,2} \underset{\{exec\}}{\bowtie} T^{1,2} \Big) \underset{\emptyset}{\bowtie} \Big(C^{2,2} \underset{\{exec\}}{\bowtie} T^{2,2} \Big) \underset{\{io\}}{\bowtie} U^{1,2} \Big] \Big) \underset{\{exec,io\}}{\bowtie} E^1. \end{aligned} \quad (4.2)$$

Similarly to above, we note that the superscript of a label identifies the sequential component. For instance, the label $C^{1,2}$ refers to a group of CPUs which belong to the *first* machine within the *second* application. Specifically, the length of the sequence gives the number of *nested* repetitions. For instance, C arises *in several* machines *within several* applications. We shall refer to the maximal length of all sequences in a model as the *nesting depth*.

The fact that *Sys* has a nesting depth of two allows us to consider two tuple partitions whose exactly fluid lumpable partitions can be merged by Theorem 11. To see this, we first fix

$$\begin{aligned} \mathcal{P}_1 &:= \big\{(C^{1,1}, T^{1,1}), (C^{2,1}, T^{2,1}), (U^{1,1}), (C^{1,2}, T^{1,2}), (C^{2,2}, T^{2,2}), (U^{1,2}), (E^1)\big\} \\ \mathcal{P}_2 &:= \big\{(C^{1,1}, T^{1,1}, C^{2,1}, T^{2,1}, U^{1,1}), (C^{1,2}, T^{1,2}, C^{2,2}, T^{2,2}, U^{1,2}), (E^1)\big\}. \end{aligned}$$

Then, using the notion of label equivalence from Chapter 3, we show that

$$\begin{aligned} \mathcal{P}_1/\sim_{\{\mathcal{P}_1\}} &= \Big\{\big\{(C^{1,1}, T^{1,1}), (C^{2,1}, T^{2,1})\big\}, \big\{(U^{1,1})\big\}, \\ &\qquad \big\{(C^{1,2}, T^{1,2}), (C^{2,2}, T^{2,2})\big\}, \big\{(U^{1,2})\big\}, \big\{(E^1)\big\}\Big\}, \\ \mathcal{P}_2/\sim_{\{\mathcal{P}_2\}} &= \Big\{\big\{(C^{1,1}, T^{1,1}, C^{2,1}, T^{2,1}, U^{1,1}), (C^{1,2}, T^{1,2}, C^{2,2}, T^{2,2}, U^{1,2})\big\}, \big\{(E^1)\big\}\Big\}. \end{aligned}$$

Thus, we finally conclude that

$$\begin{aligned} \mathcal{G}(Sys)/(\approx_{\{\mathcal{P}_1\}} \cup \approx_{\{\mathcal{P}_2\}})^* = \Big\{\big\{C^{1,1}, C^{2,1}, C^{1,2}, C^{2,2}\big\}, \\ \big\{T^{1,1}, T^{2,1}, T^{1,2}, T^{2,2}\big\}, \big\{U^{1,1}, U^{1,2}\big\}, \big\{E^1\big\}\Big\}. \end{aligned}$$

This shows that the ODE system of *Sys*, which *depends* on the number of machines and applications, can be aggregated to an ODE system which does *not* depend on those multiplicities.

In order to systematically construct FPA models with (nested) repetitions, we abbreviate by $[\![M]\!]_L^N$ the cooperation of N replicas of a given model M with respect to some action set L. For instance, (4.1) is induced by the *nested* FPA model

$$\widetilde{Sys}_0 := \Big[\!\Big[C \underset{\{exec\}}{\bowtie} T\Big]\!\Big]_{\emptyset}^{N_M} \underset{\{io\}}{\bowtie} [\![U]\!]_{\emptyset}^{1}, \tag{4.3}$$

with $N_M = 2$, whereas Sys is induced by the nested FPA model

$$\widetilde{Sys} := \Big[\!\Big[\Big[\!\Big[C \underset{\{exec\}}{\bowtie} T\Big]\!\Big]_{\emptyset}^{N_M} \underset{\{io\}}{\bowtie} [\![U]\!]_{\emptyset}^{1}\Big]\!\Big]_{\emptyset}^{N_I} \underset{\{exec,io\}}{\bowtie} [\![E]\!]_{\emptyset}^{1}, \tag{4.4}$$

with $N_M = 2$ and $N_I = 2$. Note that in (4.4) the replication operator $[\![\cdot]\!]$ is applied to $\widetilde{Sys}_0$, leading to labels with sequences of length two. Moreover, the fluid approximation of $\widetilde{Sys}$ is given by an ODE system of size

$$N_I\big(N_M(|ds(C)| + |ds(T)|) + |ds(U)|\big) + |ds(E)| = N_I(4N_M + 2) + 2.$$

That is, the ODE representation grows polynomially with the nesting depth and may hinder the practical feasibility of the analysis of large-scale models.

Using exact fluid lumpability, we show in this chapter that the ODE system of a nested FPA model may be exactly related to a lumped ODE system whose size does not depend on the multiplicities. For instance, the lumped ODE system of (4.4) will have a size of $1 \cdot (4 \cdot 1 + 2) + 2 = 8$.

4.2 Definitions and Results

We start with a definition that provides the syntactic means to modelling systems with arbitrarily nested repetitions.

Definition 25 (Nested FPA Model)**.** *The syntax of a nested FPA model is given by the grammar*

$$\tilde{M} ::= \tilde{M} \underset{L}{\bowtie} \tilde{M} \mid [\![\tilde{M}]\!]_L^N \mid [\![M]\!]_L^N,$$

where M is an FPA model, $L \subseteq \mathcal{A}$ and $N \in \mathbb{N}$. We assume that in a nested FPA model all constituent FPA models have disjoint label sets and that $L = \emptyset$ if $N = 1$ for all terms $[\![\tilde{M}]\!]_L^N$ and $[\![M]\!]_L^N$.

As discussed in Section 4.1, $[\![M]\!]_L^N$ describes a cooperation of N copies of the FPA model M over the action set L, whereas $[\![\tilde{M}]\!]_L^N$ refers to a cooperation of N copies of processes which itself consists of replicated processes, thus capturing multiple levels of nesting. Throughout this section, we use $\tilde{M}$ to denote a nested FPA model, and M to denote an FPA model. Before giving the semantics, we define the set of fluid atoms of a nested FPA model.

Definition 26. *Fix a nested FPA model $\tilde{M}$. The label set of $\tilde{M}$, $\tilde{\mathcal{G}}(\tilde{M})$, is given by*

$$\tilde{\mathcal{G}}(\tilde{M}) := \begin{cases} \tilde{\mathcal{G}}(\tilde{M}_0) \cup \tilde{\mathcal{G}}(\tilde{M}_1) & , \ \tilde{M} = \tilde{M}_0 \underset{L}{\bowtie} \tilde{M}_1 \\ \tilde{\mathcal{G}}(\tilde{M}_0) & , \ \tilde{M} = [\![\tilde{M}_0]\!]_L^N \\ \mathcal{G}(M_0) & , \ \tilde{M} = [\![M_0]\!]_L^N \end{cases}$$

For instance, it holds that $\tilde{\mathcal{G}}(\widetilde{Sys}) = \{C, T, U, E\}$.

Next, we introduce the *copies* of the fluid atoms of a nested FPA model.

Definition 27. *Fix a nested FPA model $\tilde{M}$. The set of* replicated constants *of $\tilde{M}$ is $\{Q^{\vec{i}} \mid \vec{i} \in \mathbb{N}^{<\omega}$ and $Q \in ds(P)$ for some $P \in \tilde{\mathcal{G}}(\tilde{M})\}$ with*

$$Q^{\vec{i}} \stackrel{\text{def}}{=} \sum_{j \in J} (\alpha_j, r_j).Q_j^{\vec{i}} \quad \text{if} \quad Q \stackrel{\text{def}}{=} \sum_{j \in J} (\alpha_j, r_j).Q_j.$$

For instance, the sequential processes C^1 and $C^{1,1}$ in (4.2) are copies of C. Finally, the following definition permits to replace fluid atoms within an FPA model.

Definition 28. *Let M be an FPA model and $\mathcal{G}(M) = \{P_1, \ldots, P_n\}$. For a set of labels $\{Q_1, \ldots, Q_n\}$, the FPA model $M[P_1/Q_1, \ldots, P_n/Q_n]$ (alternatively, $M[P_i/Q_i \mid 1 \leq i \leq n]$) is obtained from M by replacing P_k with Q_k, for $1 \leq k \leq n$.*

For instance, it holds that $(C \underset{L}{\bowtie} T)[C/C^1, T/T^1] = C^1 \underset{L}{\bowtie} T^1$.

We are now in the position to define the semantics of a nested FPA model.

Definition 29 (Interpretation Function)**.** *A nested FPA model $\tilde{M}$ is interpreted as the ordinary FPA model $\mathcal{I}(\tilde{M})$, which is recursively given by*

$$\begin{cases} \mathcal{I}(\tilde{M}_0) \underset{L}{\bowtie} \mathcal{I}(\tilde{M}_1) & , \ \tilde{M} = \tilde{M}_0 \underset{L}{\bowtie} \tilde{M}_1 \\ \mathcal{I}\left([\![\mathcal{I}(\tilde{M}_0)]\!]_L^N\right) & , \ \tilde{M} = [\![\tilde{M}_0]\!]_L^N \\ M[P_1/\Lambda(P_1,1), \ldots, P_m/\Lambda(P_m,1)] & , \ \tilde{M} = [\![M]\!]_L^N \wedge N = 1 \wedge \\ & \quad \mathcal{G}(M) = \{P_1, \ldots, P_m\} \\ M[P_1/\Lambda(P_1,1), \ldots, P_m/\Lambda(P_m,1)] \underset{L}{\bowtie} \cdots & \\ \quad \cdots \underset{L}{\bowtie} M[P_1/\Lambda(P_1,N), \ldots, P_m/\Lambda(P_m,N)] & , \ \tilde{M} = [\![M]\!]_L^N \wedge N > 1 \wedge \\ & \quad \mathcal{G}(M) = \{P_1, \ldots, P_m\}, \end{cases}$$

where

$$\Lambda(P,i) := \begin{cases} Q^i & , \ \exists Q \in \tilde{\mathcal{G}}(\tilde{M}).\ \big(P = Q\big) \\ Q^{\vec{j},i} & , \ \exists Q \in \tilde{\mathcal{G}}(\tilde{M}).\ \exists \vec{j} \in \mathbb{N}^{<\omega}.\ \big(P = Q^{\vec{j}}\big) \end{cases}$$

denotes the superscript appending function.

A simple inductive argument shows that $\mathcal{I}(\tilde{M})$ is indeed an ordinary FPA model if $\tilde{M}$ is a nested FPA model. Crucially, the interpretation function is such

that the labels preserve all the information about the replication structure of the nested model. The function Λ carries out a suitable manipulation of labels which keeps track of the nesting hierarchy by appending unique sequences as superscripts.

For instance, by applying $\mathcal{I}$ to the motivating example (4.4), one infers

$$\begin{aligned}
\mathcal{I}(\widetilde{Sys}) &= \mathcal{I}\left(\left[\!\!\left[\mathcal{I}\left(\left[\!\!\left[C \underset{\{exec\}}{\bowtie} T\right]\!\!\right]^2_{\emptyset}\right) \underset{\{io\}}{\bowtie} \mathcal{I}\left(\llbracket U \rrbracket^1_{\emptyset}\right)\right]\!\!\right]^2_{\emptyset}\right) \underset{\{exec,io\}}{\bowtie} \mathcal{I}\left(\llbracket E \rrbracket^1_{\emptyset}\right) \\
&= \mathcal{I}\left(\left[\!\!\left[\left(C^1 \underset{\{exec\}}{\bowtie} T^1\right) \underset{\emptyset}{\bowtie} \left(C^2 \underset{\{exec\}}{\bowtie} T^2\right) \underset{\{io\}}{\bowtie} U^1\right]\!\!\right]^2_{\emptyset}\right) \underset{\{exec,io\}}{\bowtie} E^1 \\
&= \Big(\Big[\Big(C^{1,1} \underset{\{exec\}}{\bowtie} T^{1,1}\Big) \underset{\emptyset}{\bowtie} \Big(C^{2,1} \underset{\{exec\}}{\bowtie} T^{2,1}\Big) \underset{\{io\}}{\bowtie} U^{1,1}\Big] \underset{\emptyset}{\bowtie} \\
&\qquad \Big[\Big(C^{1,2} \underset{\{exec\}}{\bowtie} T^{1,2}\Big) \underset{\emptyset}{\bowtie} \Big(C^{2,2} \underset{\{exec\}}{\bowtie} T^{2,2}\Big) \underset{\{io\}}{\bowtie} U^{1,2}\Big] \Big) \underset{\{exec,io\}}{\bowtie} E^1
\end{aligned}$$

In particular, $\mathcal{I}(\widetilde{Sys})$ is, as expected, the FPA model Sys.

The following notions will be needed to state the main result of the chapter.

Definition 30. *Fix a nested FPA model $\tilde{M}$ and let $P \in \tilde{\mathcal{G}}(\tilde{M})$. Then, $P(\tilde{M})$ denotes the set of copies of P.*

For instance, it holds that $C(\widetilde{Sys}) = \{C^{1,1}, C^{2,1}, C^{1,2}, C^{2,2}\}$ and $U(\widetilde{Sys}) = \{U^{1,1}, U^{1,2}\}$.

Definition 31. *Fix a nested FPA model $\tilde{M}$. Then, for all $P \in \tilde{\mathcal{G}}(\tilde{M})$ and $P^{\vec{i}}, P^{\vec{j}} \in P(\tilde{M})$, the bijections*

$$ds(P^{\vec{i}}) \to ds(P^{\vec{j}}), \quad Q^{\vec{i}} \mapsto Q^{\vec{j}}, \qquad \textit{where} \quad Q \in ds(P),$$

are called copy-isomorphisms.

Let us fix a nested FPA model $\tilde{M}$ such that $\mathcal{I}(\tilde{M})$ is well-posed and $\tilde{\mathcal{G}}(\tilde{M}) = \{P_1, \ldots, P_n\}$. In the following, we show that $\{P_i(\tilde{M}) \mid 1 \leq i \leq n\}$ is an exactly fluid lumpable partition of $\mathcal{G}(\mathcal{I}(\tilde{M}))$ established by copy-isomorphisms, cf. Theorem 14. We do so by proving first that there exist tuple partitions $\mathcal{P}_1, \ldots, \mathcal{P}_m$ of $\mathcal{G}(\mathcal{I}(\tilde{M}))$ and partitions $\mathfrak{P}_1, \ldots, \mathfrak{P}_m$ of $\mathcal{P}_1, \ldots, \mathcal{P}_m$, respectively, such that

$$\begin{aligned}
&1) \quad \mathcal{P}_l \,/\, \sim_{\mathfrak{P}_l} \text{ is established by copy-isomorphisms for all } 1 \leq l \leq m \\
&2) \quad \mathcal{G}(\mathcal{I}(\tilde{M})) \,/\, (\approx_{\mathfrak{P}_1} \cup \ldots \cup \approx_{\mathfrak{P}_m})^* = \{P_i(\tilde{M}) \mid 1 \leq i \leq n\}
\end{aligned} \tag{4.5}$$

This and Theorem 11 yield then the claim. Before establishing (4.5), however, one has first to prove the following special case of it.

Theorem 12. *Fix an FPA model M and let $\{P_1, \ldots, P_n\}$ be the labels of $\mathcal{G}(M)$. Then for the tuple partition $\mathcal{P} := \{(P_1^1, \ldots, P_n^1), \ldots, (P_1^N, \ldots, P_n^N)\}$*

of $\mathcal{G}(\mathcal{I}([\![M]\!]_L^N))$ *and two arbitrary tuples* $\left(P_1^i,\dots,P_n^i\right)$ *and* $\left(P_1^j,\dots,P_n^j\right)$*, the copy-isomorphisms*

$$\sigma_k : ds(P_k^i) \to ds(P_k^j), \quad P^i \mapsto P^j, \quad P \in ds(P_k),$$

where $1 \leq k \leq n$*, establish* $\left(P_1^i,\dots,P_n^i\right) \sim_{\{\mathcal{P}\}} \left(P_1^j,\dots,P_n^j\right)$.

Proof. Let us write $M^1 \underset{L}{\bowtie} \dots \underset{L}{\bowtie} M^N$ for $\mathcal{I}([\![M]\!]_L^N)$ and define $Sys := \mathcal{I}([\![M]\!]_L^N)$. Then, for an arbitrary concentration function v of Sys, it holds that

$$\begin{aligned} r_\alpha(Sys, v) &= \min\{r_\alpha(M^1, v), \dots, r_\alpha(M^N, v)\} \\ &= \min\{r_\alpha(M^1, v^\sigma), \dots, r_\alpha(M^N, v^\sigma)\} = r_\alpha(Sys, v^\sigma) \end{aligned}$$

for all $\alpha \in L$ and

$$\begin{aligned} r_\alpha(Sys, v) &= r_\alpha(M^1, v) + \dots + r_\alpha(M^N, v) \\ &= r_\alpha(M^1, v^\sigma) + \dots + r_\alpha(M^N, v^\sigma) = r_\alpha(Sys, v^\sigma) \end{aligned}$$

for all all $\alpha \notin L$, where v^σ is as in Definition 23. Moreover, if $\alpha \in L$, it holds that

$$\mathcal{R}_\alpha(Sys, v, P) = \frac{\mathcal{R}_\alpha(M^l, v, P)}{r_\alpha(M^l, v)} r_\alpha(Sys, v)$$

for all $1 \leq l \leq N$, $1 \leq k \leq n$ and $P \in ds(P_k^l)$. We show this by induction on N:

- $N = 1$: Clear.
- $N \to N+1$: Since the case is obvious if $l = N+1$, we focus on the case $1 \leq l \leq N$. Then it holds that

  $$\mathcal{R}_\alpha(\mathcal{I}([\![M]\!]_L^{N+1}), v, P) = \frac{\mathcal{R}_\alpha(\mathcal{I}([\![M]\!]_L^N), v, P)}{r_\alpha(\mathcal{I}([\![M]\!]_L^N), v)} r_\alpha(\mathcal{I}([\![M]\!]_L^{N+1}), v)$$

  and the induction hypothesis

  $$\mathcal{R}_\alpha(\mathcal{I}([\![M]\!]_L^N), v, P) = \frac{\mathcal{R}_\alpha(M^l, v, P)}{r_\alpha(M^l, v)} r_\alpha(\mathcal{I}([\![M]\!]_L^N), v)$$

  yields the claim.

Using this auxiliary result, we infer in the case of $\alpha \in L$ that

$$\begin{aligned} \mathcal{R}_\alpha(Sys, v, P^i) &= \frac{\mathcal{R}_\alpha(M^i, v, P^i)}{r_\alpha(M^i, v)} r_\alpha(Sys, v) \\ &= \frac{\mathcal{R}_\alpha(M^j, v^\sigma, P^j)}{r_\alpha(M^j, v^\sigma)} r_\alpha(Sys, v^\sigma) = \mathcal{R}_\alpha(Sys, v^\sigma, P^j) \end{aligned}$$

for all $1 \leq k \leq n$, $P^i \in ds(P^i_k)$ and

$$\begin{aligned}\mathcal{R}_\alpha(Sys, v, P^l) &= \frac{\mathcal{R}_\alpha(M^l, v, P^l)}{r_\alpha(M^l, v)} r_\alpha(Sys, v) \\ &= \frac{\mathcal{R}_\alpha(M^l, v^\sigma, P^l)}{r_\alpha(M^l, v^\sigma)} r_\alpha(Sys, v^\sigma) = \mathcal{R}_\alpha(Sys, v^\sigma, P^l)\end{aligned}$$

for all $1 \leq k \leq n$, $l \in \{1, \ldots, N\} \setminus \{i, j\}$ and $P^l \in ds(P^l_k)$. Since in the case of $\alpha \notin L$ it also holds that

$$\mathcal{R}_\alpha(Sys, v, P^i) = \mathcal{R}_\alpha(M^i, v, P^i) = \mathcal{R}_\alpha(M^j, v^\sigma, P^j) = \mathcal{R}_\alpha(Sys, v^\sigma, P^j)$$

for all $1 \leq k \leq n$, $P^i \in ds(P^i_k)$ and

$$\mathcal{R}_\alpha(Sys, v, P^l) = \mathcal{R}_\alpha(M^l, v, P^l) = \mathcal{R}_\alpha(M^l, v^\sigma, P^l) = \mathcal{R}_\alpha(Sys, v^\sigma, P^l)$$

for all $1 \leq k \leq n$, $l \in \{1, \ldots, N\} \setminus \{i, j\}$ and $P^l \in ds(P^l_k)$, the proof is complete. □

Equipped with Theorem 12, (4.5) can be shown by means of structural induction.

Theorem 13. *Fix a nested FPA model $\tilde{M}_0$ and let $\{P_1, \ldots, P_n\}$ be the labels $\tilde{\mathcal{G}}(\tilde{M}_0)$. Then, under the assumption that $\mathcal{I}(\tilde{M}_0)$ is well-posed, there exist tuple partitions $\mathcal{P}_1, \ldots, \mathcal{P}_m$ of $\mathcal{G}(\mathcal{I}(\tilde{M}_0))$ and partitions $\mathfrak{P}_1, \ldots, \mathfrak{P}_m$ of $\mathcal{P}_1, \ldots, \mathcal{P}_m$, respectively, such that*

1) $\mathcal{P}_l \,/\, \sim_{\mathfrak{P}_l}$, where $1 \leq l \leq m$, is established by copy-isomorphisms

2) $\mathcal{G}(\mathcal{I}(\tilde{M}_0)) \,/\, (\approx_{\mathfrak{P}_1} \cup \ldots \cup \approx_{\mathfrak{P}_m})^* = \{P_i(\tilde{M}_0) \mid 1 \leq i \leq n\}$

Proof. We prove this by induction on $\tilde{M}_0$.

- $\tilde{M}_0 = [\![M]\!]^N_L$: Follows from Theorem 12.
- $\tilde{M}_0 = [\![\tilde{M}]\!]^N_L$: Clearly, the well-posedness of $\mathcal{I}([\![\tilde{M}]\!]^N_L)$ induces that of $\mathcal{I}(\tilde{M})$ and one can apply the induction hypothesis which ensures that there are tuple partitions $\mathcal{P}_1, \ldots, \mathcal{P}_m$ of $\mathcal{G}(\mathcal{I}(\tilde{M}))$ and partitions $\mathfrak{P}_1, \ldots, \mathfrak{P}_m$ of $\mathcal{P}_1, \ldots, \mathcal{P}_m$, respectively, witnessing property 1) and 2) of $\tilde{M}$. We define

$$\begin{aligned}\mathcal{P}^k_l &:= \{\Lambda(\vec{P}, k) \mid \vec{P} \in \mathcal{P}_l\} \\ \mathfrak{P}^k_l &:= \left\{\{\Lambda(\vec{P}, k) \mid \vec{P} \in \mathfrak{p}\} \;\middle|\; \mathfrak{p} \in \mathfrak{P}_l\right\}\end{aligned}$$

  for all $1 \leq l \leq m$ and $1 \leq k \leq N$, where Λ caries over to tuples of labels in straightforward manner. Using Theorem 8, one can prove by induction on N that $\vec{P}' \sim_{\mathfrak{P}_l} \vec{P}''$ induces $\Lambda(\vec{P}', k) \sim_{\mathfrak{P}^1_l \cup \ldots \cup \mathfrak{P}^N_l} \Lambda(\vec{P}'', k)$ for all $1 \leq k \leq N$. Moreover, since also the converse can be shown by induction on N, property 2) yields

$$\begin{aligned}&\mathcal{G}\big(\mathcal{I}\big([\![\tilde{M}]\!]^N_L\big)\big) \,/\, (\approx_{\mathfrak{P}^1_1 \cup \ldots \cup \mathfrak{P}^N_1} \cup \ldots \cup \approx_{\mathfrak{P}^1_m \cup \ldots \cup \mathfrak{P}^N_m})^* = \\ &= \big\{\Lambda(P_1(\tilde{M}), 1), \ldots, \Lambda(P_n(\tilde{M}), 1), \ldots, \Lambda(P_1(\tilde{M}), N), \ldots, \Lambda(P_n(\tilde{M}), N)\big\}\,.\end{aligned}$$

Let us identify the labels of $\mathcal{G}(\mathcal{I}(\tilde{M}))$ by $\{Y_1, \ldots, Y_\nu\}$ and define

$$\mathcal{P} := \big\{\big(\Lambda(Y_1,1),\ldots,\Lambda(Y_\nu,1)\big),\ldots,\big(\Lambda(Y_1,N),\ldots,\Lambda(Y_\nu,N)\big)\big\}.$$

Then, as Theorem 12 induces

$$\mathcal{P} \,/\sim_{\{\mathcal{P}\}} = \Big\{\big\{\big(\Lambda(Y_1,1),\ldots,\Lambda(Y_\nu,1)\big),\ldots,\big(\Lambda(Y_1,N),\ldots,\Lambda(Y_\nu,N)\big)\big\}\Big\}$$

and

$$\{\Lambda(Y_i,k) \mid 1 \le i \le \nu\} = \bigcup\{\Lambda(P_i(\tilde{M}),k) \mid 1 \le i \le n\}$$

for all $1 \le k \le N$, one infers that

$$\mathcal{G}\big(\mathcal{I}\big([\![\tilde{M}]\!]_L^N\big)\big) \,/\, (\approx_{\{\mathcal{P}\}} \cup \approx_{\mathfrak{P}_1^1 \cup \ldots \cup \mathfrak{P}_1^N} \cup \ldots \cup \approx_{\mathfrak{P}_m^1 \cup \ldots \cup \mathfrak{P}_m^N})^* = \\ = \{P_i([\![\tilde{M}]\!]_L^N) \mid 1 \le i \le n\}\ .$$

Since $(\mathcal{P}_l^1 \cup \ldots \cup \mathcal{P}_l^N) \,/\sim_{\mathfrak{P}_l^1 \cup \ldots \cup \mathfrak{P}_l^N}$, where $1 \le l \le m$, is established by copy-isomorphisms thanks to property 1) and the same obviously holds for $\mathcal{P} \,/\sim_{\{\mathcal{P}\}}$, the case is complete.

- $\tilde{M}_0 = \tilde{M}^0 \underset{L}{\bowtie} \tilde{M}^1$: Assume without loss of generality that $\{P_1, \ldots, P_{n'}\}$ and $\{P_{n'+1}, \ldots, P_n\}$ are the labels of $\tilde{\mathcal{G}}(\tilde{M}^0)$ and $\tilde{\mathcal{G}}(\tilde{M}^1)$, respectively. Since the well-posedness of $\mathcal{I}(\tilde{M}_0)$ induces that of $\mathcal{I}(\tilde{M}^j)$, the induction hypothesis may be applied and ensures that there exist tuple partitions $\mathcal{P}_1^j, \ldots, \mathcal{P}_{m^j}^j$ of $\mathcal{G}(\mathcal{I}(\tilde{M}^j))$ and partitions $\mathfrak{P}_1^j, \ldots, \mathfrak{P}_{m^j}^j$ of $\mathcal{P}_1^j, \ldots, \mathcal{P}_{m^j}^j$, respectively, which witness property 1) and 2) of $\tilde{M}^j$, where $j = 0, 1$. Identifying the labels of $\mathcal{G}(\mathcal{I}(\tilde{M}^j))$ by $\{Y_1^j, \ldots, Y_{\nu_j}^j\}$, we define

$$\overline{\mathcal{P}}_l^j := \mathcal{P}_l^j \cup \{(Y_1^{1-j}, \ldots, Y_{\nu_{1-j}}^{1-j})\} \quad \text{and} \quad \overline{\mathfrak{P}}_l^j := \mathfrak{P}_l^j \cup \big\{\{(Y_1^{1-j}, \ldots, Y_{\nu_{1-j}}^{1-j})\}\big\},$$

where $1 \le l \le m^j$, and observe using Theorem 8 that $\vec{P}' \sim_{\mathfrak{P}_l^j} \vec{P}''$ implies $\vec{P}' \sim_{\overline{\mathfrak{P}}_l^j} \vec{P}''$ for all $1 \le l \le m^j$ and $\vec{P}', \vec{P}'' \in \mathcal{P}_l^j$. Since also the converse holds thanks to the well-posedness of $\mathcal{I}(\tilde{M}_0)$, property 2) yields

$$\mathcal{G}(\mathcal{I}(\tilde{M}_0)) \,/\, (\approx_{\overline{\mathfrak{P}}_1^j} \cup \ldots \cup \approx_{\overline{\mathfrak{P}}_{m^j}^j})^* = \\ \begin{cases} \big\{P_i(\tilde{M}^0) \mid 1 \le i \le n'\big\} \cup \big\{\{Y_k^1\} \mid 1 \le k \le \nu_1\big\} & ,\ j = 0 \\ \big\{P_i(\tilde{M}^1) \mid n'+1 \le i \le n\big\} \cup \big\{\{Y_k^0\} \mid 1 \le k \le \nu_0\big\} & ,\ j = 1 \end{cases}$$

and we infer

$$\mathcal{G}(\mathcal{I}(\tilde{M}_0)) \,/\, (\approx_{\overline{\mathfrak{P}}_1^0} \cup \ldots \cup \approx_{\overline{\mathfrak{P}}_{m^0}^0} \cup \approx_{\overline{\mathfrak{P}}_1^1} \cup \ldots \cup \approx_{\overline{\mathfrak{P}}_{m^1}^1})^* = \\ = \{P_i(\tilde{M}^0) \mid 1 \le i \le n'\} \cup \{P_i(\tilde{M}^1) \mid n'+1 \le i \le n\} \\ = \{P_i(\tilde{M}_0) \mid 1 \le i \le n\}.$$

Since 1) ensures that $\overline{\mathcal{P}}_l^j \,/\, \sim_{\overline{\mathfrak{P}}_l^j}$, where $j = 0, 1$ and $1 \le l \le m^j$, is established by copy-isomorphisms, the case is complete.

□

We are now in a position to state the main result of the chapter.

Theorem 14. *Fix a nested FPA model $\tilde{M}$ and let $\tilde{\mathcal{G}}(\tilde{M}) = \{P_1, \ldots, P_n\}$. Then, if $\mathcal{I}(\tilde{M})$ is well-posed, $\{P_i(\tilde{M}) \mid 1 \leq i \leq n\}$ is an exactly fluid lumpable partition of $\mathcal{G}(\mathcal{I}(\tilde{M}))$ and one can choose copy-isomorphisms as the establishing bijections.*

Proof. The claim follows by Theorem 13, Theorem 11 and the fact that all bijections in Figure 3.1 can be chosen as copy-isomorphisms. □

4.3 Related Work

An alternative route for an efficient analysis of PEPA models with replications of composite processes is to identify classes of models that enjoy a *product form* solution, whereby the steady-state joint probability distribution of a component-based model can be expressed as the product of the marginal probability distributions of the constituting components, which are often sensibly easier to obtain. Originally researched in the context of queueing networks (e.g., [59]), product forms have been also studied in the context of stochastic Petri nets [60] and more general compositions of Markov chains [61]. In PEPA, [62, 63] syntactically characterise classes of models that admit a product form. Instead, [64] studies a class of queueing-network type PEPA models that are amenable to mean value analysis [64], which makes the analysis only linearly dependent on job populations, as opposed to a generally polynomial growth with lumping techniques. A general framework for product forms for PEPA is that of Harrison's *Reversed Compound Agent Theorem* [65]. In all these works, the PEPA model must satisfy certain syntactical conditions which restrict the applicability of those results; for instance, in general (4.3) does not admit a product form [66].

In the context of layered queueing networks [67], Woodside *et al.* have developed a method for efficiently analysing replicated subsystems, which are defined in a similar fashion as our nested models in terms replicas of non-elementary components of the network [68]. Their approach scales very well with increasing number of replicas because the solution method is based on approximate mean value analysis (e.g., [69, 70]), which is insensitive to the network's customer populations. Despite being analogous in spirit, our approach is starkly different for two reasons: first, it is an exact form of approximation in the sense that the original ODE solution can be fully recovered from the aggregated one; second, the relationship between the fluid trajectories of the original and the aggregated model is valid for the entire time horizon for which the ODE is defined, unlike in layered queues or in exact product-form solutions where only steady-state estimates are available.

In the remainder of this section, we compare the theory of this chapter to its predecessor [58]. There, we study families of models that, though being structurally different, are all related to the same underlying ODE system. This is done by systematically simplifying, under certain assumptions, a given model

into one with fewer fluid atoms. Although the original and simplified models share a common ODE system, it can be shown that they are, in general, not semi-isomorphic, not strongly bisimilar and not strongly equivalent. A numerical study motivated by this observation suggests that simplified models are approximated better by the common ODE system. Since not all ODE aggregations can be expressed in terms of a model-to-model simplification, we conclude that the theory of this chapter improves [58].

Example We relate [58] to the approach of this chapter using our running example. Specifically, let us consider the variation

$$\Big(\big(C^1 \underset{\{exec\}}{\bowtie} T^1\big) \underset{\emptyset}{\bowtie} \ldots \underset{\emptyset}{\bowtie} \big(C^D \underset{\{exec\}}{\bowtie} T^D\big)\Big) \underset{\{io\}}{\bowtie} U^1 \tag{4.6}$$

of (3.1) where $U^1 \stackrel{def}{=} (io, z).U^1$ and C^d, T^d are as before, that is

$$C^d \stackrel{def}{=} (exec, r).\widehat{C}^d, \quad \widehat{C}^d \stackrel{def}{=} (reset, s).C^d, \quad T^d \stackrel{def}{=} (exec, r).\widehat{T}^d, \quad \widehat{T}^d \stackrel{def}{=} (io, s').T^d.$$

Then, similarly to the running example (3.1), it can be shown that the partition $\big\{\{C^1, \ldots, C^D\}, \{T^1, \ldots, T^D\}, \{U^1\}\big\}$ is exactly fluid lumpable. This implies that the fluid approximation of (4.6)

$$\dot{v}_{C^d} = -r \min\big(v_{C^d}, v_{T^d}\big) + s v_{\widehat{C}^d} \qquad \dot{v}_{\widehat{C}^d} = -\dot{v}_{C^d}$$

$$\dot{v}_{T^d} = -r \min\big(v_{C^d}, v_{T^d}\big) + \frac{s' v_{\widehat{T}^d}}{s' \sum_{d'=1}^{D} v_{\widehat{T}^{d'}}} \min\Big(s' \sum_{d'=1}^{D} v_{\widehat{T}^{d'}}, z v_{U^1}\Big) \quad \dot{v}_{\widehat{T}^d} = -\dot{v}_{T^d}$$

$$\dot{v}_{U^1} = 0,$$

where $1 \leq d \leq D$, can be recovered by solving

$$\begin{aligned}
&\dot{v}_{C^1} = -r \min\big(v_{C^1}, v_{T^1}\big) + s v_{\widehat{C}^1} && \dot{v}_{\widehat{C}^1} = -\dot{v}_{C^1} \\
&\dot{v}_{T^1} = -r \min\big(v_{C^1}, v_{T^1}\big) + (1/D) \min\big(s' D \cdot v_{\widehat{T}^1}, z v_{U^1}\big) && \dot{v}_{\widehat{T}^1} = -\dot{v}_{T^1} \\
&\dot{v}_{U^1} = 0, && \qquad (4.7)
\end{aligned}$$

if it holds that $v_{P^d}(0) = v_{P^{d'}}(0)$ for all $1 \leq d, d' \leq D$ and $P \in \{C, \widehat{C}, T, \widehat{T}\}$.

Note that by setting

$$v'_{U^1} = v_{U^1} \quad \text{and} \quad v'_{P^1} = D \cdot v_{P^1}, \qquad P \in \{C, \widehat{C}, T, \widehat{T}\},$$

and multiplying the first four ODEs of (4.7) by D, one infers that

$$\begin{aligned}
&\dot{v}'_{C^1} = -r \min\big(v'_{C^1}, v'_{T^1}\big) + s v'_{\widehat{C}^1} && \dot{v}'_{\widehat{C}^1} = -\dot{v}'_{C^1} \\
&\dot{v}'_{T^1} = -r \min\big(v'_{C^1}, v'_{T^1}\big) + \min\Big(s' \cdot v'_{\widehat{T}^1}, z v'_{U^1}\Big) && \dot{v}'_{\widehat{T}^1} = -\dot{v}'_{T^1} \\
&\dot{v}'_{U^1} = 0 && \qquad (4.8)
\end{aligned}$$

This is remarkable in that the above ODE system describes the fluid approximation of

$$\big(C^1 \underset{\{exec\}}{\bowtie} T^1\big) \underset{\{io\}}{\bowtie} U^1.$$

From this, we infer that the fluid approximations of the nested FPA models

$$\Big[\!\Big[C \underset{\{exec\}}{\bowtie} T\Big]\!\Big]_{\emptyset}^{D} \underset{\{io\}}{\bowtie} [\![U]\!]_{\emptyset}^{1} \quad \text{and} \quad \Big[\!\Big[C \underset{\{exec\}}{\bowtie} T\Big]\!\Big]_{\emptyset}^{1} \underset{\{io\}}{\bowtie} [\![U]\!]_{\emptyset}^{1}, \tag{4.9}$$

are related by

$$v'_{U^1} = v_{U^1} \quad \text{and} \quad v'_{P^1} = D \cdot v_{P^d}, \qquad P \in \{C, \widehat{C}, T, \widehat{T}\}, \quad 1 \le d \le D. \tag{4.10}$$

Stochastic Difference Next, we show that, in general, the original and simplified models are stochastically different. For this, let us denote by

$$Sys := \Big(\big(C[N_C] \underset{\{exec\}}{\bowtie} T[N_T]\big) \underset{\emptyset}{\bowtie} \ldots \underset{\emptyset}{\bowtie} \big(C[N_C] \underset{\{exec\}}{\bowtie} T[N_T]\big)\Big) \underset{\{io\}}{\bowtie} U[N_U]$$

and

$$Sys' := \big(C[D \cdot N_C] \underset{\{exec\}}{\bowtie} T[D \cdot N_T]\big) \underset{\{io\}}{\bowtie} U[N_U]$$

the PEPA models induced by (4.9) and (4.10). We proceed by noting that, although the total number of sequential components is equal in both models, Sys' has, intuitively, a higher communication potential than Sys. To see this, assume for the sake of simplicity that $N_C = N_T = N_U = 1$ and $D = 2$. Then, although the models

$$\big(C \underset{\{exec\}}{\bowtie} \widehat{T}\big) \underset{\emptyset}{\bowtie} \big(\widehat{C} \underset{\{exec\}}{\bowtie} T\big) \underset{\{io\}}{\bowtie} U \qquad \text{and} \qquad \big(C \parallel \widehat{C}\big) \underset{\{exec\}}{\bowtie} \big(T \parallel \widehat{T}\big) \underset{\{io\}}{\bowtie} U$$

have the same number of sequential components, the first model, in contrast to the second one, cannot perform an *exec* action. This observation is at the basis of the proof that, in general, Sys and Sys' are not strongly bisimilar. Indeed, the following can be shown.

Proposition 2. *In general, Sys and Sys′ are*

i) Not semi-isomorphic.

ii) Not strongly bisimilar.

iii) Not strongly equivalent.

Proof. We start by observing that Sys and Sys' cannot be semi-isomorphic because of $|ds(Sys')| < |ds(Sys)|$ and proceed by providing a winning strategy for the attacker in a bisimulation game, as illustrated in Figure 4.1. Each line in this figure denotes a move of the game in the case of $D = 2$; the strategy, however, can be easily generalised for arbitrary D. The transitions are labelled with the role (where *A:* and *D:* stand for *attacker* and *defender*, respectively) and the action type chosen. The rates are suppressed, as they are not relevant for the game.

Statements *i*) and *ii*) hold for any values of the rates r, s, and s', any $D \ge 2$ and any initial populations N_C, N_T and N_U. Instead, in order to show that in general Sys is not strongly equivalent to Sys', we resort to numerical solution

of the two CTMCs in the specific case where $r = 4$, $s = s' = 1$, $D = 2$ and $N_C = N_T = N_U = 1$. Let us assume towards a contradiction that *Sys* and *Sys*$'$ are strongly equivalent, that is, we can fix strong equivalence relations R on $ds(Sys)$ and R' on $ds(Sys')$ such that the corresponding lumped CTMCs stand in an one-to-one correspondence, cf. Section 8.5 in [7].

Next, we fix an arbitrary $E'_0 \in [Sys']_{R'}$. As pointed out in the proof of Proposition 8.3.1 in [7], it must hold that $r_{exec}(Sys') = r_{exec}(E'_0)$. Hence, we infer $E'_0 = Sys'$, because *Sys*$'$ is the only state in $ds(Sys')$ with an *exec* apparent rate of $\min(2r, 2r) = 2r$. Consequently, $[Sys']_{R'} = \{Sys'\}$.

Since R and R' are strong equivalence relations, there exists an $S \subseteq ds(Sys)$ such that $\pi(Sys') = \sum_{s \in S} \pi(s)$, where $\pi(s)$ denotes the steady-state probability of s in the corresponding CTMC. (In essence, S is the macro state in $ds(Sys)/R$ which corresponds to the macro state $[Sys']_{R'}$ in $ds(Sys')/R'$.) We found that $\pi(Sys')$ was equal to 0.01345 and $\min\{\pi(s) \mid s \in ds(Sys)\}$ was equal to 0.01640 up to the fifth decimal digit across a range of solution algorithms such as Gaussian elimination and the methods of generalised minimal residual and biconjugate gradient [71]. Since this is a contradiction to $\pi(Sys') = \sum_{s \in S} \pi(s)$, the proof is complete. □

Remark 4. *Among being of interest on its own, the above result shows that the notion of exact fluid lumpability cannot be captured by common stochastic equivalence relations.*

Numerical Study Above, we have established that the fluid approximation of *Sys* can be recovered from that of *Sys*$'$. Moreover, *Sys* and *Sys*$'$ were identified as stochastically different. Since their common ODE system (4.8) approximates the concentration trajectories of the sequential components, it is interesting to assess which CTMC model between *Sys* and *Sys*$'$ is best approximated by the ODE solution.

This study is here conducted by means of a large numerical assessment over five thousand instances of *Sys* which differed in the actual values for the rate parameters r, s, and s', and in the initial population levels N_C, N_T, and N_U. These parameters were all drawn from uniform distributions. The range for N_C, N_T, and N_U was set to $1, \ldots, 20$, the range for D was $1, \ldots, 10$, whereas the range for all rate values was $[0.01, 100.0]$. For each such pair, we computed the steady-state distributions of the CTMC of *Sys* and that of *Sys*$'$, using a stochastic simulation algorithm with the method of batch means and imposing a stopping condition of 5% radius at 95% confidence intervals in both cases. (Standard numerical solution of the CTMC by linear algebra was not possible with this data set due to the extremely large state spaces involved.) The expectations of the total number of components in state C, $\widehat{C}$, T, $\widehat{T}$, hereby denoted by $\mathbb{E}[C], \ldots, \mathbb{E}[\widehat{T}]$, were compared against the solution to the ODE $v_C, \ldots, v_{\widehat{T}}$. The following percentage errors were computed:

$$\text{Error} = 100 \cdot \max_{P \in \{C, \widehat{C}, T, \widehat{T}\}} \big\{ |\mathbb{E}[P] - v_P| \;/\; \mathbb{E}[P] \big\}.$$

$$\Big([N_C,0] \underset{\{exec\}}{\bowtie} [N_T,0]\Big) \parallel \Big([N_C,0] \underset{\{exec\}}{\bowtie} [N_T,0]\Big) \underset{\{io\}}{\bowtie} [N_U] \xrightarrow{A:exec}$$
$$\Big([N_C-1,1] \underset{\{exec\}}{\bowtie} [N_T-1,1]\Big) \parallel \Big([N_C,0] \underset{\{exec\}}{\bowtie} [N_T,0]\Big) \underset{\{io\}}{\bowtie} [N_U]$$
$$\Big([2N_C,0] \underset{\{exec\}}{\bowtie} [2N_T,0]\Big) \underset{\{io\}}{\bowtie} [N_U] \xrightarrow{D:exec}$$
$$\Big([2N_C-1,1] \underset{\{exec\}}{\bowtie} [2N_T-1,1]\Big) \underset{\{io\}}{\bowtie} [N_U]$$
$$\Big([N_C-1,1] \underset{\{exec\}}{\bowtie} [N_T-1,1]\Big) \parallel \Big([N_C,0] \underset{\{exec\}}{\bowtie} [N_T,0]\Big) \underset{\{io\}}{\bowtie} [N_U] \xrightarrow{A:exec}$$
$$\Big([N_C-1,1] \underset{\{exec\}}{\bowtie} [N_T-1,1]\Big) \parallel \Big([N_C-1,1] \underset{\{exec\}}{\bowtie} [N_T-1,1]\Big) \underset{\{io\}}{\bowtie} [N_U]$$
$$\Big([2N_C-1,1] \underset{\{exec\}}{\bowtie} [2N_T-1,1]\Big) \underset{\{io\}}{\bowtie} [N_U] \xrightarrow{D:exec}$$
$$\Big([2N_C-2,2] \underset{\{exec\}}{\bowtie} [2N_T-2,2]\Big) \underset{\{io\}}{\bowtie} [N_U]$$
$$\vdots$$
$$\Big([0,N_C] \underset{\{exec\}}{\bowtie} [0,N_T]\Big) \parallel \Big([1,N_C-1] \underset{\{exec\}}{\bowtie} [1,N_T-1]\Big) \underset{\{io\}}{\bowtie} [N_U] \xrightarrow{A:exec}$$
$$\Big([0,N_C] \underset{\{exec\}}{\bowtie} [0,N_T]\Big) \parallel \Big([0,N_C] \underset{\{exec\}}{\bowtie} [0,N_T]\Big) \underset{\{io\}}{\bowtie} [N_U]$$
$$\Big([1,2N_C-1] \underset{\{exec\}}{\bowtie} [1,2N_T-1]\Big) \underset{\{io\}}{\bowtie} [N_U] \xrightarrow{D:exec}$$
$$\Big([0,2N_C] \underset{\{exec\}}{\bowtie} [0,2N_T]\Big) \underset{\{io\}}{\bowtie} [N_U]$$
$$\Big([0,N_C] \underset{\{exec\}}{\bowtie} [0,N_T]\Big) \parallel \Big([0,N_C] \underset{\{exec\}}{\bowtie} [0,N_T]\Big) \underset{\{io\}}{\bowtie} [N_U] \xrightarrow{A:reset}$$
$$\Big([1,N_C-1] \underset{\{exec\}}{\bowtie} [0,N_T]\Big) \parallel \Big([0,N_C] \underset{\{exec\}}{\bowtie} [0,N_T]\Big) \underset{\{io\}}{\bowtie} [N_U]$$
$$\Big([0,2N_C] \underset{\{exec\}}{\bowtie} [0,2N_T]\Big) \underset{\{io\}}{\bowtie} [N_U] \xrightarrow{D:reset}$$
$$\Big([1,2N_C-1] \underset{\{exec\}}{\bowtie} [0,2N_T]\Big) \underset{\{io\}}{\bowtie} [N_U]$$
$$\Big([1,N_C-1] \underset{\{exec\}}{\bowtie} [0,N_T]\Big) \parallel \Big([0,N_C] \underset{\{exec\}}{\bowtie} [0,N_T]\Big) \underset{\{io\}}{\bowtie} [N_U] \xrightarrow{A:io}$$
$$\Big([1,N_C-1] \underset{\{exec\}}{\bowtie} [0,N_T]\Big) \parallel \Big([0,N_C] \underset{\{exec\}}{\bowtie} [1,N_T-1]\Big) \underset{\{io\}}{\bowtie} [N_U]$$
$$[1,2N_C-1] \underset{\{exec\}}{\bowtie} [0,2N_T] \underset{\{io\}}{\bowtie} [N_U] \xrightarrow{D:io}$$
$$\Big([1,2N_C-1] \underset{\{exec\}}{\bowtie} [1,2N_T-1]\Big) \underset{\{io\}}{\bowtie} [N_U]$$
$$\Big([1,2N_C-1] \underset{\{exec\}}{\bowtie} [1,2N_T-1]\Big) \underset{\{io\}}{\bowtie} [N_U] \xrightarrow{A:exec}$$
$$\Big([0,2N_C] \underset{\{exec\}}{\bowtie} [,2N_T]\Big) \underset{\{io\}}{\bowtie} [N_U]$$
$$\Big([1,N_C-1] \underset{\{exec\}}{\bowtie} [0,N_T]\Big) \parallel \Big([0,N_C] \underset{\{exec\}}{\bowtie} [1,N_T-1]\Big) \underset{\{io\}}{\bowtie} [N_U] \xrightarrow{D:exec} \not\downarrow$$

Figure 4.1: Bisimulation game for *Sys* and *Sys′*. For the sake of readability we assume that $D = 2$, introduce the abbreviations $[M_C, M_{C'}] := C[M_C] \parallel C'[M_{C'}]$, $[M_T, M_{T'}] := T[M_T] \parallel T'[M_{T'}]$, $[N_U] := U[N_U]$ and use the canonical form of PEPA [13], where $C \parallel C'$ is the representative of $C \parallel C'$ and $C' \parallel C$, $T \parallel T'$ is the representative (in lexicographical order) of $T \parallel T'$ and $T' \parallel T$, and so on (i.e., we disregard the order of independent components).

Model	5%	50%	Avg.	95%
Error of the CTMCs Sys	0.055	0.372	4.924	32.554
Error of the simplified CTMCs Sys'	0.047	0.294	3.057	16.355

Table 4.1: 5% quantile, median, average and 95% quantile for the approximation error of over the 5000 randomly generated instances of Sys and Sys'.

Table 4.1 shows the statistics of the as-defined errors across all 5000 randomly generated models. For both groups of CTMCs, the ODE accuracy is acceptable, although the simplified CTMCs tend to be better approximated. The fact that the median is one order of magnitude smaller than the average error indicates that the error distribution is more concentrated at low values. The rather large errors reported for a small percentage of the models can be explained by the fact that the population sizes considered in this study are relatively low, which makes the fluid approximation less precise in general.

Expressiveness of [58] Using similar arguments as in the case of Sys and Sys', nested FPA models with nesting depth greater than one can be simplified. For instance, the nested FPA model

$$\left[\left[C \underset{\{exec\}}{\bowtie} T\right]_{\emptyset}^{N_M} \underset{\{io\}}{\bowtie} [\![U]\!]_{\emptyset}^{1}\right]_{\emptyset}^{N_I} \underset{\{exec,io\}}{\bowtie} [\![E]\!]_{\emptyset}^{1}$$

may be first related to

$$\left[\left[C \underset{\{exec\}}{\bowtie} T\right]_{\emptyset}^{N_M} \underset{\{io\}}{\bowtie} [\![U]\!]_{\emptyset}^{1}\right]_{\emptyset}^{1} \underset{\{exec,io\}}{\bowtie} [\![E]\!]_{\emptyset}^{1}$$

via

$$\begin{aligned} v'_{P^{i,1}} &= N_I \cdot v_{P^{i,j}}, && 1 \le i \le N_M, && 1 \le j \le N_I, && P \in \{C, \widehat{C}, T, \widehat{T}\}, \\ v'_{U^{1,1}} &= N_I \cdot v_{U^{1,j}}, && && 1 \le j \le N_I, && \\ v'_{P} &= v_P, && && && P \in \{E^1, \widehat{E}^1\}. \end{aligned}$$

Afterwards, the model

$$\left[\left[C \underset{\{exec\}}{\bowtie} T\right]_{\emptyset}^{N_M} \underset{\{io\}}{\bowtie} [\![U]\!]_{\emptyset}^{1}\right]_{\emptyset}^{1} \underset{\{exec,io\}}{\bowtie} [\![E]\!]_{\emptyset}^{1},$$

can be related to

$$\left[\left[C \underset{\{exec\}}{\bowtie} T\right]_{\emptyset}^{1} \underset{\{io\}}{\bowtie} [\![U]\!]_{\emptyset}^{1}\right]_{\emptyset}^{1} \underset{\{exec,io\}}{\bowtie} [\![E]\!]_{\emptyset}^{1}$$

via

$$\begin{aligned} v''_{P^{1,1}} &= N_M \cdot v'_{P^{i,1}}, && 1 \leq i \leq N_M, && P \in \{C, \widehat{C}, T, \widehat{T}\}, \\ v''_{U^{1,1}} &= v'_{U^{1,1}}, \\ v''_P &= v'_P, && && P \in \{E^1, \widehat{E}^1\}. \end{aligned}$$

Indeed, [58] identifies, essentially, a class of nested FPA models whose members are amenable to such an *iterative* simplification strategy. In contrast to the aggregation technique of this chapter, however, not all nested FPA models can be simplified. To see this, let us consider the FPA model

$$\mathcal{I}\Big([\![T]\!]^2_{\{exec\}} \underset{\{exec,io\}}{\bowtie} [\![E]\!]^1_{\emptyset}\Big) = \big(T^1 \underset{\{exec\}}{\bowtie} T^2\big) \underset{\{exec,io\}}{\bowtie} E^1$$

with T and E as before, meaning that

$$T \stackrel{def}{=} (exec, r).\widehat{T}, \quad \widehat{T} \stackrel{def}{=} (io, s').T, \quad E \stackrel{def}{=} (exec, r).\widehat{E}, \quad \widehat{E} \stackrel{def}{=} (io, s').E.$$

Then, since the partition $\big\{\{T^1, T^2\}, \{E^1\}\big\}$ is exactly fluid lumpable thanks to Theorem 14, the underlying ODE system

$$\begin{aligned} \dot{v}_{T^1} &= -r \min(v_{T^1}, v_{T^2}, v_{E^1}) + s' \frac{v_{\widehat{T}^1}}{v_{\widehat{T}^1} + v_{\widehat{T}^2}} \min(v_{\widehat{T}^1} + v_{\widehat{T}^2}, v_{\widehat{E}^1}), \quad \dot{v}_{\widehat{T}^1} = -\dot{v}_{T^1}, \\ \dot{v}_{T^2} &= -r \min(v_{T^1}, v_{T^2}, v_{E^1}) + s' \frac{v_{\widehat{T}^2}}{v_{\widehat{T}^1} + v_{\widehat{T}^2}} \min(v_{\widehat{T}^1} + v_{\widehat{T}^2}, v_{\widehat{E}^1}), \quad \dot{v}_{\widehat{T}^2} = -\dot{v}_{T^2}, \\ \dot{v}_{E^1} &= -r \min(v_{T^1}, v_{T^2}, v_{E^1}) + s' \min(v_{\widehat{T}^1} + v_{\widehat{T}^2}, v_{\widehat{E}^1}), \qquad \dot{v}_{\widehat{E}^1} = -\dot{v}_{E^1}. \end{aligned}$$

can be aggregated to

$$\begin{aligned} \dot{v}_{T^1} &= -r \min(v_{T^1}, v_{E^1}) + s'(1/2) \min(2v_{\widehat{T}^1}, v_{\widehat{E}^1}), \qquad \dot{v}_{\widehat{T}^1} = -\dot{v}_{T^1}, \\ \dot{v}_{E^1} &= -r \min(v_{T^1}, v_{E^1}) + s' \min(2v_{\widehat{T}^1}, v_{\widehat{E}^1}), \qquad \dot{v}_{\widehat{E}^1} = -\dot{v}_{E^1}. \end{aligned}$$

In contrast to (4.9), however, the above ODE system cannot be related to the model $[\![T]\!]^1_{\emptyset} \underset{\{exec,io\}}{\bowtie} [\![E]\!]^1_{\emptyset}$. To see this, note that minima arise in FPA only in the case of synchronisation. Thus, the definitions of T and E imply that the flux underlying *io* must be the same, but

$$s'(1/2) \min(2v_{\widehat{T}^1}, v_{\widehat{E}^1}) < s' \min(2v_{\widehat{T}^1}, v_{\widehat{E}^1}).$$

Chapter 5

Ordinary Fluid Lumpability

As discussed, exact fluid lumpability considers a partition of labels such that elements in the same part have the *same solution*. Instead, in the case of ordinary fluid lumpability which was introduced in [44] for an extension of FPA, the *sums of the solutions* of the 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. The name stems from the parallel with the theory of ordinary lumpability for Markov chains, where the probabilities of all micro states sum up to the probability of the underlying macro state in the lumped CTMC, cf. Theorem 2 in Section 2.1.

The structure of this chapter is as follows. We first build on intuition by discussing a motivating example in Section 5.1 and then continue by presenting the general theory in Section 5.2. In Section 5.3, instead, we show that ordinary fluid lumpability implies, under the assumption of well-posedness, the notion of semi-isomorphism.

5.1 Motivating Example

Using the same sequential component as in (3.1), that is

$$T_d \stackrel{def}{=} (exec, r).\widehat{T}_d, \quad \widehat{T}_d \stackrel{def}{=} (io, s').T_d, \quad C \stackrel{def}{=} (exec, r).\widehat{C}, \quad \widehat{C} \stackrel{def}{=} (reset, s).C,$$

let us consider the FPA process

$$Sys := \left(T_1 \underset{\emptyset}{\bowtie} \ldots \underset{\emptyset}{\bowtie} T_D\right) \underset{\{exec\}}{\bowtie} C, \tag{5.1}$$

with initial concentrations

$$v_{T_d}(0) = \mathfrak{c}_d, \qquad v_{\widehat{T}_d}(0) = 0, \qquad v_C(0) = \mathfrak{c}_{D+1}, \qquad v_{\widehat{C}}(0) = 0 \tag{5.2}$$

for $1 \leq d \leq D$. Note that, unlike exact fluid lumpability, the initial concentrations $\mathfrak{c}_1, \ldots, \mathfrak{c}_D$ may be different. Informally, *Sys* models a single machine where a group of CPUs serves D groups of threads. Since each T_d, with $1 \leq d \leq D$,

contributes $|ds(T_d)| = 2$ ODEs, the fluid approximation of (5.1) is given by the following $2D + 2$ ODEs:

$$\dot{v}_{T_d} = -\frac{rv_{T_d}}{\sum_{1\le d'\le D} rv_{T_{d'}}} \min\Big(\sum_{1\le d'\le D} rv_{T_{d'}}, rv_C\Big) + s'v_{\widehat{T}_d}, \quad \dot{v}_{\widehat{T}_d} = -\dot{v}_{T_d},$$
$$\dot{v}_C = -\min\Big(\sum_{1\le d'\le D} rv_{T_{d'}}, rv_C\Big) + sv_{\widehat{C}}, \qquad \dot{v}_{\widehat{C}} = -\dot{v}_C. \quad (5.3)$$

Clearly, the ODE analysis may become numerically tedious if D is large. Note, however, that the above ODE system yields

$$\sum_{1\le d\le D} \dot{v}_{T_d} = -r\min\Big(\sum_{1\le d\le D} v_{T_d}, v_C\Big) + s'\sum_{1\le d\le D} v_{\widehat{T}_d},$$
$$\sum_{1\le d\le D} \dot{v}_{\widehat{T}_d} = -\sum_{1\le d\le D} \dot{v}_{T_d},$$
$$\dot{v}_C = -r\min\Big(\sum_{1\le d\le D} v_{T_d}, v_C\Big) + sv_{\widehat{C}},$$
$$\dot{v}_{\widehat{C}} = -\dot{v}_C.$$

Consequently, the solution of the lumped ODE system

$$\dot{\mathfrak{v}}_T = -r\min(\mathfrak{v}_T, \mathfrak{v}_C) + s'\mathfrak{v}_{\widehat{T}}, \qquad \dot{\mathfrak{v}}_{\widehat{T}} = -\dot{\mathfrak{v}}_T, \quad (5.4)$$
$$\dot{\mathfrak{v}}_C = -r\min(\mathfrak{v}_T, \mathfrak{v}_C) + s\mathfrak{v}_{\widehat{C}}, \qquad \dot{\mathfrak{v}}_{\widehat{C}} = -\dot{\mathfrak{v}}_C,$$

subjected to

$$\mathfrak{v}_T(0) = \sum_{1\le d\le D} \mathfrak{c}_d, \quad \mathfrak{v}_{\widehat{T}}(0) = 0, \quad \mathfrak{v}_C(0) = \mathfrak{c}_{D+1}, \quad \mathfrak{v}_{\widehat{C}}(0) = 0$$

and the solution of (5.3) and (5.2) satisfy for all $t \ge 0$:

$$\mathfrak{v}_T(t) = \sum_{1\le d\le D} v_{T_d}(t), \qquad \mathfrak{v}_{\widehat{T}}(t) = \sum_{1\le d\le D} v_{\widehat{T}_d}(t),$$
$$\mathfrak{v}_C(t) = v_C(t), \qquad \mathfrak{v}_{\widehat{C}}(t) = v_{\widehat{C}}(t).$$

Note that $\mathfrak{v}_T(t) = \sum_{d=1}^{D} v_{T_d}(t)$, but each individual solution $v_{T_d}(t)$ cannot be recovered. This is, in essence, the price which one has to pay if one wants to allow *different* initial concentrations. It is worth noting that $\big\{\{T_1, \ldots, T_D\}, \{C\}\big\}$ is also exactly fluid lumpable, meaning that $\mathfrak{c}_1 = \ldots = \mathfrak{c}_D$ induces

$$v_{T_d}(t) = v_{T_{d'}}(t), \quad v_{\widehat{T}_d}(t) = v_{\widehat{T}_{d'}}(t), \qquad 1 \le d, d' \le D.$$

5.2 Ordinarily Fluid Lumpable Partitions

The ideas presented in the previous section are now generalised for any FPA model. Each formal definition will be accompanied by a simple application to our motivating example. We begin with the notion of ordinary fluid lumpability.

Definition 32 (Ordinary Fluid Lumpability)**.** *Let M be an FPA model and let $\{\overline{P}^1, \ldots, \overline{P}^n\}$ be a partition of $\mathcal{G}(M)$, where $\overline{P}^i = \{P^i_j \mid 1 \leq j \leq k_i\}$ as in Definition 21. The partition is called* ordinarily fluid lumpable *if there exist bijections*

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

such that $\sigma_{P^i_1} \equiv id_{ds(P^i_1)}$ and for all $\alpha \in \mathcal{A}$, $1 \leq i \leq n$, v and

$$v^\sigma_P := \begin{cases} \sum\limits_{1 \leq j \leq k_i} v_{\sigma_{P^i_j}(P)} & , \exists 1 \leq i \leq n.\ \big(P \in ds(P^i_1)\big) \\ 0 & , \textit{otherwise} \end{cases}$$

it holds that

i) $$\sum_{1 \leq j \leq k_i} \mathcal{R}_\alpha(M, v, \sigma_{P^i_j}(P)) = \mathcal{R}_\alpha(M, v^\sigma, P), \quad \forall P \in ds(P^i_1)$$

ii) $$\sum_{1 \leq j \leq k_i} \sum_{P' \in ds(P^i_1)} p_\alpha(\sigma_{P^i_j}(P'), \sigma_{P^i_j}(P)) \mathcal{R}_\alpha(M, v, \sigma_{P^i_j}(P')) = \sum_{P' \in ds(P^i_1)} p_\alpha(P', P) \mathcal{R}_\alpha(M, v^\sigma, P'), \quad \forall P \in ds(P^i_1)$$

iii) $r_\alpha(M, v) = r_\alpha(M, v^\sigma)$

Informally, a partition $\{\overline{P}^1, \ldots, \overline{P}^n\}$ is ordinarily fluid lumpable, if the component rates are linear on the blocks $\overline{P}^i$, $1 \leq i \leq n$.

For instance, the partition $\big\{\{T_1, \ldots, T_D\}, \{C\}\big\}$ of the FPA model *Sys* given in (5.1) is ordinarily fluid lumpable. To see this, we first define $\sigma_C := \mathrm{id}_{ds(C)}$ and

$$\sigma_{T_d} : ds(T_1) \to ds(T_d), \quad T_1 \mapsto T_d,\ \widehat{T}_1 \mapsto \widehat{T}_d, \qquad 1 \leq d \leq D.$$

For an arbitrary concentration function v of *Sys* this induces

$$v^\sigma_P = \begin{cases} \sum_{d=1}^D v_{T_d} & ,\ P = T_1 \\ \sum_{d=1}^D v_{\widehat{T}_d} & ,\ P = \widehat{T}_1 \\ 0 & ,\ P \in \{T_2, \widehat{T}_2, \ldots, T_D, \widehat{T}_D\} \\ v_C & ,\ P = C \\ v_{\widehat{C}} & ,\ P = \widehat{C} \end{cases}$$

That is, the concentrations of all thread atoms $T_1, \ldots, T_D$ are accumulated in the first thread atom T_1. Intuitively, in order to apply the notion of ordinary

fluid lumpability, the sum of all α component rates of $T_1, \ldots, T_D$ underlying v must match the α component rate of the single atom T_1 underlying v^σ. As in the case of exact fluid lumpability, we stress that this must hold *for all* concentration functions v, meaning that an algorithm for establishing ordinary fluid lumpability has to perform *symbolic* calculations in the style of a computer algebra system. We next check that $r_\alpha(Sys, v) = r_\alpha(Sys, v^\sigma)$ and

$$\sum_{1 \leq d \leq D} \mathcal{R}_\alpha(Sys, v, \sigma_{T_d}(T_1)) = \mathcal{R}_\alpha(Sys, v^\sigma, T_1)$$

for all concentrations functions v and actions α. Since the remaining equalities of component rates are shown similarly, this shows the ordinary fluid lumpability of $\big\{\{T_1, \ldots, T_D\}, \{C\}\big\}$. To see this, we first infer

$$r_\alpha(Sys, v) = \min(\sum_{d=1}^{D} r_\alpha(T_d, v), r_\alpha(C, v)) = \min(r_\alpha(T_1, v^\sigma), r_\alpha(C, v^\sigma)) =$$
$$= \min(\sum_{d=1}^{D} r_\alpha(T_d, v^\sigma), r_\alpha(C, v^\sigma)) = r_\alpha(Sys, v^\sigma)$$

if $\alpha = exec$ and

$$r_\alpha(Sys, v) = \sum_{d=1}^{D} r_\alpha(T_d, v) + r_\alpha(C, v) = r_\alpha(T_1, v^\sigma) + r_\alpha(C, v^\sigma) =$$
$$= \sum_{d=1}^{D} r_\alpha(T_d, v^\sigma) + r_\alpha(C, v^\sigma) = r_\alpha(Sys, v^\sigma)$$

otherwise. Using this, one notes

$$\begin{aligned}
\sum_{d=1}^{D} \mathcal{R}_\alpha(Sys, v, T_d) &= \sum_{d=1}^{D} \frac{\mathcal{R}_\alpha(T_d, v, T_d)}{\sum_{d'=1}^{D} r_\alpha(T_{d'}, v)} r_\alpha(Sys, v) \\
&= r_\alpha(Sys, v^\sigma) \\
&= \frac{\mathcal{R}_\alpha(T_1, v^\sigma, T_1)}{r_\alpha(T_1, v^\sigma)} r_\alpha(Sys, v^\sigma) \\
&= \frac{\mathcal{R}_\alpha(T_1, v^\sigma, T_1)}{\sum_{d=1}^{D} r_\alpha(T_d, v^\sigma)} r_\alpha(Sys, v^\sigma) \\
&= \mathcal{R}_\alpha(Sys, v^\sigma, T_1)
\end{aligned}$$

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

Theorem 15 (ODE Lumping)**.** *Let M be an FPA model, $\{\overline{P}^1, \ldots, \overline{P}^n\}$ an ordinarily fluid lumpable partition of $\mathcal{G}(M)$ with $\overline{P}^i$ as in Definition 32 and v the ODE solution of M for a given initial condition $v(0)$. Define*

$$\mathfrak{v}_P := \sum_{1 \leq j \leq k_i} v_{\sigma_{P_j^i}(P)}, \qquad 1 \leq i \leq n, \quad P \in ds(P_1^i)$$

and

$$\overline{\mathfrak{v}}_P := \begin{cases} \mathfrak{v}_P & , \ \exists 1 \leq i \leq n.\ \big(P \in ds(P_1^i)\big) \\ 0 & , \ \textit{otherwise} \end{cases}$$

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

$$\begin{aligned} \dot{\mathfrak{v}}_P &= \sum_{\alpha \in \mathcal{A}} \Big(\sum_{P' \in ds(P_1^i)} p_\alpha(P', P) \mathcal{R}_\alpha(M, \overline{\mathfrak{v}}, P') - \mathcal{R}_\alpha(M, \overline{\mathfrak{v}}, P) \Big), \\ \mathfrak{v}_P(0) &= \sum_{1 \leq j \leq k_i} v_{\sigma_{P_j^i}(P)}(0), \end{aligned} \tag{5.5}$$

where $1 \leq i \leq n$ *and* $P \in ds(P_1^i)$. *Hence,*

$$\sum_{1 \leq j \leq k_i} v_{\sigma_{P_j^i}(P)}, \qquad 1 \leq i \leq n, \quad P \in ds(P_1^i),$$

can be recovered by solving the lumped ODE system (5.5).

Proof. As the ODE system of a PEPA model is Lipschitz [54], the lumped ODE system (5.5) is Lipschitz too. The theorem of Picard-Lindelöf asserts then that (5.5) has a unique solution. Moreover, for all $1 \leq i \leq n$ and $P \in ds(P_1^i)$, Definition 32 yields

$$\begin{aligned} \dot{\mathfrak{v}}_P &= \sum_{1 \leq j \leq k_i} \dot{v}_{\sigma_{P_j^i}(P)} = \sum_{1 \leq j \leq k_i} \sum_{\alpha \in \mathcal{A}} \Big(- \mathcal{R}_\alpha(M, v, \sigma_{P_j^i}(P)) \\ &\qquad + \sum_{P' \in ds(P_1^i)} p_\alpha(\sigma_{P_j^i}(P'), \sigma_{P_j^i}(P)) \mathcal{R}_\alpha(M, v, \sigma_{P_j^i}(P')) \Big) \\ &\overset{\text{i),ii)}{=} \sum_{\alpha \in \mathcal{A}} \Big(\sum_{P' \in ds(P_1^i)} p_\alpha(P', P) \mathcal{R}_\alpha(M, v^\sigma, P') - \mathcal{R}_\alpha(M, v^\sigma, P) \Big) \\ &= \sum_{\alpha \in \mathcal{A}} \Big(\sum_{P' \in ds(P_1^i)} p_\alpha(P', P) \mathcal{R}_\alpha(M, \overline{\mathfrak{v}}, P') - \mathcal{R}_\alpha(M, \overline{\mathfrak{v}}, P) \Big) \end{aligned}$$

and $\mathfrak{v}_P(0) = \sum_{1 \leq j \leq k_i} v_{\sigma_{P_j^i}(P))}(0)$. This induces the claim. □

For instance, the aggregated ODE system of the FPA model *Sys* given in (5.1) is (5.4) and has four ODEs. It holds that $\mathfrak{v}_T(t) = \sum_{d=1}^{D} v_{T_d}(t)$, but each individual solution $v_{T_d}(t)$ cannot be recovered. Let us remark that the same partition is ordinarily as well exactly fluid lumpable, leading however to two distinct aggregated ODE systems. That is, while *ordinary* fluid lumping of $\big\{\{T_1, \ldots, T_D\}, \{C\}\big\}$ leads to the aggregated ODE system (5.4), the *exact* fluid lumping of $\big\{\{T_1, \ldots, T_D\}, \{C\}\big\}$ aggregates the original ODE system to

$$\begin{aligned} \dot{v}_{T_1} &= -r \frac{1}{D} \min(D v_{T_1}, v_C) + s' v_{\widehat{T}_1} & \dot{v}_{\widehat{T}_1} &= +r \frac{1}{D} \min(D v_{T_1}, v_C) - s' v_{\widehat{T}_1} \\ \dot{v}_C &= -r \min(D v_{T_1}, v_C) + s v_{\widehat{C}} & \dot{v}_{\widehat{C}} &= +r \min(D v_{T_1}, v_C) - s v_{\widehat{C}} \end{aligned}$$

The next theorem can be seen as a congruence property of ordinary fluid lumpability with respect to the parallel composition of FPA.

Theorem 16. *Let us fix two FPA models M_1, M_2 and assume that $\{\overline{P}^1, \ldots, \overline{P}^n\}$ and $\{\overline{P}^{n+1}, \ldots, \overline{P}^{n+m+1}\}$ are ordinarily fluid lumpable partitions of $\mathcal{G}(M_1)$ and $\mathcal{G}(M_2)$, respectively. Then, thanks to the set of bijections*

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

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

Proof. Let us fix an arbitrary v of $M := M_1 \underset{L}{\bowtie} M_2$. Then, Definition 32 yields in the case $\alpha \in L$

$$\begin{aligned} r_\alpha(M_1 \underset{L}{\bowtie} M_2, v) &= \min(r_\alpha(M_1, v), r_\alpha(M_2, v)) \\ &\overset{\text{iii)}}{=} \min(r_\alpha(M_1, v^\sigma), r_\alpha(M_2, v^\sigma)) = r_\alpha(M_1 \underset{L}{\bowtie} M_2, v^\sigma) \end{aligned}$$

and in the case $\alpha \notin L$

$$\begin{aligned} r_\alpha(M_1 \underset{L}{\bowtie} M_2, v) &= r_\alpha(M_1, v) + r_\alpha(M_2, v) \\ &\overset{\text{iii)}}{=} r_\alpha(M_1, v^\sigma) + r_\alpha(M_2, v^\sigma) = r_\alpha(M_1 \underset{L}{\bowtie} M_2, v^\sigma)\ . \end{aligned}$$

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

$$\begin{aligned} \sum_{1 \leq j \leq k_i} \mathcal{R}_\alpha(M, v, \sigma_{P_j^i}(P)) &= \sum_{1 \leq j \leq k_i} \frac{\mathcal{R}_\alpha(M_1, v, \sigma_{P_j^i}(P))}{r_\alpha(M_1, v)} r_\alpha(M_1 \underset{L}{\bowtie} M_2, v) \\ &\overset{\text{iii)}}{=} \sum_{1 \leq j \leq k_i} \frac{\mathcal{R}_\alpha(M_1, v, \sigma_{P_j^i}(P))}{r_\alpha(M_1, v^\sigma)} r_\alpha(M_1 \underset{L}{\bowtie} M_2, v^\sigma) \\ &\overset{\text{ii)}}{=} \sum_{1 \leq j \leq k_i} \frac{\mathcal{R}_\alpha(M_1, v^\sigma, \sigma_{P_j^i}(P))}{r_\alpha(M_1, v^\sigma)} r_\alpha(M_1 \underset{L}{\bowtie} M_2, v^\sigma) \\ &= \sum_{1 \leq j \leq k_i} \mathcal{R}_\alpha(M, v^\sigma, \sigma_{P_j^i}(P)) \end{aligned}$$

and

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

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

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

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

and

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

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

For instance, since $\big\{\{T_1,\dots,T_D\}\big\}$ is clearly an ordinarily fluid lumpable partition of $T_1 \underset{\emptyset}{\bowtie} \dots \underset{\emptyset}{\bowtie} T_D$, Theorem 16 immediately implies that the partition $\big\{\{T_1,\dots,T_D\},\{C\}\big\}$ of $(T_1 \underset{\emptyset}{\bowtie} \dots \underset{\emptyset}{\bowtie} T_D) \underset{\{exec\}}{\bowtie} C$ is ordinary fluid lumpable.

5.3 Ordinary Fluid Lumpability and Semi-Isomorphism

Recall that in Section 3.3.2 we were able to show that projected label equivalence induces semi-isomorphism if the model is well-posed. It is therefore natural to ask whether a similar result holds for ordinary fluid lumpability. We show next that in the case of a well-posed FPA model M and an ordinarily fluid lumpable partition $\{\overline{P}^1,\dots,\overline{P}^n\}$ of $\mathcal{G}(M)$, the sequential components P_1^i and P_j^i are semi-isomorphic for all $1 \le i \le n$ and $1 \le j \le k_i$. To build on intuition, we start with a sketch of the proof strategy used to achieve this result, which is stated as Theorem 17. In the remainder of this section, $i) - iii)$ refer to Definition 32.

Similarly to exact fluid lumpability, we have to prove that

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

for all $\alpha \in \mathcal{A}$, $1 \le i \le n$, $1 \le j \le k_i$ and $P_0, P_1 \in ds(P_1^i)$. The case $r_\alpha(P_0) = 0$ is shown by proving that the well-posedness of M implies $r_\alpha(P_0) = r_\alpha(\sigma_{P_j^i}(P_0))$, cf. Lemma 11. For the case $r_\alpha(P_0) > 0$, instead, we note that $i)$ and $ii)$ imply

$$\mathcal{R}_\alpha(M,v,\sigma_{P_j^i}(P_0)) = \mathcal{R}_\alpha(M,v^\sigma,P_0)$$
$$p_\alpha(\sigma_{P_j^i}(P_0),\sigma_{P_j^i}(P_1))\mathcal{R}_\alpha(M,v,\sigma_{P_j^i}(P_0)) = p_\alpha(P_0,P_1)\mathcal{R}_\alpha(M,v^\sigma,P_0)$$

for all v which satisfy

$$v_P = \begin{cases} 1 & , \ P \in ds(P_j^i) \wedge P = \sigma_{P_j^i}(P_0) \\ 0 & , \ P \in ds(P_j^i) \wedge P \neq \sigma_{P_j^i}(P_0) \\ 0 & , \ P \in \bigcup_{l \neq j} ds(P_l^i) \end{cases} \tag{5.6}$$

We proceed by inferring from the well-posedness of M the existence of a v which satisfies (5.6) and $\mathcal{R}_\alpha(M, v^\sigma, P_0) > 0$. Since this yields $p_\alpha(P_0, P_1) = p_\alpha(\sigma_{P_j^i}(P_0), \sigma_{P_j^i}(P_1))$, the claim readily follows from $r_\alpha(P_0) = r_\alpha(\sigma_{P_j^i}(P_0))$.

The remainder of this section formalises these ideas. The next two lemmas are used to show the existence of a v which satisfies (5.6) and $\mathcal{R}_\alpha(M, v^\sigma, P_0) > 0$.

Lemma 7. *Let M be an FPA model, $P^0 \in \mathcal{G}(M)$, $P' \in ds(P^0)$ satisfying $r_\alpha(P') > 0$ and v a concentration 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 by $r_\alpha(P') > 0$.
- $M = M_1 \underset{L}{\bowtie} M_2$: 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 $0 < r_\alpha(M_1 \underset{L}{\bowtie} M_2, v) = \min(r_\alpha(M_1, v), r_\alpha(M_2, v))$ 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 $\min(r_\alpha(M_1, \widehat{v}), r_\alpha(M_2, \widehat{v})) > 0$.
  - $\alpha \notin L$: 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, $r_\alpha(M_1 \underset{L}{\bowtie} M_2, \widehat{v}) = r_\alpha(M_1, \widehat{v})$ and the claim follows by the induction hypothesis.

□

Lemma 8. *Let M be an FPA model, $P^0 \in \mathcal{G}(M)$, $P' \in ds(P^0)$ satisfying $r_\alpha(P') > 0$ and v a concentration 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 by $r_\alpha(P') > 0$.

- $M = M_1 \underset{L}{\bowtie} M_2$: 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 7 and
    $$0 < \mathcal{R}_\alpha(M, v, P') = \frac{\mathcal{R}_\alpha(M_1, v, P')}{r_\alpha(M_1, v)} \min(r_\alpha(M_1, v), r_\alpha(M_2, v))$$
    imply then
    $$0 < \frac{\mathcal{R}_\alpha(M_1, \widehat{v}, P')}{r_\alpha(M_1, \widehat{v})} \min(r_\alpha(M_1, \widehat{v}), r_\alpha(M_2, \widehat{v})) = \mathcal{R}_\alpha(M, \widehat{v}, P')$$
  - $\alpha \notin L$: We observe first 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.

□

Recall that our goal it to show that

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

for all $\alpha \in \mathcal{A}$, $1 \leq i \leq n$, $1 \leq j \leq k_i$ and $P_0, P_1 \in ds(P_1^i)$. For this, we first have to establish that $r_\alpha(P_0) = r_\alpha(\sigma_{P_j^i}(P_0))$, which is addressed in the next three lemmas.

Lemma 9. *Let M be an FPA model and P^0 a fluid atom of it. Assume further that there exist $\alpha \in \mathcal{A}$ and $\delta, c > 0$ such that $r_\alpha(M, v^\eta) = c\eta$ for all $0 \leq \eta \leq \delta$, where*

$$v^\eta_{P'} := \begin{cases} \hat{c} + \eta & , \ P' \in ds(P^0) \wedge P' = P \\ \hat{c} & , \ P' \in ds(P^0) \wedge P' \neq P \\ v_{P'} & , \ P' \notin ds(P^0) \end{cases}$$

for some $\hat{c} \geq 0$ and $P \in ds(P^0)$. Then it holds that $\hat{c} = 0$.

Proof. We prove the claim using structural induction.

- $M = P^0$: The claim is trivial.
- $M = M_1 \underset{L}{\bowtie} M_2$: Let us assume without loss of generality that $P^0 \in \mathcal{G}(M_1)$. By writing $v^\eta = (v_1^\eta, v_2^\eta)$, where v_i^η denotes the concentrations of M_i, one observes that v_2^η does not depend on η. Hence, there is a concentration function v_2 of M_2 such that $v_2 \equiv v_2^\eta$.
  - $\alpha \in L$: As $c\eta = \min(r_\alpha(M_1, v_1^\eta), r_\alpha(M_2, v_2))$ and $\delta, c > 0$, it holds that $r_\alpha(M_2, v_2) > 0$. Hence, $r_\alpha(M_1, v_1^\eta) = c\eta$ for all η such that $c\eta < r_\alpha(M_2, v_2)$ and the I.H. yields the claim.

– $\alpha \notin L$: As $c\eta = r_\alpha(M_1, v_1^\eta) + r_\alpha(M_2, v_2)$ for all $0 \leq \eta \leq \delta$, it holds that $r_\alpha(M_2, v_2) = 0$. Hence, $c\eta = r_\alpha(M_1, v_1^\eta)$ and the I.H. yields the claim.

□

Lemma 10. *For a fixed FPA model M, assume that $\{\overline{P}^1, \ldots, \overline{P}^n\}$ is an ordinary fluid lumpable partition of $\mathcal{G}(M)$ which is established by the bijections*

$$\sigma_{P_j^i} : ds(P_1^i) \to ds(P_j^i), \qquad 1 \leq i \leq n,\ 1 \leq j \leq k_i.$$

Then, for arbitrary $1 \leq j_i \leq k_i$, where $1 \leq i \leq n$, the bijections

$$\rho_{P_j^i} := \sigma_{P_j^i} \circ \sigma_{P_{j_i}^i}^{-1} : ds(P_{j_i}^i) \to ds(P_j^i), \qquad \forall 1 \leq i \leq n,\ 1 \leq j \leq k_i,$$

establish also the ordinary fluid lumpability of $\{\overline{P}^1, \ldots, \overline{P}^n\}$. That is, similarly to the notion of exact fluid lumpability, cf. Remark 2, the notion of ordinary fluid lumpability does not depend on the choice of the representatives.

Proof. We show first that $(v^\rho)^\sigma = v^\sigma$ for an arbitrary concentration function v of M. Let us fix for this a $P \in \mathcal{B}(M)$. Then, $(v^\rho)^\sigma_P = 0 = v^\sigma_P$ if there is no $1 \leq i \leq n$ such that $P \in ds(P_1^i)$. In the case where $P \in ds(P_1^i)$ for some $1 \leq i \leq n$, instead, it holds that

$$\begin{aligned}(v^\rho)^\sigma_P &= \sum_{1 \leq j \leq k_i} v^\rho_{\sigma_{P_j^i}(P)} = v^\rho_{\left(\sigma_{P_{j_i}^i}(P)\right)} \\ &= \sum_{1 \leq j \leq k_i} v_{\left(\rho_{P_j^i}(\sigma_{P_{j_i}^i}(P))\right)} = \sum_{1 \leq j \leq k_i} v_{\left(\sigma_{P_j^i}(P)\right)} = v^\sigma_P.\end{aligned}$$

This yields

$$r_\alpha(M, v^\rho) \overset{\text{iii)}}{=} r_\alpha(M, (v^\rho)^\sigma) = r_\alpha(M, v^\sigma) \overset{\text{iii)}}{=} r_\alpha(M, v)$$

and, for $P \in ds(P_{j_i}^i)$,

$$\begin{aligned}\sum_{1 \leq j \leq k_i} \mathcal{R}_\alpha(M, v, \rho_{P_j^i}(P)) &= \sum_{1 \leq j \leq k_i} \mathcal{R}_\alpha\big(M, v, \sigma_{P_j^i}(\sigma^{-1}_{P_{j_i}^i}(P))\big) \\ &\overset{\text{i)}}{=} \sum_{1 \leq j \leq k_i} \mathcal{R}_\alpha\big(M, v^\sigma, \sigma_{P_j^i}(\sigma^{-1}_{P_{j_i}^i}(P))\big) \\ &= \sum_{1 \leq j \leq k_i} \mathcal{R}_\alpha\big(M, (v^\rho)^\sigma, \sigma_{P_j^i}(\sigma^{-1}_{P_{j_i}^i}(P))\big) \\ &\overset{\text{i)}}{=} \sum_{1 \leq j \leq k_i} \mathcal{R}_\alpha\big(M, v^\rho, \sigma_{P_j^i}(\sigma^{-1}_{P_{j_i}^i}(P))\big) \\ &= \sum_{1 \leq j \leq k_i} \mathcal{R}_\alpha\big(M, v^\rho, \rho_{P_j^i}(P)\big)\end{aligned}$$

and

$$\begin{aligned}
&\sum_{1\le j\le k_i}\sum_{P'\in ds(P^i_{j_i})} p_\alpha(\rho_{P^i_j}(P'),\rho_{P^i_j}(P))\mathcal{R}_\alpha(M,v,\rho_{P^i_j}(P'))\\
&=\sum_{1\le j\le k_i}\sum_{P'\in ds(P^i_{j_i})} p_\alpha\big(\sigma_{P^i_j}(\sigma^{-1}_{P^i_{j_i}}(P')),\sigma_{P^i_j}(\sigma^{-1}_{P^i_{j_i}}(P))\big)\mathcal{R}_\alpha\big(M,v,\sigma_{P^i_j}(\sigma^{-1}_{P^i_{j_i}}(P'))\big)\\
&=\sum_{1\le j\le k_i}\sum_{P'\in ds(P^i_1)} p_\alpha\big(\sigma_{P^i_j}(P'),\sigma_{P^i_j}(\sigma^{-1}_{P^i_{j_i}}(P))\big)\mathcal{R}_\alpha\big(M,v,\sigma_{P^i_j}(P')\big)\\
&\overset{\text{ii)}}{=}\sum_{1\le j\le k_i}\sum_{P'\in ds(P^i_1)} p_\alpha\big(\sigma_{P^i_j}(P'),\sigma_{P^i_j}(\sigma^{-1}_{P^i_{j_i}}(P))\big)\mathcal{R}_\alpha\big(M,v^\sigma,\sigma_{P^i_j}(P')\big)\\
&=\sum_{1\le j\le k_i}\sum_{P'\in ds(P^i_1)} p_\alpha\big(\sigma_{P^i_j}(P'),\sigma_{P^i_j}(\sigma^{-1}_{P^i_{j_i}}(P))\big)\mathcal{R}_\alpha\big(M,(v^\rho)^\sigma,\sigma_{P^i_j}(P')\big)\\
&\overset{\text{ii)}}{=}\sum_{1\le j\le k_i}\sum_{P'\in ds(P^i_1)} p_\alpha\big(\sigma_{P^i_j}(P'),\sigma_{P^i_j}(\sigma^{-1}_{P^i_{j_i}}(P))\big)\mathcal{R}_\alpha\big(M,v^\rho,\sigma_{P^i_j}(P')\big)\\
&=\sum_{1\le j\le k_i}\sum_{P'\in ds(P^i_{j_i})} p_\alpha(\rho_{P^i_j}(P'),\rho_{P^i_j}(P))\mathcal{R}_\alpha(M,v^\rho,\rho_{P^i_j}(P')).
\end{aligned}$$

□

We are now in a position to prove that $r_\alpha(P_0)=r_\alpha(\sigma_{P^i_j}(P_0))$.

Lemma 11. *Let M be a well-posed FPA model and assume that $\{\overline{P}^1,\dots,\overline{P}^n\}$ is an ordinarily fluid lumpable partition of $\mathcal{G}(M)$. Then, it holds that $r_\alpha(\sigma_{P^i_j}(P))=r_\alpha(P)$ for all $1\le i\le n$, $2\le j\le k_i$ and $P\in ds(P^i_1)$.*

Proof. We assume first that $r_\alpha(\sigma_{P^i_j}(P))>0$. As M is well-posed, Lemma 4 ensures that there exist a $\delta>0$ and a set of concentrations $\{v_E \mid E\in\mathcal{B}(M)\wedge E\notin ds(P^i_j)\}$ such that

$$v^\eta_E:=\begin{cases}\eta & ,\ E\in ds(P^i_j)\wedge E=\sigma_{P^i_j}(P)\\ 0 & ,\ E\in ds(P^i_j)\wedge E\neq\sigma_{P^i_j}(P)\\ v_E & ,\ E\notin ds(P^i_j)\end{cases}$$

where

$$v_E=v_{E'},\quad \forall Q\in\mathcal{G}(M),Q\neq P^i_j.\ \forall E,E'\in ds(Q),$$

satisfies for all $0\le\eta\le\delta$

$$r_\alpha(M,v^\eta)=r_\alpha(P^i_j,v^\eta)=r_\alpha(\sigma_{P^i_j}(P))v_{\sigma_{P^i_j}(P)}=r_\alpha(\sigma_{P^i_j}(P))\eta.$$

Then, $c:=r_\alpha(\sigma_{P^i_j}(P))$, $\hat{c}:=\sum_{l\neq j}^{k_i}v_{\sigma_{P^i_l}(E)}$, where $E\in ds(P^i_1)$ is arbitrary, and $\mathfrak{v}^\eta:=(v^\eta)^\sigma$ fulfill the assumptions of Lemma 9, since

$$\mathfrak{v}^\eta_E=(v^\eta)^\sigma_E=\begin{cases}\hat{c} & ,\ E\in ds(P^i_1)\wedge E\neq P\\ \hat{c}+\eta & ,\ E\in ds(P^i_1)\wedge E=P\end{cases}$$

and

$$r_\alpha(\sigma_{P_j^i}(P))\eta = r_\alpha(M, v^\eta) \overset{\text{iii)}}{=} r_\alpha(M, (v^\eta)^\sigma) = r_\alpha(M, \mathfrak{v}^\eta)$$

for all $0 \leq \eta \leq \delta$. As Lemma 9 ensures $\hat{c} = 0$, Lemma 5 yields $r_\alpha(\sigma_{P_j^i}(P)) = r_\alpha(P)$. This finishes the first case where we assumed that $r_\alpha(\sigma_{P_j^i}(P)) > 0$. For the case $r_\alpha(\sigma_{P_j^i}(P)) = 0$, instead, we have to show that

$$r_\alpha(\sigma_{P_j^i}(P)) = 0 \quad \Rightarrow \quad r_\alpha(\sigma_{P_j^i}(P)) = r_\alpha(P),$$

which is obviously equivalent to

$$r_\alpha(\sigma_{P_j^i}(P)) = 0 \quad \Rightarrow \quad r_\alpha(P) = 0.$$

By building the contraposition of the last statement, we infer that the claim of the second case is equivalent to

$$r_\alpha(P) > 0 \quad \Rightarrow \quad r_\alpha(\sigma_{P_j^i}(P)) > 0.$$

To prove the last statement, we first define

$$\rho_{P_l^\iota} := \begin{cases} \sigma_{P_l^i} \circ \sigma_{P_j^i}^{-1} & , \ \iota = i \\ \sigma_{P_l^\iota} & , \ \iota \neq i \end{cases}$$

for all $1 \leq \iota \leq n$ and $1 \leq l \leq k_\iota$. Informally, the above definition changes the representative of $\overline{P}^i$ from P_1^i to P_j^i, while keeping at the same time the representatives of $\overline{P}^\iota$, where $\iota \neq i$, fixed. Since Lemma 10 ensures that also the family $\rho_\bullet$ establishes the ordinary fluid lumpability of $\{\overline{P}^1, \ldots, \overline{P}^n\}$, we can apply the first case to the process $\sigma_{P_j^i}(P)$ instead of P, which implies

$$r_\alpha(\rho_{P_1^i}(\sigma_{P_j^i}(P)) > 0 \ \Rightarrow \ r_\alpha(\rho_{P_1^i}(\sigma_{P_j^i}(P)) = r_\alpha(\sigma_{P_j^i}(P)).$$

By exploiting the definition of $\rho_\bullet$, the last statement rewrites to

$$r_\alpha(P) > 0 \ \Rightarrow \ r_\alpha(P) = r_\alpha(\sigma_{P_j^i}(P)),$$

yielding the claim. □

The preceding auxiliary results are used to establish the connection between ordinary fluid lumpability and semi-isomorphism.

Theorem 17. *Fix a well-posed FPA model M and assume that the partition $\{\overline{P}^1, \ldots, \overline{P}^n\}$ of $\mathcal{G}(M)$ is ordinarily fluid lumpable. Then, P_1^i is semi-isomorphic to P_j^i for all $2 \leq j \leq k_i$ and $1 \leq i \leq n$.*

Proof. Let us fix arbitrary $P_0, P_1 \in ds(P_1^i)$ and some $\alpha \in \mathcal{A}$ and assume first $r_\alpha(\sigma_{P_j^i}(P_0)) > 0$. Then, Lemma 3 asserts that the concentration function

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

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

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

Observing that Lemma 11 implies $r_\alpha(P_0) = r_\alpha(\sigma_{P_j^i}(P_0)) > 0$, we conclude using Lemma 8 that $\mathcal{R}_\alpha(M, \widehat{v}, P_0) > 0$, where

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

Using

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

we infer

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

and

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

Hence, since the equality $\mathcal{R}_\alpha(M, v^\sigma, P_0) = \mathcal{R}_\alpha(M, \widehat{v}, P_0) > 0$ implies $p_\alpha(P_0, P_1) = p_\alpha(\sigma_{P_j^i}(P_0), \sigma_{P_j^i}(P_1))$, Lemma 11 yields the desired equality

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

As in the case $r_\alpha(\sigma_{P_j^i}(P_0)) = 0$ the claim follows by observing that Lemma 11 implies $r_\alpha(P_0) = 0$, the proof is complete. □

Similarly to exact fluid lumpability, the above theorem states that well-posedness and ordinary fluid lumpability imply the notion of semi-isomorphism. We end this section by stressing that in the case of ill-posed models no such statement can be made.

To see this, let us consider the ill-posed model

$$(T_0 \underset{\emptyset}{\bowtie} T_1) \underset{\{exec,\gamma\}}{\bowtie} C,$$

where C and T_1 are as in (3.1), whereas

$$T_0 \stackrel{def}{=} (exec, r).\widehat{T}_0 + (\gamma, x).\widehat{T}_0, \qquad \widehat{T}_0 \stackrel{def}{=} (io, s').T_0.$$

Then, the partition $\big\{\{T_0, T_1\}, \{C\}\big\}$ is ordinarily fluid lumpable, but T_0 can perform a γ-action, while T_1 cannot. Since each of the relations from Section 2.3 distinguishes between the types of action performed by a process, we conclude that, in general, ordinary fluid lumpability implies none of the behavioural equivalences of Section 2.3.

On the other hand, even isomorphism between fluid atoms is, in general, not *sufficient* for the atoms belong to the the same element of an ordinary fluid lumpable partition. To see this, consider the model $C_1 \underset{\{exec\}}{\bowtie} C_2$, where C_d is as in (3.1). Then, the partition $\big\{\{C_1, C_2\}\big\}$ cannot be ordinarily fluid lumpable. To see this, let us assume towards a contradiction that $\big\{\{C_1, C_2\}\big\}$ is ordinarily fluid lumpable. If C_1 is the representative of $\{C_1, C_2\}$, there exists a bijection $\sigma_{C_2} : ds(C_1) \to ds(C_2)$ which satisfies $i) - iii)$ from Definition 32 for all concentration functions v. However, $v_{C_1} = v_{C_1'} = v_{C_2} = v_{C_2'} = 1$ implies that

$$r_{exec}(C_1 \underset{\{exec\}}{\bowtie} C_2, v^\sigma) = 0 < r_{exec}(C_1 \underset{\{exec\}}{\bowtie} C_2, v),$$

which violates $iii)$. Since the very same argumentation can be applied in the case where C_2 is the representative of $\{C_1, C_2\}$, we infer the claim.

5.4 Related Work

The closest work to ours is [44] where ordinary fluid lumpability is discussed for a generalised version of FPA which supports among the minimum semantics of PEPA also the law of mass action known from chemistry [72], theoretical biology [73] and epidemic routing [74]. This is achieved by replacing the minimum $\min(r_\alpha(M_0, v), r_\alpha(M_1, v))$ in Definition 14 with the product $r_\alpha(M_0, v) r_\alpha(M_1, v)$. However, in order to show that the fluid lumpability implies the notion of semi-isomorphism and the merging theorem from Section 3.3.3, [44] assumes an additional property in the definition of exactly and ordinary fluid lumpability. That is, by focusing on the minimum semantics, we are able to state our fluid notions under milder requirements. Apart from that, the notion of ordinary fluid lumpability is related to the best of our knowledge only to the aggregation technique from [36] and its enhancement [40]. Indeed, ordinary fluid lumpability can be

seen as a special case of this technique. To see this, we briefly sketch the idea behind [40]. Let us start with the ODE system

$$\dot{x}_i = f_i(x_1, \ldots, x_n), \qquad 1 \leq i \leq n, \tag{5.7}$$

where each f_i is assumed to be continuous on $\mathbb{R}^n$. We then aggregate $x_1, \ldots, x_n$ to $y_1, \ldots, y_m$, with $m \leq n$, by setting

$$y_j := g_j(x_1, \ldots, x_n), \qquad 1 \leq j \leq m,$$

where each $g_j : \mathbb{R}^n \to \mathbb{R}$ is differentiable. Then, the chain rule shows that

$$\dot{y}_j = \sum_{k=1}^{n} \big(\partial_{x_k} g_j\big)(x_1, \ldots, x_n) \cdot f_k(x_1, \ldots, x_n), \qquad 1 \leq j \leq m.$$

Consequently, if for each $1 \leq j \leq m$ there exists an $F_j : \mathbb{R}^m \to \mathbb{R}$ such that

$$\sum_{k=1}^{n} \big(\partial_{x_k} g_j\big)(x_1, \ldots, x_n) \cdot f_k(x_1, \ldots, x_n) \equiv F_j(y_1, \ldots, y_m),$$

the original ODE system (5.7) is related to the aggregated ODE system

$$\dot{y}_j = F_j(y_1, \ldots, y_m), \qquad 1 \leq j \leq m$$

by means of $y_j = g_j(x_1, \ldots, x_n)$. Indeed, the ODE systems (3.18) and (5.3) are instances of such an aggregation with g_j being of the form $\sum_{i \in S_j} x_i$. Although such an approach is more general than ordinary fluid lumpability, the latter is easier to check, allows for compositional reasoning on the level of process terms and implies the notion of semi-isomorphism in the case of well-posedness. Worthy of remark is that, in contrast to the notion of exact fluid lumpability, one cannot *fully* recover the solution of the original ODE system by means of the above aggregation technique when $m < n$. To see this, let us assume towards a contradiction that there is such an aggregation. Then, one of the functions g_j induces a continuous *bijection* $g : \mathbb{R}^k \to \mathbb{R}$ for some $k \geq 2$. Since $B := \{x \in \mathbb{R}^k \mid \|x\|_2 \leq 1\}$ is connected and compact, the continuity of g implies that $g(B)$ is connected and compact as well. Hence, $g(B) \subseteq \mathbb{R}$ yields $g(B) = [a; b]$ for some $a \leq b$. Moreover, the bijectivity of g enforces $a < b$ and allows us to define $x_0 := g^{-1}(c)$ for some arbitrary $c \in (a; b)$. Then, $B \setminus \{x_0\}$ is connected, since it is obviously path-connected, and the continuity of g implies that $g(B \setminus \{x_0\})$ is connected as well. This is, however, false, for $g(B \setminus \{x_0\}) = [a; b] \setminus \{c\}$.

Chapter 6

Fluid ε-Lumpability

This chapter studies aggregations when the fluid atoms of an FPA model can be grouped to a fluid lumpable partition *after* a suitable perturbation of their parameters. In the case of exact fluid lumpability, we perturbate initial populations and rates of sequential components. In the case of ordinary fluid lumpability, instead, we only consider the latter because there is no requirement on identical initial populations for aggregated fluid atoms.

The structure is as follows. After building on intuition in terms of a motivating example in Section 6.1, we define exact and ordinary fluid ε-lumpable partitions in Section 6.2. There, we also show that the error depends *linearly* on the perturbation ε and that fluid ε-lumpability implies, in the case of well-posed models, the notion of ε-semi-isomorphism. In Section 6.3 we consider a numerical evaluation to study the impact of ε on the ODEs in the context of the motivating example.

6.1 Motivating Example

Let us consider again a variation of the model

$$Sys := \left(T_1 \underset{\emptyset}{\bowtie} \ldots \underset{\emptyset}{\bowtie} T_D\right) \underset{\{exec\}}{\bowtie} C$$

given in (5.1), but now with different T_d. More specifically, let us assume that $T_d \stackrel{def}{=} (exec, r_d).\widehat{T}_d$ and $\widehat{T}_d \stackrel{def}{=} (io, s').T_d$ for $r_d := r + \varepsilon_d$, with $1 \leq d \leq D$. In such a case, the underlying ODE system

$$\begin{aligned}
\dot{v}_{T_d} &= -\frac{r_d v_{T_d}}{\sum\limits_{1 \leq d' \leq D} r_{d'} v_{T_{d'}}} \min\left(\sum_{1 \leq d' \leq D} r_{d'} v_{T_{d'}}, r v_C\right) + s' v_{\widehat{T}_d}, \\
\dot{v}_{\widehat{T}_d} &= -\dot{v}_{T_d}, \\
\dot{v}_C &= -\min\left(\sum_{1 \leq d' \leq D} r_{d'} v_{T_{d'}}, r v_C\right) + s v_{\widehat{C}},
\end{aligned}$$

$$\dot{v}_{\widehat{C}} = -\dot{v}_C \tag{6.1}$$

cannot be aggregated to (5.4), unless $\varepsilon_1 = \ldots = \varepsilon_D = 0$. However, it is reasonable to ask whether one can bound the difference between the solutions of (5.3) and (6.1) in terms of the rate perturbation $\varepsilon = \|(\varepsilon_1, \ldots, \varepsilon_D)\|$.

A similar question can be stated in the context of exact fluid lumpability which makes, in contrast to ordinary fluid lumpability, assumptions on the fluid atoms *as well as* the initial conditions. For instance, recall the running example of Chapter 3 given in (3.1)

$$Sys' := \Big(\big(C_1 \underset{\{exec\}}{\bowtie} C_1' \underset{\{exec\}}{\bowtie} T_1 \big) \underset{\emptyset}{\bowtie} \ldots \underset{\emptyset}{\bowtie} \big(C_D \underset{\{exec\}}{\bowtie} C_D' \underset{\{exec\}}{\bowtie} T_D \big) \Big) \underset{\{io\}}{\bowtie} U,$$

where it was assumed that

$$\begin{array}{lll} C_d \stackrel{def}{=} (exec, r).\widehat{C}_d, & C_d' \stackrel{def}{=} (exec, r/2).\widehat{C}_d' + (exec, r/2).\widehat{C}_d', & T_d \stackrel{def}{=} (exec, r).\widehat{T}_d, \\ \widehat{C}_d \stackrel{def}{=} (reset, s).C_d, & \widehat{C}_d' \stackrel{def}{=} (reset, s).C_d', & \widehat{T}_d \stackrel{def}{=} (io, s').T_d \end{array} \tag{6.2}$$

and

$$\begin{array}{lll} v_{C_d}(0) = \mathfrak{c}_C & v_{C_d'}(0) = \mathfrak{c}_C & v_{T_d}(0) = \mathfrak{c}_T \\ v_{\widehat{C}_d}(0) = 0 & v_{\widehat{C}_d'}(0) = 0 & v_{\widehat{T}_d}(0) = 0 \\ v_U(0) = \mathfrak{c}_U & v_{\widehat{U}}(0) = 0 & \end{array} \tag{6.3}$$

for all $1 \leq d \leq D$. Then, one could ask whether the difference between the solution underlying (6.2), (6.3) and those underlying

$$\begin{array}{lll} C_d \stackrel{def}{=} (exec, r).\widehat{C}_d, & C_d' \stackrel{def}{=} (exec, r/2).\widehat{C}_d' + (exec, r/2).\widehat{C}_d', & T_d \stackrel{def}{=} (exec, r).\widehat{T}_d, \\ \widehat{C}_d \stackrel{def}{=} (reset, s + \varepsilon_d).C_d, & \widehat{C}_d' \stackrel{def}{=} (reset, s).C_d', & \widehat{T}_d \stackrel{def}{=} (io, s').T_d \end{array}$$

and

$$\begin{array}{lll} v_{C_d}(0) = \mathfrak{c}_C + \eta_d & v_{C_d'}(0) = \mathfrak{c}_C & v_{T_d}(0) = \mathfrak{c}_T \\ v_{\widehat{C}_d}(0) = 0 & v_{\widehat{C}_d'}(0) = 0 & v_{\widehat{T}_d}(0) = 0 \\ v_U(0) = \mathfrak{c}_U & v_{\widehat{U}}(0) = 0 & \end{array}$$

can be bounded in terms of $\|(\varepsilon_1, \ldots, \varepsilon_D, \eta_1, \ldots, \eta_D)\|$.

6.2 Definitions and Results

At the basis of our investigation stands a standard result from the area of ODEs which relates two ODE systems of the same size, where the vector field is made dependent on a pair of vectors, 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 $\underline{x}_\xi$, with $\delta = \left\|\underline{x}_\xi - \underline{x}_\zeta\right\|$. This will be used to define our approximate version of exact fluid lumpability.

The theorem below states that, on a fixed time interval $[0;t]$, the distance between the two solutions depends *linearly* on both ε and δ, if the ODE system is Lipschitz in x and ξ.

Theorem 18. *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 $\mathbb{R}^{n+m}$, with respect to both x and ζ, i.e.

$$\forall \zeta \in \mathbb{R}^n.\ \exists L_\zeta > 0.\ \forall x, x' \in \mathbb{R}^m.\ \left(\|f(\zeta, x) - f(\zeta, x')\| \leq L_\zeta \|x - x'\| \right)$$
$$\forall x \in \mathbb{R}^m.\ \exists K_x > 0.\ \forall \zeta, \zeta' \in \mathbb{R}^n.\ \left(\|f(\zeta, x) - f(\zeta', x)\| \leq K_x \|\zeta - \zeta'\| \right)$$

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

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

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

Proof. We first show an auxiliary result. Let c_1, c_2, c_3 be positive constants and u a continuous function on $0 \leq t < \infty$ such that

$$u(t) \leq c_3 + c_2 t + c_1 \int_0^t u(s) ds \tag{6.4}$$

Then, it holds that

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

To see this, note that (6.4) can be rewritten into

$$\underbrace{u(t) + \frac{c_2}{c_1}}_{\tilde{u}(t) =} \leq \underbrace{\left(\frac{c_2}{c_1} + c_3 \right)}_{\tilde{\alpha} =} + \int_0^t \underbrace{c_1 \left(u(s) + \frac{c_2}{c_1} \right)}_{\tilde{v}(s)\tilde{u}(s) =} ds.$$

By applying Gronwall's inequality to

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

we infer that $\tilde{u}(t) \leq \tilde{\alpha} \cdot \mathrm{e}^{\int_0^t \tilde{v}(s) ds}$ and the auxiliary claim follows.

Let us focus now on the main claim. We observe first

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

By applying the auxiliary result for $u(s) := \|x_\zeta(s) - x_\xi(s)\|$, $c_3 := \delta$, $c_1 := L_\zeta$ and $c_2 := \varepsilon K$, this yields the claim. □

Next, we formally introduce the notion of perturbation on rates.

Definition 33. *For an FPA 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.*

We wish to point out that it is not important how the vector $\nu(M)$ is calculated, as long as it uniquely relates the action rates within the model. To build on intuition, we sketch one possible way to achieve this. We first construct an auxiliary vector $\mathfrak{N}(M)$: if M is a fluid atom P, we initialise $\mathfrak{N}(P)$ with the empty vector and enhance the while-loop of the common algorithm which constructs the derivation graph of P by one additional operation: if X denotes the graph that has been constructed so far by the algorithm and a new transition $(P', (\alpha, r), P'')$ is added to X, we also append $(P', (\alpha, r), P'', i)$ to $\mathfrak{N}(P)$, where i denotes the number of the (α, r) arcs between P' and P'' in X. In the case of $M = M_0 \underset{L}{\bowtie} M_1$, instead, we append to the sequence $\mathfrak{N}(M_1)$ to the sequence $\mathfrak{N}(M_0)$. Note that $\mathfrak{N}(M_0)$ and $\mathfrak{N}(M_1)$ have pairwise different elements, since Definition 12 ensures that any two fluid atoms of M have disjoint derivative sets. The vector $\nu(M)$ arises then directly from $\mathfrak{N}(M)$ by replacing each element $(P', (\alpha, r), P'', i)$ with r.

For instance, given

$$P \stackrel{def}{=} (\alpha, r).P' + (\alpha, r).P', \quad P' \stackrel{def}{=} (\beta, s).P, \quad Q \stackrel{def}{=} (\gamma, u).Q', \quad Q' \stackrel{def}{=} (\delta, w).Q,$$

we first derive $\mathfrak{N}(P) = ((P, (\alpha, r), P', 1), (P, (\alpha, r), P', 2), (P', (\beta, s), P, 1))$ and $\mathfrak{N}(Q) = ((Q, (\gamma, u), Q', 1), (Q', (\delta, w), Q, 1))$. This yields then $\nu(P \underset{\{\alpha\}}{\bowtie} Q) = (r, r, s, u, w)$.

Before Theorem 18 can be applied to FPA, we have to show that FPA models induce globally Lipschitz ODE systems.

Proposition 3. *For an FPA model $M \equiv M(\xi)$ and*

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

$F(\xi,\cdot)$ and $F(\cdot,v)$ are globally Lipschitz. Moreover, if 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 proof is similar to the one of Lemma B.1 in [54] and is given in Appendix A.3. □

Equipped with Theorem 18, we are in a position to state the aforementioned perturbation result.

Theorem 19. *Fix an FPA model M, a $\zeta \in \mathbb{R}_{>0}^{|\nu(M)|}$, a concentration function $v^\zeta(0)$ and $c, t > 0$. Then there exist $C_1, C_2 > 0$ such that $\|v^\xi(0) - v^\zeta(0)\| \leq c$ implies*

$$\max_{0\leq s\leq t} \|v^\xi(s) - v^\zeta(s)\| \leq C_1\|\xi - \zeta\| + C_2\|v^\xi(0) - v^\zeta(0)\|$$

for all $\xi \in \mathbb{R}_{>0}^{|\nu(M)|}$, where v^ξ and v^ζ refer to the ODE solutions of $M(\xi)$ and $M(\zeta)$, respectively.

Proof. The claim follows by Lemma 12 in Appendix A.1, Proposition 3 and Theorem 18. □

Note that in the above theorem $M(\zeta)$ is arbitrary but fixed, whereas $M(\xi)$ varies. We now focus on the situation where $M(\zeta)$ has either an exactly or an ordinarily fluid lumpable partition.

Definition 34 (Fluid ε-Lumpability)**.** *Fix an FPA model M and $\xi \in \mathbb{R}_{>0}^{|\nu(M)|}$. If $M(\zeta)$ has an exactly/ordinarily fluid lumpable partition $\{\overline{P}^1, \ldots, \overline{P}^n\}$ 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 $\|\cdot\|$.*

We build on intuition by considering the FPA model

$$Sys' := \Big((T_1 \underset{\{exec\}}{\bowtie} R_1) \underset{\emptyset}{\bowtie} \ldots \underset{\emptyset}{\bowtie} (T_D \underset{\{exec\}}{\bowtie} R_D)\Big) \underset{\{exec\}}{\bowtie} C, \tag{6.5}$$

where $R_d \stackrel{def}{=} (exec, r').R_d$, with $1 \leq d \leq D$, and for which it can be shown that $\big\{\{T_1, \ldots, T_D\}, \{R_1, \ldots, R_D\}, \{C\}\big\}$ is exactly fluid lumpable. Then, together with

$$\xi = (r+\varepsilon_1, s'+\varepsilon_2, r'+\varepsilon_3, \ldots, r+\varepsilon_{3D+1}, s'+\varepsilon_{3D+2}, r'+\varepsilon_{3D+3}, r, s) \in \mathbb{R}_{>0}^{|\nu(Sys')|},$$

$Sys'(\xi)$ is exactly fluid ε-lumpable with

$$\varepsilon = \|(\varepsilon_1, \varepsilon_2, \varepsilon_3, \ldots, \varepsilon_{3D+1}, \varepsilon_{3D+2}, \varepsilon_{3D+3}, 0, 0)\|.$$

On the other hand, the partition $\{\overline{P}^1, \overline{P}^2\} = \big\{\{T_1, \ldots, T_D\}, \{C\}\big\}$ of $Sys(\zeta)$ defined in (5.1) is ordinarily fluid lumpable if $\zeta = (r, s', \ldots, r, s', r, s)$. Consequently, it holds that $Sys(\xi)$ is ε-ordinarily fluid lumpable, where

$$\varepsilon = \|(\xi_1 - r, \xi_2 - s', \ldots, \xi_{2D-1} - r, \xi_{2D} - s', \xi_{2D+1} - r, \xi_{2D+2} - s)\|.$$

That is, an exactly/ordinarily fluid lumpable partition admits an infinity of ε-lumpable partitions and ε gives the measure of how close a given model is to error-free fluid lumping.

Both exact and ordinary fluid ε-lumpability enjoy congruence. In the case of exact fluid ε-lumpability, however, the following assumption has to be made.

Remark 5. *Usually, exact fluid lumpable partitions are constructed using the notion of* label equivalence*, cf. Section 3.3. Throughout the chapter we will assume that this is always the case.*

Theorem 20 (Congruence)**.** *Fix two FPA models M_1, M_2 and assume that $\{\overline{P}_k^1, \ldots, \overline{P}_k^{n_k}\}$ 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 $L \subseteq \mathcal{A}$, $\bigcup_{k=1}^{2}\{\overline{P}_k^1, \ldots, \overline{P}_k^{n_k}\}$ is $\|(\xi_1, \xi_2) - (\zeta_1, \zeta_2)\|$-exactly/ordinarily fluid lumpable in $\mathcal{G}(M_1 \underset{L}{\bowtie} M_2)$.*

Proof. Theorem 8 shows the case of exact fluid lumpability, whereas Theorem 16 yields the case of ordinary fluid lumpability. □

Clearly, since an ordinarily fluid lumpable partition does not depend on the initial values, a perturbation of initial values is interesting only in the case of exact fluid lumpability.

We turn now to a classification of exact and ordinary fluid ε-lumpability, where labels within blocks of a fluid ε-lumpable partition are related. For this, we define the notion of ε-semi-isomorphism, which regards two sequential components to be equal, if a change of the underlying rates not greater than ε makes them semi-isomorphic.

Definition 35 (ε-Semi-Isomorphism)**.** *Two sequential components P and Q are ε-semi-isomorphic for some $\varepsilon > 0$, if there is a bijection $\sigma : ds(P) \to ds(Q)$ which satisfies*

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

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

Analogously to exact and ordinary fluid lumpability, the following characterises ε-lumpability with respect to ε-semi-isomorphism.

Theorem 21. *For any well-posed FPA model M and norm $\|\cdot\|$, there exists a $C > 0$ such that: assume that $\{\overline{P}^1, \ldots, \overline{P}^n\}$ is an $\|\xi - \zeta\|$-exactly/ordinarily fluid lumpable partition of $M(\xi)$, where $\xi, \zeta \in \mathbb{R}_{>0}^{|\nu(M)|}$. Then, it holds that:*

a) Any two fluid atoms $P_j^i, P_{j'}^i$ of $M(\xi)$ are $C\,\|\xi - \zeta\|$-semi-isomorphic;

b) 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 $\|\cdot\| = \|\cdot\|_\infty$, a) holds for $C = 1$.

Δ	0.00	0.01	0.02	0.03	0.04	0.05
$D = 2$	0.41%	0.70%	1.02%	1.33%	1.64%	1.94%
$D = 3$	0.82%	1.24%	1.71%	2.17%	2.62%	3.07%
$D = 4$	1.23%	1.78%	2.39%	2.99%	3.59%	4.17%
$D = 5$	1.63%	2.31%	3.06%	3.81%	4.53%	5.25%

Table 6.1: Approximation errors for exact fluid lumpability, by perturbations of initial conditions and rates: D enumerates different models, while Δ accounts for the discrepancy in the rates. In the case of $\Delta = 0$, the error is stemming from different initial conditions.

Δ	0.01	0.02	0.03	0.04	0.05
$D = 2, 3, 4, 5$	0.16%	0.32%	0.47%	0.63%	0.78%

Table 6.2: Approximation errors for ordinary fluid lumpability, by perturbations of rates: D enumerates different models, while Δ accounts for the discrepancy in the rates.

Proof. Thanks to the fact that $\{\overline{P}^1, \ldots, \overline{P}^n\}$ is an ordinary/exact fluid lumpable partition of $\mathcal{G}(M(\zeta))$, Theorem 10 and 17 ensure that the fluid atoms $P^i_j, P^i_{j'}$ in $M(\zeta)$ are semi-isomorphic. Moreover, by a standard theorem from calculus, 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 T_d, $T_{d'}$ are $\|\xi - \zeta\|_\infty$-semi-isomorphic in $Sys(\xi)$ for all $\xi \in \mathbb{R}^{|\nu(Sys)|}_{>0}$, if $\zeta = (r, s', \ldots, r, s', r, s)$.

6.3 Numerical Examples

We provide some numerical evidence of the aggregation error on the models presented in the previous section. For exact fluid lumpability, we considered the model (6.5) with $T_d \stackrel{def}{=} (exec, r_d).\widehat{T}_d$, $\widehat{T}_d \stackrel{def}{=} (io, s').T_d$, $R_d \stackrel{def}{=} (exec, r_d).R_d$, $C = (exec, r_1).\widehat{C}$, $\widehat{C} = (reset, s).C$, where we fixed $s' = 0.5$, $s = 0.2$ and set $r_d = 1.0 + (d-1)\Delta$; Δ was varied between 0.00 and 0.05 at 0.01 steps. The models were analysed for different values of D. For each value, we set $v_{T_d}(0) = 200 + (d-1)$, $v_{\widehat{T}_d}(0) = 0$, $v_{R_d} = 300$, $v_C(0) = 300$, and $v_{\widehat{C}} = 0$. This corresponds to a situation where the initial concentrations of T_d-components are different and separated by a few percent. This model was compared against the solution of a perturbed model with rates and initial concentrations such that all are set equal to the averages in the original model, i.e., $1.0 + (\Delta/D)\sum_{d=1}^{D}(d-1)$

and $200 + (1/D)\sum_{d=1}^{D}(d-1)$. Note that these changes allow for exact fluid lumpability.

Both the original and the perturbed model were numerically solved over the time interval $[0; 30]$ (ensuring convergence to equilibria) with solutions registered with 0.2 time unit steps. The approximation relative error is defined as:

$$\max_{P\in\{T_d,\widehat{T}_d,R_d,C,\widehat{C}\}} \max_{t\in\{0,0.02,\ldots,30\}} \frac{|v_P(t) - v_P^{\varepsilon}(t)|}{\sum_{P'\in ds(P)} v_{P'}(0)} \times 100,$$

where $v_P(t)$ is the solution of the original model and $v_P^{\varepsilon}(t)$ is the corresponding estimate in the exactly fluid ε-lumpable one. The absolute difference is normalised with respect to the total concentration of the fluid atom to which derivative P belongs. The results are presented in Table 6.1.

The model used for the numerical examples with ordinary fluid lumpability is *Sys*, which was parametrised as in the previous case, except for $v_C(0)$ which was set to 1500. (For $v_C(0) = 300$ the approximation errors were found to be of the same order of magnitude as the tolerance of the numerical solution, i.e. 1e-8.) The results are shown in Table 6.2, where the numerical approximation error is computed with respect to an ε-ordinarily fluid lumpable partition where all T_d have the same average rate as the original model, similarly to above.

Overall, with this parametrisation exact fluid ε-lumpability shows good accuracy across all tests. The case for $\Delta = 0.00$ measures the impact on the approximation error of the heterogeneity only due to the initial conditions of the aggregated components. Instead, in these examples, ordinary fluid ε-lumpability appears to be more robust in practice, with errors that were found to be independent (up to numerical precision) from the number of aggregated components. With the same relative perturbation on the rates by Δ, the approximation errors are suitably lower. (The parametrisation for $v_C(0) = 300$ does show dependence on D for the approximation, however, as discussed, the actual errors are negligible.)

6.4 Related Work

Several *approximate* aggregation techniques for ODE systems have been proposed. For instance, [32] splits the original ODE system into a *fast* and a *slow* part, while [33, 34] identify parts of the ODE system with a *negligible* impact on the overall trajectory. The methods [35] and [75], instead, look for an aggregated ODE system of certain size which minimises the distance to the original one. However, apart from [32], none of these works considers ODE systems which can be exactly aggregated after a small perturbation. Specifically, [32] studies ODE systems with equations which can be set to zero by means of small perturbations. As a reduction technique which is based on the Centre Manifold Theorem [76], the aggregations arising from [32] usually lead to good approximations for all $t \geq 0$. At the heart of fluid ε-lumpability, instead, stands Gronwall's inequality with a bound which grows exponentially as t increases. However, it is fair to say that in order to perform an aggregation in the style

of [32], the underlying ODE system has to be differentiable. Thus, [32] does not apply to the minimum function, which is at the heart of PEPA. The work [77], instead, considers exact aggregation according to [40] after a perturbation of the parameters of the original ODE system. Similarly to fluid ε-lumpability, the bounds of [77] can be traced back to Gronwall's inequality. In this respect, [77] is closely related to the notion of ordinary fluid ε-lumpability and can be seen as an extension of [40], meaning that it applies also to ODE systems which do not underly an FPA model. On the other hand, [77] does not cover ε-semi-isomorphism or exact fluid lumpability, and so our work here can be seen as more general in some respects.

Chapter 7

Spatial Aggregation

Fluid lumpability, and in particular nested FPA models, yield ODE aggregations that exploit structural symmetries such as hierarchically composed processes. In this chapter, instead, we want to study FPA processes endowed with an explicit notion of mobility and location. The sequential components live in a two-dimensional lattice in the unit square where they may perform *stationary* actions with other processes in the same region in the lattice. In addition, they perform *spatial* actions which allow them to move across the lattice independently from each other. In Section 7.1, we achieve this by defining, for each FPA model M, its *spatial* version $\mathcal{S}(M)$, which is an FPA model itself and is constructed as follows. First, one defines the spatial version $\mathcal{S}(P)$ of any sequential component in M, i.e. $P \in \mathcal{G}(M)$. Then, the sequential component $\mathcal{S}(P)$ arises from P by augmenting the latter with spatial actions which allow for a random walk on the lattice. Having this, we define $\mathcal{S}(M)$ by replacing each $P \in \mathcal{G}(M)$ in M by $\mathcal{S}(P)$. With such a construction, it is possible to model mobile systems such as, for instance, personal communication services [45]: the base stations can be modelled as regions of the lattice, which can contain potentially many mobile nodes that may migrate across the lattice. Another interesting application would be the modelling of spread patterns of smartphone viruses [46]. Unfortunately, the incorporation of locality leads to a blow-up not only of the CTMC, but also of the underlying ODE system. Specifically, if $1/K$ is the step-size of the regular lattice, it consists of $(K+1)^2$ regions and leads to an ODE system of size $\mathcal{O}(K^2)$, making an efficient numerical analysis infeasible in the case of fine grained lattices. This problem is addressed in Sections 7.2 and 7.3, where conditions are identified under which the aforementioned ODE systems converge, as $K \to \infty$, to a system of partial differential equations (PDEs) whose size does not depend on K. Note that the restriction to interact in the same region becomes more and more restrictive as K tends to infinity. However, if the unit square describes from the perspective of a single agent a large enough area, a good approximation of the stochastic model by the PDE system may be achieved while maintaining a realistic distance between neighbouring regions. By performing a numerical evaluation in Section 7.4, we argue that the ODE

systems are already numerically indistinguishable for moderate sizes of K. The chapter concludes with an overview of related work in Section 7.5.

7.1 Spatial FPA

Let us begin with the definition of the two-dimensional lattice

$$\mathcal{R} \equiv \mathcal{R}_K = \{(i/K, j/K) \mid 0 \leq i, j \leq K\} \subseteq [0;1]^2, \qquad K \geq 1.$$

We illustrate our intent by defining the spatial version of

$$\mathcal{M} := C \underset{\{exec\}}{\bowtie} T,$$

where

$$C \stackrel{def}{=} (exec, r).\widehat{C}, \quad \widehat{C} \stackrel{def}{=} (reset, s).C, \quad T \stackrel{def}{=} (exec, r).\widehat{T}, \quad \widehat{T} \stackrel{def}{=} (io, s').T.$$

For this, let $\mathcal{N}(x, y) \equiv \mathcal{N}_K(x, y)$ be the von Neumann neighbourhood[1] of the region (x, y),

$$\Omega \equiv \Omega_K = \big\{(i/K, j/K) \mid i \in \{0, 1\} \vee j \in \{0, 1\}\big\}$$

be the set of boundary regions and $\Delta s = 1/K$. For instance, for $K = 2$, it holds that $\mathcal{N}(0, 0) = \{(0, 1/2), (1/2, 0)\}$ and $\mathcal{R} \backslash \Omega = \{(1/2, 1/2)\}$. Our transformation will yield $\mathcal{S}(\mathcal{M})$ defined as

$$\mathcal{S}(\mathcal{M}) = C^{(\Delta s, \Delta s)} \underset{L}{\bowtie} T^{(\Delta s, \Delta s)}, \qquad L = \{exec^l \mid l \in \mathcal{R} \setminus \Omega\}, \tag{7.1}$$

with

$$\begin{aligned}
C^l &\stackrel{def}{=} (exec^l, r).\widehat{C}^l + \sum_{\widetilde{l} \in \mathcal{N}(l) \setminus \Omega} (\delta, \mu_C^{l,\widetilde{l}}(K)).C^{\widetilde{l}} + \sum_{\widetilde{l} \in \mathcal{N}(l) \cap \Omega} (\delta, \mu_C^{l,\widetilde{l}}(K)).O \\
\widehat{C}^l &\stackrel{def}{=} (reset^l, s).C^l + \sum_{\widetilde{l} \in \mathcal{N}(l) \setminus \Omega} (\delta, \mu_{\widehat{C}}^{l,\widetilde{l}}(K)).\widehat{C}^{\widetilde{l}} + \sum_{\widetilde{l} \in \mathcal{N}(l) \cap \Omega} (\delta, \mu_{\widehat{C}}^{l,\widetilde{l}}(K)).O \\
T^l &\stackrel{def}{=} (exec^l, r).\widehat{T}^l + \sum_{\widetilde{l} \in \mathcal{N}(l) \setminus \Omega} (\delta, \mu_T^{l,\widetilde{l}}(K)).T^{\widetilde{l}} + \sum_{\widetilde{l} \in \mathcal{N}(l) \cap \Omega} (\delta, \mu_T^{l,\widetilde{l}}(K)).O \\
\widehat{T}^l &\stackrel{def}{=} (io^l, s').T^l + \sum_{\widetilde{l} \in \mathcal{N}(l) \setminus \Omega} (\delta, \mu_{\widehat{T}}^{l,\widetilde{l}}(K)).\widehat{T}^{\widetilde{l}} + \sum_{\widetilde{l} \in \mathcal{N}(l) \cap \Omega} (\delta, \mu_{\widehat{T}}^{l,\widetilde{l}}(K)).O \\
O &\stackrel{def}{=} (\tau, 1.0).O
\end{aligned}$$

for all $l \in \mathcal{R} \setminus \Omega$. Intuitively, $\mathcal{S}(\mathcal{M})$ models a situation where sequential components of type $\mathcal{B}(\mathcal{M}) = \{C, \widehat{C}, T, \widehat{T}\}$ move across $\mathcal{R} \setminus \Omega$ via the spatial *diffusion* action δ and exit it as soon as they hit the boundary Ω. Formally, departures

[1] Other neighbourhoods types may be considered, e.g. the one of Moore. However, it is not clear whether those allow for a spatial aggregation resulting in PDEs.

are modelled by transitions to an absorbing sequential component O. (The rate 1.0 was chosen arbitrarily; indeed, any rate would be fine because the action models a self-loop.) The rates $\mu_P^{l,\widetilde{l}}(K) \geq 0$ may depend, in general, on the sequential component P that is moving, on the origin and target region, i.e. l and $\widetilde{l}$, respectively, and on K. The actions originally available in $\mathcal{M}$, i.e. *exec*, *reset* and *io*, are instead performed locally, hence their superscript which signals in which region they are taking place. In particular, enforcing synchronisation only between processes in the same region is achieved by appending l to each action type, modifying the synchronisation sets accordingly in the model equation.

Remark 6. *It is worth noting that the usage of location $(\Delta s, \Delta s)$ in the definition of $\mathcal{S}(M)$ is arbitrary, essentially because any two locations of the lattice are interconnected.*

For an FPA model M, we assume in the following without loss of generality that $\delta, \tau \notin \mathcal{A}$ and $O \notin \mathcal{B}(M)$. The spatial version of M, $\mathcal{S}(M)$, is then as follows.

Definition 36 (Spatial FPA)**.** *For a given FPA model M, the spatial version of M over the lattice $\mathcal{R}$, denoted by $\mathcal{S}(M) \equiv \mathcal{S}_K(M)$, is inductively given by*

$$\mathcal{S}(P) := P^{(\Delta s, \Delta s)}, \qquad \mathcal{S}(M_0 \underset{L}{\bowtie} M_1) := \mathcal{S}(M_0) \underset{\mathcal{S}(L)}{\bowtie} \mathcal{S}(M_1),$$

where $\mathcal{S}(L) = \{\alpha^l \mid \alpha \in L \wedge l \in \mathcal{R} \setminus \Omega\}$ and

$$P^l \stackrel{\text{def}}{=} \sum_{\widetilde{l} \in \mathcal{N}(l) \setminus \Omega} (\delta, \mu_P^{l,\widetilde{l}}(K)).P^{\widetilde{l}} + \sum_{\widetilde{l} \in \mathcal{N}(l) \cap \Omega} (\delta, \mu_P^{l,\widetilde{l}}(K)).O + \sum_{(\alpha,r,i) \in X} (\alpha^l, r).P_i^l$$

for all $l \in \mathcal{R} \setminus \Omega$ and $\mu_P^{l,\widetilde{l}}(K) \geq 0$, provided that $P \stackrel{\text{def}}{=} \sum_{(\alpha,r,i) \in X} (\alpha, r).P_i$. (Notice that the case $\mu_P^{l,\widetilde{l}}(K) = 0$ corresponds to removing the respective summand in the definition of P^l). Moreover, the absorbing sequential component is defined by $O \stackrel{\text{def}}{=} (\tau, 1.0).O$, whereas $\mathcal{A}^+ := \{\alpha^l \mid \alpha \in \mathcal{A} \wedge l \in \mathcal{R} \setminus \Omega\} \cup \{\delta, \tau\}$ denotes the set of actions of $\mathcal{S}(M)$.

From the above definition it becomes evident that, for any FPA model M, $\mathcal{S}(M)$ is an FPA model, with actions from $\mathcal{A}^+$, admitting a limit ODE system. For example, the ODEs of $\mathcal{B}(\mathcal{S}(\mathcal{M})) \setminus \{O\}$ are

$$\begin{aligned}
\dot{v}_{C^l} &= -r \min(v_{C^l}, v_{T^l}) + s v_{\widehat{C}^l} + \sum_{\widetilde{l} \in \mathcal{N}(l) \setminus \Omega} \mu_C^{\widetilde{l},l}(K) v_{C^{\widetilde{l}}} - \sum_{\widetilde{l} \in \mathcal{N}(l)} \mu_C^{l,\widetilde{l}}(K) v_{C^l}, \\
\dot{v}_{\widehat{C}^l} &= +r \min(v_{C^l}, v_{T^l}) - s v_{\widehat{C}^l} + \sum_{\widetilde{l} \in \mathcal{N}(l) \setminus \Omega} \mu_{\widehat{C}}^{\widetilde{l},l}(K) v_{\widehat{C}^{\widetilde{l}}} - \sum_{\widetilde{l} \in \mathcal{N}(l)} \mu_{\widehat{C}}^{l,\widetilde{l}}(K) v_{\widehat{C}^l}, \\
\dot{v}_{T^l} &= -r \min(v_{C^l}, v_{T^l}) + s' v_{\widehat{T}^l} + \sum_{\widetilde{l} \in \mathcal{N}(l) \setminus \Omega} \mu_T^{\widetilde{l},l}(K) v_{T^{\widetilde{l}}} - \sum_{\widetilde{l} \in \mathcal{N}(l)} \mu_T^{l,\widetilde{l}}(K) v_{T^l}, \\
\dot{v}_{\widehat{T}^l} &= +r \min(v_{C^l}, v_{T^l}) - s' v_{\widehat{T}^l} + \sum_{\widetilde{l} \in \mathcal{N}(l) \setminus \Omega} \mu_{\widehat{T}}^{\widetilde{l},l}(K) v_{\widehat{T}^{\widetilde{l}}} - \sum_{\widetilde{l} \in \mathcal{N}(l)} \mu_{\widehat{T}}^{l,\widetilde{l}}(K) v_{\widehat{T}^l}, \quad (7.2)
\end{aligned}$$

for all $l \in \mathcal{R} \setminus \Omega$. Note that *none* of the $|\mathcal{B}(\mathcal{S}(\mathcal{M})) \setminus \{O\}| = (K-1)^2|\mathcal{B}(M)|$ ODEs depends on the ODE of v_O. In general, such a derivation is formally obtained through the following.

Theorem 22. *Let us fix an FPA model M, a concentration function v of $\mathcal{S}(M)$ and some $l \in \mathcal{R} \setminus \Omega$. Then, the concentration function $v_{|l}$ of M, given by $(v_{|l})_P := v_{P^l}$ for all $P \in \mathcal{B}(M)$, satisfies*

$$F(\mathcal{S}(M), v)_{P^l} = F(M, v_{|l})_P + \sum_{\widetilde{l} \in \mathcal{N}(l) \setminus \Omega} \mu_P^{\widetilde{l},l}(K) v_{P^{\widetilde{l}}} - \sum_{\widetilde{l} \in \mathcal{N}(l)} \mu_P^{l,\widetilde{l}}(K) v_{P^l}$$

for all $P \in \mathcal{B}(M)$.

Proof. We first show by induction on M that

$$r_{\alpha^l}(\mathcal{S}(M), v) = r_\alpha(M, v_{|l}) \quad \text{and} \quad \mathcal{R}_{\alpha^l}(\mathcal{S}(M), v, P^l) = \mathcal{R}_\alpha(M, v_{|l}, P)$$

for all $P \in \mathcal{B}(M)$, $\alpha \in \mathcal{A}$, $l \in \mathcal{R} \setminus \Omega$ and concentration functions v of $\mathcal{S}(M)$.

- $M = P_0$: The claim follows by

$$r_{\alpha^l}\big(\mathcal{S}(P_0), v\big) = \sum_{P_i \in ds(P_0)} r_\alpha(P_i) v_{P_i^l} = r_\alpha(P_0, v_{|l}), \tag{7.3}$$

$$\mathcal{R}_{\alpha^l}\big(\mathcal{S}(P_0), v, P^l\big) = r_\alpha(P) v_{P^l} = \mathcal{R}_\alpha(P_0, v_{|l}, P). \tag{7.4}$$

- $M = M_0 \underset{L}{\bowtie} M_1$: We assume without loss of generality that $P \in \mathcal{B}(M_0)$, which yields also $P^l \in \mathcal{B}(\mathcal{S}(M_0))$. Let us first consider the case $\alpha \in L$. Then, together with $\alpha^l \in \mathcal{S}(L)$, we infer

$$\begin{aligned} r_{\alpha^l}(\mathcal{S}(M_0 \underset{L}{\bowtie} M_1), v) &= \min\big(r_{\alpha^l}(\mathcal{S}(M_0), v), r_{\alpha^l}(\mathcal{S}(M_1), v)\big) \\ &\overset{\text{I.H.}}{=} \min\big(r_\alpha(M_0, v_{|l}), r_\alpha(M_1, v_{|l})\big) = r_\alpha(M_0 \underset{L}{\bowtie} M_1, v_{|l}) \end{aligned}$$

and

$$\begin{aligned} \mathcal{R}_{\alpha^l}\big(\mathcal{S}(M_0 \underset{L}{\bowtie} M_1), v, P^l\big) &= \frac{\mathcal{R}_{\alpha^l}\big(\mathcal{S}(M_0), v, P^l\big)}{r_{\alpha^l}(\mathcal{S}(M_0), v)} r_{\alpha^l}\big(\mathcal{S}(M_0 \underset{L}{\bowtie} M_1), v\big) \\ &\overset{\text{I.H.}}{=} \frac{\mathcal{R}_\alpha(M_0, v_{|l}, P)}{r_\alpha(M_0, v_{|l})} r_\alpha(M_0 \underset{L}{\bowtie} M_1, v_{|l}) \\ &= \mathcal{R}_\alpha(M_0 \underset{L}{\bowtie} M_1, v_{|l}, P). \end{aligned}$$

If $\alpha \notin L$, it holds that $\alpha^l \notin \mathcal{S}(L)$, yielding

$$\begin{aligned} r_{\alpha^l}(\mathcal{S}(M_0 \underset{L}{\bowtie} M_1), v) &= r_{\alpha^l}(\mathcal{S}(M_0), v) + r_{\alpha^l}(\mathcal{S}(M_1), v) \\ &\overset{\text{I.H.}}{=} r_\alpha(M_0, v_{|l}) + r_\alpha(M_1, v_{|l}) = r_\alpha(M_0 \underset{L}{\bowtie} M_1, v_{|l}) \end{aligned}$$

and

$$\begin{aligned} \mathcal{R}_{\alpha^l}\big(\mathcal{S}(M_0 \underset{L}{\bowtie} M_1), v, P^l\big) &= \mathcal{R}_{\alpha^l}\big(\mathcal{S}(M_0), v, P^l\big) \\ &\overset{\text{I.H.}}{=} \mathcal{R}_\alpha(M_0, v_{|l}, P) = \mathcal{R}_\alpha(M_0 \underset{L}{\bowtie} M_1, v_{|l}, P). \end{aligned}$$

Equipped with the auxiliary result, we are in a position to prove the actual claim. For this, let us fix the unique $Q \in \mathcal{G}(M)$ such that $P \in ds(Q)$. Then it holds that

$$\begin{aligned}
F(\mathcal{S}(M), v)_{P^l} &= \sum_{\alpha \in \mathcal{A}^+} \Big(\sum_{P' \in \mathcal{B}(\mathcal{S}(M))} p_\alpha(P', P^l) \mathcal{R}_\alpha(\mathcal{S}(M), v, P') \\
&\qquad\qquad - \mathcal{R}_\alpha(\mathcal{S}(M), v, P^l) \Big) \\
&= \sum_{\alpha \in \mathcal{A}} \Big(\sum_{\tilde{P} \in ds(Q)} p_{\alpha^l}(\tilde{P}^l, P^l) \mathcal{R}_{\alpha^l}(\mathcal{S}(M), v, \tilde{P}^l) - \mathcal{R}_{\alpha^l}(\mathcal{S}(M), v, P^l) \Big) \\
&\qquad + \sum_{\widetilde{l} \in \mathcal{N}(l) \setminus \Omega} p_\delta(P^{\widetilde{l}}, P^l) \mathcal{R}_\delta(\mathcal{S}(M), v, P^{\widetilde{l}}) - \mathcal{R}_\delta(\mathcal{S}(M), v, P^l) \\
&= \sum_{\alpha \in \mathcal{A}} \Big(\sum_{\tilde{P} \in ds(Q)} p_\alpha(\tilde{P}, P) \mathcal{R}_\alpha(M, v_{|l}, \tilde{P}) - \mathcal{R}_\alpha(M, v_{|l}, P) \Big) \\
&\qquad + \sum_{\widetilde{l} \in \mathcal{N}(l) \setminus \Omega} \mu_P^{\widetilde{l},l}(K) v_{P^{\widetilde{l}}} - \sum_{\widetilde{l} \in \mathcal{N}(l)} \mu_P^{l,\widetilde{l}}(K) v_{P^l} \\
&= F(M, v_{|l})_P + \sum_{\widetilde{l} \in \mathcal{N}(l) \setminus \Omega} \mu_P^{\widetilde{l},l}(K) v_{P^{\widetilde{l}}} - \sum_{\widetilde{l} \in \mathcal{N}(l)} \mu_P^{l,\widetilde{l}}(K) v_{P^l}.
\end{aligned}$$

□

Informally, Theorem 22 says that each ODE in $\mathcal{S}(M)$ has two contributions. The first contribution is a *reactive* part $F(M, v_{|l})_P$, which corresponds to the behaviour of the model M. The *diffusive* part, instead, is due to the migration across regions. As in the example (7.2), the ODE of the absorbing state O is not coupled to the ODEs of $\mathcal{B}(\mathcal{S}(M)) \setminus \{O\}$. This allows one to ignore $\dot{v}_O$ altogether.

7.2 Underlying PDE System

A direct consequence of Theorem 22 is that the ODE system of an FPA model M over $\mathcal{R}$ has $|\mathcal{B}(M)|(K-1)^2 + 1$ equations, meaning that the analysis becomes computationally more difficult with larger K. Now, similarly to the fluid semantics where one wants to make the analysis independent from N, in this case we wish to study the conditions under which the analysis of $\mathcal{S}(M)$ is also independent from K. Intuitively, we would like to make space *continuous* by sending K to infinity. Continuing with the analogy with the fluid model where certain scaling conditions for the transition rates are to be satisfied, a suitable scaling of the rates needs to be found also with respect to K. In addition, unlike the ODE case, we need to make assumptions on the initial concentration function for $\mathcal{S}(M)$, in particular how it scales with K.

Overall, we make three assumptions, which we discuss in detail next.

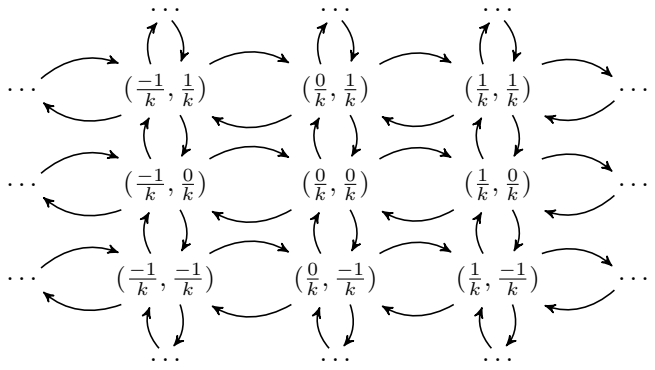

Figure 7.1: Continuous-time random walk $(W_k(t))_{t\geq 0}$ on the lattice $\frac{1}{k}\mathbb{Z} \times \frac{1}{k}\mathbb{Z}$. The rate of each transition is $r_k/4$ and was suppressed to enhance readability. In particular, the average sojourn time in each state is $1/r_k$.

Assumption 1: Unbiased Random Walk. We assume that each sequential component is subjected to an *unbiased random walk*, i.e., it may migrate with equal likelihood to any of its neighbours. More formally, we require that

$$\mu_P^{l,\widetilde{l}}(K) = \mu_P(K), \quad \text{for all} \quad P \in \mathcal{B}(M), \quad l \in \mathcal{R} \setminus \Omega \quad \text{and} \quad \widetilde{l} \in \mathcal{N}(l). \tag{7.5}$$

Notice, however, that our assumption still allows distinct sequential components to perform migrations with different rates.

Assumption 2: Scaling of $\mu_P(K)$. Since a migration activity covers the distance $1/K$ in our lattice $\mathcal{R}$ in the unit square, each $\mu_P(K)$ should scale with K in a reasonable way. To motivate our forthcoming scaling, let us consider an unbiased random walk in the two-dimensional unbounded grid $\frac{1}{k}\mathbb{Z} \times \frac{1}{k}\mathbb{Z}$, where each migration covers the distance $1/k$ and the sojourn time at each state is exponentially distributed with mean $1/r_k$. The corresponding CTMC $(W_k(t))_{t\geq 0}$ is illustrated in Figure 7.1 and enjoys the following property.

Proposition 4. *Let us assume that $W_k(0) = (0,0)$ and denote by $d_k(t) := \|W_k(t)\|$ the Euclidian distance of $W_k(t)$ from the origin after time t. Then, it holds that*

$$\mathbb{E}(d_k(t)^2) = \left(\frac{r_k}{k^2}\right) t, \qquad \textit{for all} \quad k \geq 1 \quad \textit{and} \quad t \geq 0,$$

where $\mathbb{E}(\cdot)$ denotes the expectation value.

Proof. We give a proof which relies on the uniformisation method for CTMCs with countable state spaces [78, Ch. 8, Sec. 2.1]. Let $(\widehat{W}_k(n))_{n\geq 0}$ denote the unbiased random walk in *discrete* time on $\frac{1}{k}\mathbb{Z} \times \frac{1}{k}\mathbb{Z}$ with $\widehat{W}_k(0) = (0,0)$ and let $(N(t))_{t\geq 0}$ be the homogenous Poisson process with intensity r_k. Further,

let Π denote the transition matrix of $(\widehat{W}_k(n))_{n\geq 0}$. Then it holds that $W_k(t) = \widehat{W}_k(N(t))$ and

$$\begin{aligned}
\mathbb{E}(d_k^2(t)) &= \sum_{(x,y)\in\mathbb{Z}^2} \mathbb{P}\Big\{W_k(t) = \Big(\frac{x}{k},\frac{y}{k}\Big)\Big\}\Big[\Big(\frac{x}{k}\Big)^2 + \Big(\frac{y}{k}\Big)^2\Big] \\
&= \frac{1}{k^2}\sum_{(x,y)\in\mathbb{Z}^2}\Bigg(\sum_{n=0}^{\infty}\vec{e}^{\,T}_{\left(\frac{0}{k},\frac{0}{k}\right)}\Pi^n\frac{(r_k t)^n}{n!}e^{-r_k t}\Bigg)\vec{e}_{\left(\frac{x}{k},\frac{y}{k}\right)}\big(x^2+y^2\big) \\
&= \frac{1}{k^2}e^{-r_k t}\sum_{n=0}^{\infty}\frac{(r_k t)^n}{n!}\Bigg(\sum_{(x,y)\in\mathbb{Z}^2}\vec{e}^{\,T}_{\left(\frac{0}{k},\frac{0}{k}\right)}\Pi^n\vec{e}_{\left(\frac{x}{k},\frac{y}{k}\right)}\big(x^2+y^2\big)\Bigg) \\
&= \frac{1}{k^2}e^{-r_k t}\sum_{n=0}^{\infty}\frac{(r_k t)^n}{n!}\mathbb{E}\big(\|\widehat{W}_k(n)\|^2\big) \\
&= \frac{1}{k^2}e^{-r_k t}\sum_{n=0}^{\infty}\frac{(r_k t)^n}{n!}n \\
&= \frac{1}{k^2}e^{-r_k t}r_k t\sum_{n=1}^{\infty}\frac{(r_k t)^{n-1}}{(n-1)!} \\
&= \Big(\frac{r_k}{k^2}\Big)t.
\end{aligned}$$

□

Notice that if $r_k = k^2 r_1$ for all $k \geq 1$, Proposition 4 yields

$$\mathbb{E}(d_k(t)^2) = \mathbb{E}(d_1(t)^2), \qquad \text{for all} \quad k \geq 1 \quad \text{and} \quad t \geq 0.$$

The above relation states that if each migration of the process covers a distance of $1/k$, then the migration rate should be $k^2 r_1$, in order for the random walk to always cover *the same distance* on average independently of k.

Thus, we define the scaling of the migration rates as

$$\mu_P(K) = \mu_P K^2, \qquad \text{for all} \quad P \in \mathcal{B}(M), \tag{7.6}$$

where μ_P denotes some nonnegative constant.

Before continuing our discussion, we extend each concentration function v of $\mathcal{S}(M)$ by zero concentrations at the boundary Ω.

Definition 37. *Let M be an FPA model. In the following, any concentration function v of $\mathcal{S}(M)$ is extended by the values $v_{P^l} := 0$, where $P \in \mathcal{B}(M)$ and $l \in \Omega$.*

For instance, using the above definition and assumption (7.6), the first ODE

of (7.2) can be re-written to

$$\begin{aligned}\dot{v}_{C^l} &= -r\min(v_{C^l}, v_{T^l}) + s v_{\widehat{C}^l} + \sum_{\widetilde{l}\in\mathcal{N}(l)\setminus\Omega} \mu_C(K) v_{C^{\widetilde{l}}} - \sum_{\widetilde{l}\in\mathcal{N}(l)} \mu_C(K) v_{C^l} \\ &= -r\min(v_{C^l}, v_{T^l}) + s v_{\widehat{C}^l} + \sum_{\widetilde{l}\in\mathcal{N}(l)} \Big(\mu_C(K) v_{C^{\widetilde{l}}} - \mu_C(K) v_{C^l}\Big).\end{aligned}$$

Thus, by defining $\mathbb{1}(l) := \mathbb{1}_{\mathcal{R}\setminus\Omega}(l)$,[2] the ODE system (7.2) can be stated as

$$\begin{aligned}\dot{v}_{C^l} &= \mathbb{1}(l)\big(-r\min(v_{C^l}, v_{T^l}) + s v_{\widehat{C}^l} + \mu_C \triangle^d v_{C^l}\big) \\ \dot{v}_{\widehat{C}^l} &= \mathbb{1}(l)\big(+r\min(v_{C^l}, v_{T^l}) - s v_{\widehat{C}^l} + \mu_{\widehat{C}} \triangle^d v_{\widehat{C}^l}\big) \\ \dot{v}_{T^l} &= \mathbb{1}(l)\big(-r\min(v_{C^l}, v_{T^l}) + s' v_{\widehat{T}^l} + \mu_T \triangle^d v_{T^l}\big) \\ \dot{v}_{\widehat{T}^l} &= \mathbb{1}(l)\big(+r\min(v_{C^l}, v_{T^l}) - s' v_{\widehat{T}^l} + \mu_{\widehat{T}} \triangle^d v_{\widehat{T}^l}\big)\end{aligned}$$

for all $l \in \mathcal{R}$, where $\triangle^d v_{P^l} := \sum_{\widetilde{l}\in\mathcal{N}(l)} \left(\frac{v_{P^{\widetilde{l}}} - v_{P^l}}{(1/K)^2}\right)$. Crucially, given that $l \in \mathcal{R}\setminus\Omega$, $\triangle^d v_{P^l}$ denotes the *discrete* Laplace operator [3] thanks to Definition 37.

Our PDE approximation consists in assuming that, for sufficiently large K, the discrete Laplace operator can be approximated by the continuous one. With respect to our running example, this yields the PDE system

$$\begin{aligned}\partial_t \omega_C &= -r\min(\omega_C, \omega_T) + s\omega_{\widehat{C}} + \mu_C \triangle \omega_C \\ \partial_t \omega_{\widehat{C}} &= +r\min(\omega_C, \omega_T) - s\omega_{\widehat{C}} + \mu_{\widehat{C}} \triangle \omega_{\widehat{C}} \\ \partial_t \omega_T &= -r\min(\omega_C, \omega_T) + s'\omega_{\widehat{T}} + \mu_T \triangle \omega_T \\ \partial_t \omega_{\widehat{T}} &= +r\min(\omega_C, \omega_T) - s'\omega_{\widehat{T}} + \mu_{\widehat{T}} \triangle \omega_{\widehat{T}}\end{aligned} \tag{7.7}$$

subject to the (zero) Dirichlet boundary conditions (DBCs)

$$\omega_P(0, y, t) = \omega_P(1, y, t) = \omega_P(x, 0, t) = \omega_P(x, 1, t) = 0, \quad x, y \in [0; 1], t \geq 0,$$

where $\omega_P : [0; 1]^2 \times [0; \infty) \to \mathbb{R}_{\geq 0}$, and $\triangle = \partial_{xx} + \partial_{yy}$ denotes the *continuous* Laplace operator on $[0; 1]^2$. This is well-known in the literature as a *reaction-diffusion* PDE system, to highlight the two aforementioned contributions to the time-derivative of ω_P [73].

Thanks to Theorem 22, the above discussion carries over to the general case. To see this, we observe that

$$\begin{aligned}F(\mathcal{S}(M), v)_{P^l} &= F(M, v_{|l})_P + \sum_{\widetilde{l}\in\mathcal{N}(l)\setminus\Omega} \mu_P^{\widetilde{l},l}(K) v_{P^{\widetilde{l}}} - \sum_{\widetilde{l}\in\mathcal{N}(l)} \mu_P^{l,\widetilde{l}}(K) v_{P^l} \\ &= F(M, v_{|l})_P + \sum_{\widetilde{l}\in\mathcal{N}(l)} \Big(\mu_P(K) v_{P^{\widetilde{l}}} - \mu_P(K) v_{P^l}\Big)\end{aligned}$$

[2] $\mathbb{1}_A$ denotes the indicator function.

[3] The (two-dimensional) Laplace operator $\Delta(f) = \partial_{xx} f + \partial_{yy} f$ arises in physics.

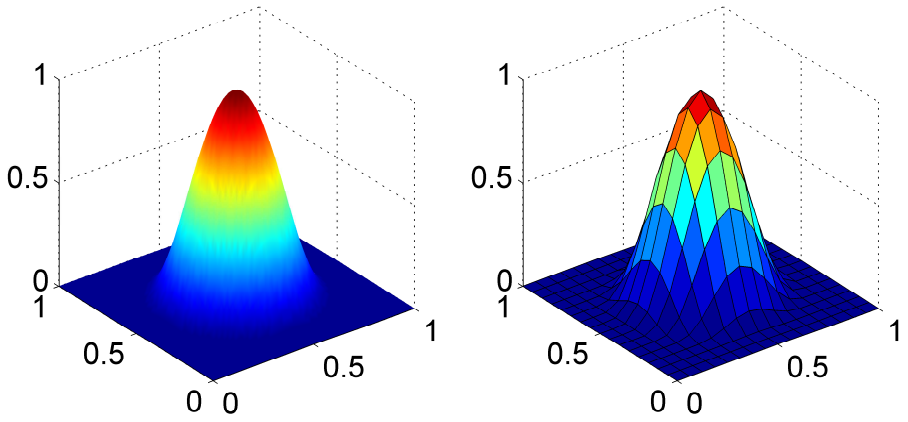

Figure 7.2: The shape of ω_C^0 and its discretisation in the case of $K = 16$.

$$\begin{aligned} &= F(M, v_{|l})_P + \frac{\mu_P(K)}{K^2} \sum_{\widetilde{l} \in \mathcal{N}(l)} \frac{v_{P^{\widetilde{l}}} - v_{P^l}}{(1/K)^2} \\ &= F(M, v_{|l})_P + \mu_P \triangle^d v_{P^l}, \end{aligned}$$

where $P \in \mathcal{B}(M)$ and $l \in \mathcal{R} \setminus \Omega$. This yields the ODE system

$$\dot{v}_{P^l} = \mathbb{1}(l)\big(F(M, v_{|l})_P + \mu_P \triangle^d v_{P^l}\big), \qquad P \in \mathcal{B}(M),\ l \in \mathcal{R}. \tag{7.8}$$

Assumption 3: Initial Conditions. Before being able to formulate the underlying PDE system, the corresponding initial conditions have to be studied carefully. Indeed, whilst in the ODE interpretation (7.8) of our spatial FPA no restriction is needed, the PDE approximation can only make sense if the initial concentration functions $v(0)$ converge, as a family of functions dependent on K, to a *differentiable* function on $[0;1]^2$ as $K \to \infty$. Thus, we fix continuously partially differentiable functions $\omega_P^0 : [0;1]^2 \to \mathbb{R}$, where $P \in \mathcal{B}(M)$, and define the initial concentrations as

$$\begin{aligned} v(0)_{P^{(x,y)}} &:= \omega_P^0(x,y), \qquad P \in \mathcal{B}(M), \quad (x,y) \in \mathcal{R}, \\ v(0)_O &:= 0 \end{aligned} \tag{7.9}$$

For instance, let us consider $\mathcal{S}(C)$ with the initial PDE conditions

$$\begin{aligned} \omega_C^0(x,y) &= \begin{cases} 0 & ,\|(x,y) - (\frac{1}{2},\frac{1}{2})\|^2 \geq \frac{1}{4} \\ \frac{\exp(4)}{\exp\left(1/(\frac{1}{4} - \|(x,y)-(\frac{1}{2},\frac{1}{2})\|^2)\right)} & ,\text{otherwise} \end{cases} \\ \omega_{\hat{C}}^0(x,y) &= 0. \end{aligned}$$

Then, for a fixed $K \geq 1$, the underlying initial ODE conditions (7.9) are discretisations of those functions, as can be seen in Figure 7.2, where the shapes of

$\omega_C^0 : [0;1]^2 \to \mathbb{R}_{\geq 0}$ and its discretisation in the case of $K = 16$ are shown. Since $\mathcal{S}(C)$ is an FPA model, the sequence of the underlying CTMCs is constructed from the initial ODE conditions as in the case of any other FPA model, cf. Theorem 5.

The combination of the three assumptions leads to the following.

Definition 38 (Reaction-Diffusion PDE)**.** *Let us fix an FPA model M and suppose that requirements (7.5), (7.6) and (7.9) are satisfied for $\mathcal{S}(M)$. Then, the underlying PDE system of $\mathcal{S}(M)$ is*

$$\partial_t \omega_P = \mu_P \triangle \omega_P + F(M, \vec{\omega})_P, \quad P \in \mathcal{B}(M). \tag{7.10}$$

The initial conditions are given by the functions $\omega_P^0 : [0;1]^2 \to \mathbb{R}_{\geq 0}$, whereas the boundary conditions are of Dirichlet type, i.e.

$$\omega_P(0, y, t) = \omega_P(1, y, t) = \omega_P(x, 0, t) = \omega_P(x, 1, t) = 0, \tag{7.11}$$

where $P \in \mathcal{B}(M)$, $x, y \in [0;1]$ and $t \geq 0$.

Similarly to Theorem 5 which establishes the convergence of $\frac{1}{N}(\mathbb{V}_N(t))_{t\geq 0}$ to (7.8) as K is fixed and $N \to \infty$, the next crucial section states that $\frac{1}{N}(\mathbb{V}_N(t))_{t\geq 0}$ converges in probability to (7.10) as $K, N \to \infty$.

7.3 Proof of Convergence

We start by recalling that the function

$$\mathbb{R}^{|\mathcal{B}(M)|} \to \mathbb{R}^{|\mathcal{B}(M)|}, \quad \vec{v} \mapsto F\big(M, \vec{v}\big)$$

is globally Lipschitz, cf. proof of Theorem 5. Since linear functions are globally Lipschitz as well, this shows that the ODE system (7.8) is globally Lipschitz. Thus, the global version of Picard-Lindelöf's theorem asserts that (7.8) subject to (7.9) has a unique solution v in $\mathbb{R}^{|\mathcal{B}(M)|(K-1)^2}$ with time domain $(-\infty; +\infty)$. Moreover, for an arbitrary but fixed $T > 0$, it can be shown [79] that the Euler sequence given by

$$\begin{aligned} v^0_{P(x,y)} &:= \omega^0_P(x, y) \\ v^{m+1}_{P(x,y)} &:= v^m_{P(x,y)} + \Delta t \cdot \mathbb{1}(x, y) \cdot \big(F(M, v^m_{|(x,y)})_P + \mu_P \triangle^d v^m_{P(x,y)}\big), \end{aligned} \tag{7.12}$$

where $P \in \mathcal{B}(M)$, $(x, y) \in \mathcal{R}$ and $\Delta t := T/\mathfrak{M}$ for an arbitrary but fixed $\mathfrak{M} \geq 1$, converges to v, as $\mathfrak{M} \to \infty$. More formally, it holds that

$$\forall K \geq 1.\ \exists C > 0.\ \forall \mathfrak{M} \geq 1.\ \Big(\max_{0 \leq m \leq \mathfrak{M}} \max_{\substack{(x,y)\in\mathcal{R}, \\ P \in \mathcal{B}(M)}} |v_{P(x,y)}(m\Delta t) - v^m_{P(x,y)}| \leq C\Delta t \Big). \tag{7.13}$$

The key observation is now that the Euler sequence (7.12) can be interpreted as a *finite difference scheme* [80] of the PDE system (7.10). Thus, we first prove

that (7.12) converges to the solution of the PDE system (7.10), as $\Delta s, \Delta t \to 0$. Recalling that (7.12) satisfies at the same time (7.13), this shows, in essence, that the sequence given in (7.12) solves the ODE and PDE systems *at the same time*. This and the fact that the family of CTMCs converges to the ODE system in probability, cf. Theorem 5, yields then the main result.

The remainder of this section consists of two theorems which realise the sketched proof strategy. We start by showing that the sequence (7.12) converges to the solution of the PDE system (7.10).

Theorem 23. *Let us assume that the functions $\vec{\omega} = (\omega_P)_{P\in\mathcal{B}(M)}$ describe on $[0;1]^2 \times [0;T]$, where $T > 0$ is arbitrary but fixed, the unique solution of (7.10) subjected to the DBCs (7.11) on $[0;1]^2 \times [0;T]$. Further, assume that*

$$\partial_{txx}\omega_P,\ \partial_{xxxx}\omega_P,\ \partial_{yxx}\omega_P,\ \partial_{tyy}\omega_P,\ \partial_{xyy}\omega_P,\ \partial_{yyyy}\omega_P, \quad P \in \mathcal{B}(M),$$

exist and are continuous. For $\mathfrak{M} \geq 1$, define $\Delta t := T/\mathfrak{M}$, $\mathfrak{q}_P := \mu_P \Delta t/\Delta s^2$ and assume that $\mathfrak{M}$ is large enough such that $\mathfrak{q}_P \leq 1/4$ for all $P \in \mathcal{B}(M)$.

Then, the Euler sequence (7.12) interpreted as a finite difference scheme of (7.10) subjected to the DBCs (7.11) converges uniformly on $[0;T]$ in the supremum norm, meaning that

$$\max_{0\leq m\leq \mathfrak{M}}\ \max_{(x,y)\in\mathcal{R},\ P\in\mathcal{B}(M)} |\omega_P(x,y,m\Delta t) - v^m_{P^{(x,y)}}| \to 0, \qquad \Delta s, \Delta t \to 0.$$

Proof. The proof uses elements from the convergence proof of the Euler method from [79] and the usual convergence proof of the heat equation [80]. Let us define

$$\triangle^d \omega_P(x,y,t) := \sum_{(\tilde{x},\tilde{y})\in\mathcal{N}(x,y)} \frac{\omega_P(\tilde{x},\tilde{y},t) - \omega_P(x,y,t)}{\Delta s^2}$$

for all $P \in \mathcal{B}(M)$, $(x,y,t) \in \mathcal{R}\setminus\Omega \times [0;T-\Delta t]$. That is, $\triangle^d\omega_P(x,y,t)$ is the approximated (i.e., discretised) version of $\triangle\omega_P(x,y,t)$. Recall that a vector in $\mathbb{R}^\nu$ is formally defined as a function from $\{1,\ldots,\nu\}$ to $\mathbb{R}$. Thus, for any $(x,y,t) \in \mathcal{R}\times[0;T]$, the vector

$$\vec{\omega}(x,y,t) = (\omega(x,y,t))_{P\in\mathcal{B}(M)}$$

is a function from $\mathcal{B}(M)$ to $\mathbb{R}$ and the statement $F(M,\vec{\omega}(x,y,t))$ is well-defined. Using this, we define the space step error and the time step error of the scheme at $(x,y,t) \in \mathcal{R}\setminus\Omega\times[0;T-\Delta t]$ by

$$\begin{aligned}
\rho_P(x,y,t) &:= \mu_P\triangle\omega_P(x,y,t) - \mu_P\triangle^d\omega_P(x,y,t)\\
\eta_P(x,y,t) &:= \omega_P(x,y,t+\Delta t) - \omega_P(x,y,t)\\
&\qquad - \Delta t\big(\mu_P\triangle\omega_P(x,y,t) + F(M,\vec{\omega}(x,y,t))_P\big),
\end{aligned}$$

respectively.

We begin by bounding the space step error. A well-known fact in numerical analysis [81, Section 6.2, Equation 5] is that a four times continuously differentiable function $f : [a; b] \to \mathbb{R}$ yields, for all $x \in (a; b)$ and $h > 0$ such that $[x - h; x + h] \subseteq [a; b]$, the existence of an $x' \in [x - h; x + h]$ with

$$\partial_{xx} f(x) = \frac{f(x-h) - 2f(x) + f(x+h)}{h^2} - h^2 \frac{\partial_{xxxx} f(x')}{12}.$$

Thus, we can fix a region $(x, y) \in \mathcal{R} \setminus \Omega$ and note that there exist $x' \in (x - \Delta s; x + \Delta s)$ and $y' \in (y - \Delta s; y + \Delta s)$ such that

$$\begin{aligned}
\frac{\rho_P(x,y,t)}{\mu_P} &= \partial_{xx}\omega_P(x,y,t) + \partial_{yy}\omega_P(x,y,t) \\
&\quad - \Bigg(\frac{\omega_P(x+\Delta s,y,t) - 2\omega_P(x,y,t) + \omega_P(x-\Delta s,y,t)}{\Delta s^2} \\
&\quad + \frac{\omega_P(x,y+\Delta s,t) - 2\omega_P(x,y,t) + \omega_P(x,y-\Delta s,t)}{\Delta s^2} \Bigg) \\
&= \frac{\partial_{xxxx}\omega_P(x',y,t)}{12}\Delta s^2 + \frac{\partial_{yyyy}\omega_P(x,y',t)}{12}\Delta s^2.
\end{aligned}$$

Consequently, there exists a $C_1 \in \mathbb{R}_{\geq 0}$ which *does not depend* on $\Delta t, \Delta s$ and satisfies $|\rho_P(x, y, t)| \leq C_1 \Delta s^2$ for all $(x, y) \in \mathcal{R} \setminus \Omega$, $0 \leq t \leq T$ and $P \in \mathcal{B}(M)$.

We now turn to the time step error. Applying the mean value theorem to $t \mapsto \omega_P(x, y, t)$ allows us to infer the existence of a $t \leq t' \leq t + \Delta t$ such that $\omega_P(x, y, t + \Delta t) - \omega_P(x, y, t) = \partial_t \omega_P(x, y, t')\Delta t$. Hence

$$\begin{aligned}
\eta_P(x,y,t) &= \omega_P(x,y,t+\Delta t) - \omega_P(x,y,t) \\
&\qquad - \Delta t\big(\mu_P \triangle \omega_P(x,y,t) + F(M,\vec{\omega}(x,y,t))_P\big) \\
&= \Delta t\big(\partial_t \omega_P(x,y,t') - \mu_P \triangle \omega_P(x,y,t) - F(M,\vec{\omega}(x,y,t))_P\big) \\
&= \Delta t\Big(\mu_P \triangle \omega_P(x,y,t') + F(M,\vec{\omega}(x,y,t'))_P \\
&\qquad - \mu_P \triangle \omega_P(x,y,t) - F(M,\vec{\omega}(x,y,t))_P\Big).
\end{aligned}$$

Let $\Lambda' > 0$ refer to the Lipschitz constant of all $\mu_P \triangle \omega_P$ on $[0; 1]^2 \times [0; T]$, with $P \in \mathcal{B}(M)$, and $\Lambda > 0$ be the *global* Lipschitz constant of

$$\mathbb{R}^{|\mathcal{B}(M)|} \to \mathbb{R}^{|\mathcal{B}(M)|}, \quad \vec{v} \mapsto F\big(M, \vec{v}\big).$$

Then the above calculation yields

$$\begin{aligned}
\frac{|\eta_P(x,y,t)|}{\Delta t} &\leq \Lambda \|\vec{\omega}(x,y,t') - \vec{\omega}(x,y,t)\|_\infty + \Lambda' \|(x,y,t') - (x,y,t)\|_\infty \\
&\leq \Lambda \|\vec{\omega}(x,y,t') - \vec{\omega}(x,y,t)\|_\infty + \Lambda' \Delta t \\
&\leq \Lambda \Delta t \max_{Q \in \mathcal{B}(M)} \max_{(x,y,t) \in [0;1]^2 \times [0;T]} |\partial_t \omega_Q(x,y,t)| + \Lambda' \Delta t,
\end{aligned}$$

where the last inequality follows again by means of the mean value theorem. Hence, there exists a $C_2 \in \mathbb{R}_{\geq 0}$ which *does not depend* on $\Delta t, \Delta s$ and satisfies $|\eta_P(x,y,t)| \leq C_2 \Delta t^2$ for all $(x,y) \in \mathcal{R}$, $0 \leq t \leq T - \Delta t$ and $P \in \mathcal{B}(M)$.

We proceed by noting that

$$\begin{aligned}\eta_P(x,y,t) = \omega_P(x,y,t+\Delta t) - \omega_P(x,y,t) \\ - \Delta t\big(\mu_P \triangle^d \omega_P(x,y,t) + \rho_P(x,y,t) + F(M,\vec{\omega}(x,y,t))_P\big)\end{aligned}$$

is equivalent to

$$\begin{aligned}\omega_P(x,y,t+\Delta t) = \omega_P(x,y,t) + \Delta t\Big(\mu_P \triangle^d \omega_P(x,y,t) \\ + F(M,\vec{\omega}(x,y,t))_P\Big) + \Delta t \rho_P(x,y,t) + \eta_P(x,y,t).\end{aligned}$$

Consequently, together with $t_m := m\Delta t$ and $e^m_{P^{(x,y)}} := \omega_P(x,y,t_m) - v^m_{P^{(x,y)}}$ it holds that

$$\begin{aligned}|e^{m+1}_{P^{(x,y)}}| &\leq \Big|(1 - |\mathcal{N}(x,y)|\mathfrak{q}_P) e^m_{P^{(x,y)}} + \mathfrak{q}_P \sum_{(\tilde{x},\tilde{y}) \in \mathcal{N}(x,y)} e^m_{P^{(\tilde{x},\tilde{y})}} \\ &\qquad + \Delta t\Big(F(M,\vec{\omega}(x,y,t_m))_P - F(M, v^m_{|(x,y)})_P\Big) \\ &\qquad + \Delta t \rho_P(x,y,t_m) + \eta_P(x,y,t_m)\Big| \\ &\leq \|\vec{e}^m\|_\infty + \Delta t \Lambda \|\vec{e}^m\|_\infty + \Delta t C_1 \Delta s^2 + C_2 \Delta t^2\end{aligned}$$

for all $0 \leq m \leq \mathfrak{M} - 1$ and $(x,y) \in \mathcal{R} \setminus \Omega$, thanks to $\mathfrak{q}_P \leq 1/4$. Noting that $e^{m+1}_{P^{(x,y)}} = 0$ for all $(x,y) \in \Omega$ because of the DBCs, we conclude that the estimation

$$|e^{m+1}_{P^{(x,y)}}| \leq (1 + \Delta t \Lambda)\|\vec{e}^m\|_\infty + \Delta t C_1 \Delta s^2 + C_2 \Delta t^2$$

holds for all $(x,y) \in \mathcal{R}$. Together with $C_3 := \max\{C_1, C_2\}$, this yields

$$\begin{aligned}\|\vec{e}^m\|_\infty &\leq (1 + \Delta t\Lambda)^m \|\vec{e}^0\|_\infty + C_3(\Delta t \Delta s^2 + \Delta t^2) \sum_{k=0}^{m-1} (1 + \Delta t \Lambda)^k \\ &\leq (1 + \Delta t\Lambda)^m \|\vec{e}^0\|_\infty + C_3(\Delta t \Delta s^2 + \Delta t^2) \frac{(1 + \Delta t\Lambda)^m - 1}{\Delta t \Lambda} \\ &\leq e^{m\Delta t \Lambda} \|\vec{e}^0\|_\infty + C_3(\Delta s^2 + \Delta t) \frac{e^{m\Delta t\Lambda} - 1}{\Lambda} \\ &\leq e^{T\Lambda} \|\vec{e}^0\|_\infty + C_3(\Delta s^2 + \Delta t) \frac{e^{T\Lambda} - 1}{\Lambda} \\ &= 0 + \frac{e^{T\Lambda} - 1}{\Lambda / C_3}(\Delta s^2 + \Delta t)\end{aligned}$$

for all $0 \leq m \leq \mathfrak{M}$. This shows the claim. □

As mentioned before, Theorem 5 and Theorem 23 can now be used to show that the CTMC sequence converges in probability to the solution of the PDE system (7.10) subjected to the DBCs (7.11) on $[0;1]^2 \times [0;T]$.

Theorem 24. *Let us assume that the functions $\vec{\omega} = (\omega_P)_{P\in\mathcal{B}(M)}$ describe on $[0;1]^2 \times [0;T]$, where $T > 0$ is arbitrary but fixed, the unique solution of (7.10) subjected to the DBCs (7.11) on $[0;1]^2 \times [0;T]$. Further, assume that*

$$\partial_{txx}\omega_P,\ \partial_{xxxx}\omega_P,\ \partial_{yxx}\omega_P,\ \partial_{tyy}\omega_P,\ \partial_{xyy}\omega_P,\ \partial_{yyyy}\omega_P, \quad P \in \mathcal{B}(M),$$

exist and are continuous. Then, for each $\varepsilon > 0$ it holds that

$$\lim_{K\to\infty}\lim_{N\to\infty}\mathbb{P}\left\{\sup_{0\le t\le T}\max_{(x,y)\in\mathcal{R},P\in\mathcal{B}(M)}\left|\frac{1}{N}(\mathbb{V}_N(t))_{P^{(x,y)}} - \omega_P(x,y,t)\right| > \varepsilon\right\} = 0,$$

where $(\mathbb{V}_N(t))_{t\ge 0}$ is as in Theorem 5.

Proof. In the following, we use the auxiliary results from the proof of Theorem 23. Define $C_1' := \frac{e^{T\Lambda}-1}{\Lambda/C_3}$ and fix a K such that $C_1'\Delta s^2 < \varepsilon/12$. The uniform continuity of v on $[0;T]$ implies the existence of a $\delta_1 > 0$ such that

$$\forall P \in \mathcal{B}(M).\ \forall (x,y) \in \mathcal{R}.\ \forall t,t' \in [0;T].\\ |t-t'| < \delta_1 \Rightarrow |v_{P^{(x,y)}}(t) - v_{P^{(x,y)}}(t')| < \frac{\varepsilon}{12}.$$

Similarly, thanks to the uniform continuity of $\vec{\omega}$ on $[0;1]^2 \times [0;T]$, there exists a $\delta_2 > 0$ such that

$$\forall P \in \mathcal{B}(M).\ \forall (x,y) \in [0;1]^2.\ \forall t,t' \in [0;T].\\ |t-t'| < \delta_2 \Rightarrow |\omega_P(x,y,t) - \omega_P(x,y,t')| < \frac{\varepsilon}{12}.$$

Moreover, by [79] there exists a $C_2' > 0$ such that

$$\max_{0\le m\le\mathfrak{M}}\max_{(x,y)\in\mathcal{R},1\le l\le L}|v_{P^{(x,y)}}(t_m) - v^m_{P^{(x,y)}}| \le C_2'\Delta t.$$

In the following, let us fix an $\mathfrak{M}$ such that

$$\Delta t = \frac{T}{\mathfrak{M}} < \min\left\{\delta_1, \delta_2, \frac{\varepsilon}{4(C_1'+C_2')}\right\}.$$

Then, for an arbitrary $t \in [0;T]$ and an $0 \le m \le \mathfrak{M}$ such that $|t - t_m| < \Delta t$, it holds that

$$\begin{aligned}|v_{P^{(x,y)}}(t) - \omega_P(x,y,t)| &\le |v_{P^{(x,y)}}(t) - v_{P^{(x,y)}}(t_m)| + |v_{P^{(x,y)}}(t_m) - v^m_{P^{(x,y)}}|\\ &\quad + |v^m_{P^{(x,y)}} - \omega_P(x,y,t_m)| + |\omega_P(x,y,t_m) - \omega_P(x,y,t)|\\ &\le \varepsilon/12 + C_2'\Delta t + C_1'(\Delta s^2 + \Delta t) + \varepsilon/12\\ &\le \varepsilon/4 + (C_1'+C_2')\Delta t\\ &\le \varepsilon/2\end{aligned}$$

for all $(x,y) \in \mathcal{R}$ and $P \in \mathcal{B}(M)$. Together with

$$\phi_1 := \sup_{0\leq t\leq T} \max_{(x,y)\in\mathcal{R},P\in\mathcal{B}(M)} \left| \frac{1}{N}(\mathbb{V}_N(t))_{P^{(x,y)}} - \omega_P(x,y,t) \right|,$$
$$\phi_2 := \sup_{0\leq t\leq T} \max_{(x,y)\in\mathcal{R},P\in\mathcal{B}(M)} \left| \frac{1}{N}(\mathbb{V}_N(t))_{P^{(x,y)}} - v_{P^{(x,y)}}(t) \right|,$$
$$\phi_3 := \sup_{0\leq t\leq T} \max_{(x,y)\in\mathcal{R},P\in\mathcal{B}(M)} \left| v_{P^{(x,y)}}(t) - \omega_P(x,y,t) \right|,$$

we infer that $\mathbb{P}\{\phi_1 > \varepsilon\} \leq \mathbb{P}\{\phi_2 + \phi_3 > \varepsilon\} \leq \mathbb{P}\{\phi_2 > \varepsilon/2 \ \vee \ \phi_3 > \varepsilon/2\} \leq \mathbb{P}\{\phi_2 > \varepsilon/2\} + \mathbb{P}\{\phi_3 > \varepsilon/2\}$. Since the choice of K from above implies that $\phi_3 \leq \varepsilon/2$, it holds that $\mathbb{P}\{\phi_3 > \varepsilon/2\} = 0$. Consequently, the equality of norms on a finite dimensional vector space and Theorem 5 yield the claim. □

7.4 Numerical Example

In this section we provide numerical confirmation of the convergence to the reaction-diffusion PDE by analysing (7.1) for the exec rate $r = 2.0$, reset rate $s = 0.5$ and io rate $s' = 0.1$. We performed tests with diffusion coefficients $\mu_C = \mu_{\widehat{C}} = \mu_T = \mu_{\widehat{T}} = \mu = 0.01$ and the initial conditions

$$\omega^0_C(x,y) = \omega^0_T(x,y) = \begin{cases} 0 & , \ \|(x,y) - (\frac{1}{2},\frac{1}{2})\|^2 \geq \frac{1}{4} \\ \frac{\exp(4)}{\exp\left(1/(\frac{1}{4} - \|(x,y)-(\frac{1}{2},\frac{1}{2})\|^2)\right)} & , \ \text{otherwise} \end{cases}$$
$$\omega^0_{\widehat{C}}(x,y) = \omega^0_{\widehat{T}}(x,y) = 0.$$

For this, we implemented the sequence (7.12) in Matlab, where, for each K, the time step Δt was set to $\Delta s^2/(8\mu)$ in order to satisfy the condition from Theorem 23 (recall that $\Delta s = 1/K$). The comparison metric was defined to be the average ratio $C/(C+\widehat{C})$ at $t = 0.50$s across the whole spatial domain. The observation time $t = 0.50$s was chosen arbitrarily, but in such a way that the numerical solution was sufficiently away from the initial condition, cf. Figure 7.3. Using this setup, K was increased until the distance between two consecutive solutions fell below the margin of 1e-4, cf. Table 7.1. The above results suggest that already moderate K lead to a stabilisation of numerical results.

7.5 Related Work

Spatial Stochastic Framework The spatial aggregation presented in this chapter can be encoded in the stochastic spatial framework [82]. There, we consider $L \geq 1$ types of sequential components, $A_1, \ldots, A_L$, which perform a random walk on the lattice $\mathcal{R}$ with rate $\mu_1(K), \ldots, \mu_L(K)$, respectively, where $\mu_l(K) = \mu_l \cdot K^2$ for some constant $\mu_l \geq 0$. In addition to migration actions, sequential components may perform local actions within the current region. In contrast to the theory presented in this chapter, local actions are given there

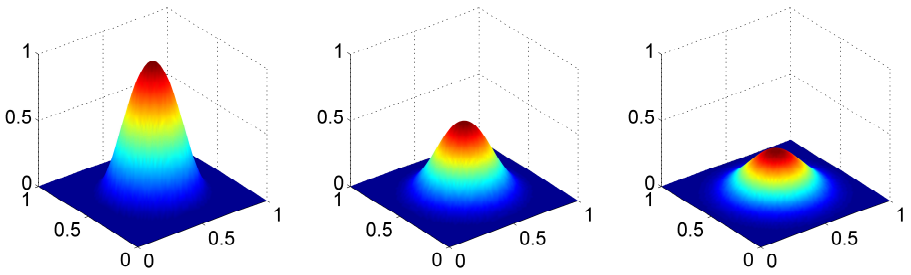

Figure 7.3: Numerical solutions for the concentration of C-processes for K=64 at t=0.00s, t=0.25s and t=0.50s.

K	*Solution*	*Distance to K - 32*	*Avg. Runtime*
32	0.439943	—	0.07s
64	0.443798	3.86 1e-3	0.57s
96	0.444528	7.30 1e-4	2.51s
128	0.444781	2.53 1e-4	8.10s
160	0.444899	1.18 1e-4	20.05s
192	0.444963	6.41 1e-5	42.10s

Table 7.1: The average ratio $C/(C+\widehat{C})$ at time $t = 0.50$s across the whole spatial domain. The calculations were performed on a single core machine with 2.21 GHz.

in the rather general notation of chemical reactions [83]. For instance, by identifying C^l, $\widehat{C}^l$, T^l, $\widehat{T}^l$ with A_1^l, A_2^l, A_3^l, A_4^l, respectively, the local actions of $\mathcal{S}(C \underset{\{exec\}}{\bowtie} T)$ in $l \in \mathcal{R} \setminus \Omega$ are captured by the rules

$$
\begin{aligned}
1: \quad & A_1^l + A_3^l \xrightarrow{F_1(A_1^l, A_3^l)} A_2^l + A_4^l, && F_1(A_1^l, A_3^l) = r \cdot \min(A_1^l, A_3^l), \\
2: \quad & A_2^l \xrightarrow{F_2(A_2^l)} A_1^l, && F_2(A_2^l) = s \cdot A_2^l, \\
3: \quad & A_4^l \xrightarrow{F_3(A_4^l)} A_3^l, && F_3(A_4^l) = s' \cdot A_4^l,
\end{aligned}
$$

whereas the migration is covered by setting $\mu_1 := \mu_C$, $\mu_2 := \mu_{\widehat{C}}$, $\mu_3 := \mu_T$ and $\mu_4 := \mu_{\widehat{T}}$.

Crucially, Theorem 23 and 24 can be shown to hold true [82] in the following, more general setting. First, we require that for each local reaction function F_j there are continuous functions $f_j : \mathbb{R}^{L+P} \to \mathbb{R}$ and $g_j : \mathbb{R}^{L+P} \to \mathbb{R}_{\geq 0}$ such that

$$
\begin{aligned}
F_j\big(Na_1, \ldots, Na_L, b_1, \ldots, b_P\big)/N = \\
= f_j\big(a_1, \ldots, a_L, b_1, \ldots, b_P\big) + \mathcal{O}\left(g_j(a_1, \ldots, a_L, b_1, \ldots, b_P)/N\right),
\end{aligned}
$$

meaning that the underlying CTMC is, in essence, density dependent. The numbers $b_1^l, \ldots, b_P^l$, where $P \geq 0$, are fixed region parameters. This implies that local actions may depend on local concentrations *and* local parameters. Second, we require that for all $\vec{z}_0 \in \mathbb{R}^{L+P}$ there exist an open neighbourhood $\mathfrak{O}$ of $\vec{z}_0$ and a $C \in \mathbb{R}_{\geq 0}$ such that

$$\left|f_j(\vec{z}_2) - f_j(\vec{z}_1)\right| \leq C\|\vec{z}_2 - \vec{z}_1\|, \qquad \forall \vec{z}_1, \vec{z}_2 \in \mathfrak{O}.$$

Since the above condition states that the function has to be *locally* Lipschitz, it is possible to describe synchronisation in terms of minima *and* polynomials. For instance, in the above example one could use $F_1(A_1^l, A_3^l) = r \cdot \frac{1}{N} \cdot A_1^l \cdot A_3^l$, which would yield an ODE system which obeys the law of mass action [73, 74].

Although being technically a special case of [82], the benefit of the theory presented in this chapter is that it allows one to define local actions from a macroscopic view. Specifically, it is possible to describe complex systems in a compositional way.

Reaction-diffusion PDEs PDEs of reaction-diffusion type are very well understood in many disciplines, such as biology [73], ecology [84], and chemistry [85]. It is beyond the scope of this thesis to provide a general overview of the literature. Instead, we focus on related work that, similarly to ours, considers PDEs as the macroscopic deterministic behaviour of a stochastic process.

In physical chemistry, one such approach is to consider the so-called *reaction-diffusion master equation*, which corresponds to the forward equations of a CTMC that models a network of biochemical reactions occurring at discrete sites, and molecular transitions across sites [86, 87]. Although the stochastic model corresponds to ours, the relationship with the PDE model is established by means of a procedure that *closes* the equations for the average populations obtained by summing across the forward equations and approximating the expected value of a function of random variables with the function of their expectations. Instead, we use a more rigourous limiting procedure in the sense of Kurtz, which also has the practical advantage of hinting at the population scaling to use for increasing the accuracy of the deterministic estimates, as confirmed by the numerical results presented in Section 7.4. The closest approach to ours is found in [88], which was subsequently worked upon in a series of papers [89, 90, 91, 92]. Their stochastic models are, however, different, in that the local reaction rates model only birth and death, i.e. interactions between multiple types of agents are not possible. Further, the convergence of the stochastic models to a system of PDEs is shown *directly*, i.e. without considering the correspondence between the fluid limit at each region and the finite difference scheme for the PDE. This suggests that our approach, which, in essence, translates a problem from the area of stochastic processes to a problem from the area of numerical analysis, reduces the underlying mathematical complexity.

Mobility models There is a substantial amount of work on mobility models, both at the analytical level and experimentally through traces. In this paragraph

we overview the literature that is most closely related to our approach based on the random walk model; for an extensive discussion, we refer to the survey [93].

Owing to its analytical tractability, the random walk model has been extensively studied in networking research. A discrete-time Markovian model was developed in [94] for the comparative evaluation of update strategies in cellular networks. The paper considers a mobility model where a node is characterised by states that determine the direction of movement. In this respect our approach is analogous, since agent types may have different movement rates. However, the results of their analysis are presented for a one-dimensional topology (over a ring) and cannot be lifted to more general local interactions; on the other hand, their mobility model is anisotropic. Unbiased random walks are instead proposed in [95] and [45] to study movements across cellular networks, and to study routing protocols [96, 97] and performance characteristics in ad hoc networks [98]. In all cases, mobility is not coupled with a model of interaction between nodes. Random walk is also used in [99] as the basic mobility model by which the authors arrive at a reaction-diffusion type equation for information propagation in ad hoc networks; their analysis is carried out at the deterministic/macroscopic level without considering a limiting regime of a counterpart microscopic/stochastic process. Instead, the PDEs used in [100] are interpreted as the deterministic limit of the empirical measure of node concentrations, by appealing to the strong law of large numbers.

Chapter 8

Conclusion

The fluid techniques developed over the past few years for high-level performance modelling techniques such as process algebra have mostly considered the case of large numbers of replicas of independent components characterised by small local state spaces. The resulting approximating mathematical object, usually a system of ordinary differential equations, has been taken as the culminating point of a line of reasoning which provides a shift from a discrete-state stochastic description to a continuous-state deterministic view whilst maintaining a well-founded relationship between the two. In this thesis we have taken the fluid approximation of a PEPA model as the starting point of an argumentation that has led to observing a rapid growth of the size of such an ODE system whenever of replication was lifted from sequential components to composite processes or spatial heterogeneity was present. We have argued that there are indeed situations of interest which call for such a form of modelling, for instance distributed computer systems or mobility models. We devised two techniques which allow for an efficient analysis in both cases.

We first introduced the technique of fluid lumpability which allows one to aggregate the ODE system belonging to a model with replication patterns into another ODE system whose size is independent from all the multiplicities of the process replicas in the model, but only depends on the local state-space sizes of the constituent sequential components. Interestingly enough, we have noted in passing that there are models which are not equivalent in terms of the common stochastic notions of behavioural equivalence but whose fluid approximations can be exactly related thanks to the notion of fluid lumpability. Similarly to near and quasi lumpability, which account for small perturbations in the transition matrix of a CTMC, we have defined the notion of fluid ε-lumpability which allows for small perturbations ε in the parameters of an ODE system. By exploiting the semantics of PEPA, we were able to derive a bound for the difference between the solutions of perturbed and original ODE systems which is *linear* in ε, allowing therefore for an analysis of almost fluid lumpable ODE systems.

To cope with the growth of ODE system size in the presence of spatial

heterogeneity, we devised a technique which applies whenever the sequential processes of a given PEPA model may perform, among local actions, a random walk on a two-dimensional lattice. We proved that the ODE system, whose size is directly proportional to the size of the lattice, converges, as the size of the lattice tends to infinity, to a spatial reaction-diffusion PDE limit of constant size. By doing so, we were able to provide an efficient analysis of large-scale mobile systems in continuous space.

Those ideas can be extended in several directions. For instance, the currently used *a-priori* error estimation in fluid ε-lumpability is rooted in Gronwall's inequality which accounts, in essence, for the worst case scenario. However, if the fluid model can be expressed by means of a kernel expansion, the *a-posteriori* error estimation can be applied, yielding much tighter bounds [101, 102].

Also, one may investigate whether models whose fluid approximations are exactly related but which fail to be equivalent with respect to common behavioural equivalences, can be related in terms of stochastic orders [103]. For instance, while the fluid approximations of the PEPA models from Section 4.3

$$M_1 := \left(C \underset{\{exec\}}{\bowtie} T\right) \underset{\emptyset}{\bowtie} \left(C \underset{\{exec\}}{\bowtie} T\right) \underset{\{io\}}{\bowtie} U \qquad M_2 := \left(C \parallel C\right) \underset{\{exec\}}{\bowtie} \left(T \parallel T\right) \underset{\{io\}}{\bowtie} U$$

are exactly related, they cannot be associated to each other by means of stochastic equivalences. Informally, this is because M_2 is capable of answering any action performed by M_1, while the converse is not true. Since this means that M_2 has, intuitively, a higher cooperation potential than M_1, a stochastic notion of inequality rather than stochastic equivalence may relate both models.

The spatial aggregation technique, on the other hand, can be extended by adding deterministic drifts. With drift rates being dependent on the current state of the agent, this would allow one to describe spatial patterns of higher complexity. For instance, one could incorporate a scenario where agents first undergo some "exploratory phase" by means of random walk. Upon locating some target, however, they wish to return to a known base station, for instance to rest/recharge. Crucially, since the location of the base station is known, the agents use a deterministic drift for their way back. One could also think of studying spatial behaviour on unbounded domains, e.g. the whole plane, or to consider reflective, instead of absorbing, boundary conditions.

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Appendix A

Proofs

A.1 Proof of Theorem 5

We start with a formal definition of the CTMC $(\mathbb{V}(t))_{t\geq 0}$.

Definition 39. *In the sequel, the following notions will be used.*

- *For all $\alpha \in \mathcal{A}$ and PEPA models G, G', let us denote by $q_\alpha(G, G')$ the sum of the rates of all α-transitions from G to G' which are induced by the PEPA semantics.*
- *Fix an FPA model M and a population function V of M. Two models $G', G'' \in ds(M_V)$ are groupwise equivalent, $G' \simeq_{M,V} G''$, if $\mathcal{C}(G', P) = \mathcal{C}(G'', P)$ for all $P \in \mathcal{B}(M)$.*

Arguing as in [17], one shows that $\simeq_{M,V}$ is an equivalence relation on $ds(M_V)$ and that

$$q_\alpha(G', E) := \sum_{G \in E} q_\alpha(G', G) = \sum_{G \in E} q_\alpha(G'', G) =: q_\alpha(G'', E)$$

for all $\alpha \in \mathcal{A}$, $E \in ds(M_V)/\simeq_{M,V}$ and $G', G'' \in ds(M_V)$ with $G' \simeq_{M,V} G''$. Also, it can be shown that $q_\alpha(G, [G]) = q_\alpha(G, G)$ for all $G \in ds(M_V)$. This yields the following.

Proposition 5. *Fix a FPA model M and a population function V of M. Together with $ds_l(M_V) := ds(M_V)/\simeq_{M,V}$, the set*

$$\mathcal{T}_l(M_V) := \left\{ \left([G], (\alpha, q_\alpha(G, [G'])), [G'] \right) \;\middle|\; [G], [G'] \in ds_l(M_V) \wedge \alpha \in \mathcal{A} \right\}$$

is well-defined. Let $(X(t))_{t\geq 0}$ and $(E(t))_{t\geq 0}$ denote the CTMCs induced by the derivation graphs $dg(M_V)$ and $(ds_l(M_V), \mathcal{T}_l(M_V))$, respectively. Then, $ds_l(M_V)$ is an ordinarily lumpable partition of $(X(t))_{t\geq 0}$ and the corresponding lumped CTMC is $(E(t))_{t\geq 0}$.

This allows us to define the following.

Definition 40. *Using the same variables as in Proposition 5, $(E(t))_{t\geq 0}$ induces $(\mathbb{V}(t))_{t\geq 0}$ by setting $(\mathbb{V}(t))_P := \mathcal{C}(G(t), P)$, where $P \in \mathcal{B}(M)$ and $G(t)$ is an arbitrary representative of $E(t)$.*

The auxiliary result stated below is needed for the proof of Theorem 5.

Lemma 12. *The underlying ODE system $\dot{v} = F(M, v)$ of a FPA model M is globally Lipschitz on $\mathbb{R}^{|\mathcal{B}(M)|}$. Moreover, for any nonnegative initial condition $v(0)$, it has a unique solution v in $\mathbb{R}^{|\mathcal{B}(M)|}$ such that its time domain contains $[0; \infty)$ and $\|v(0)\|_1 = \|v(s)\|_1$ for all $0 \leq s < \infty$.*

Proof. We cope with negative numbers by considering the ODE field $F(M, |\cdot|)$. Then, Lemma B.1 from [54] shows that $F(M, |\cdot|)$ is globally Lipschitz. Further, the global version of Picard-Lindelöf asserts that there exists a unique solution v in $\mathbb{R}^{|\mathcal{B}(M)|}$ with time domain $(-\infty; +\infty)$. To see the last claim, we first show using structural induction

i) For all $P \in \mathcal{B}(M)$ there exists a nonnegative function ρ such that $\dot{v}_P \geq -v_P \cdot \rho(v)$.

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, the proof is complete. □

We can state now the proof of Theorem 5.

Theorem 5. We first exploit Lemma 12. Let v denote the unique solution of $\dot{v} = F(M, v)$ in $\mathbb{R}^{|\mathcal{B}(M)|}$ subjected to $v(0)$. Since the time domain of v contains $[0; T]$, it holds that $c := \max_{0\leq t\leq T} \|v(t)\| + 1 < \infty$.

Let us denote by $E_N \subseteq \mathbb{R}^{|\mathcal{B}(M)|}$ the state space of $\left(\frac{1}{N}\mathbb{V}_N(t)\right)_{t\geq 0}$ subjected to the initial state $\lfloor Nv(0)\rfloor/N$. For a $\mathbb{v} \in E_N$, let $\lambda_N(\mathbb{v})$ denote the exit time distribution in state $\mathbb{v}$, meaning that

$$\mathbb{P}\Big\{\tau(\mathbb{v}) > t \;\Big|\; \frac{1}{N}\mathbb{V}_N(0) = \mathbb{v}\Big\} = e^{-\lambda_N(\mathbb{v})t}$$

with

$$\tau(\mathbb{v}) := \inf\Big\{t \geq 0 \;\Big|\; \frac{1}{N}\mathbb{V}_N(t) \neq \mathbb{v}\Big\}.$$

For every set Γ in the Borel σ-algebra of E_N, $\mathcal{B}(E_N)$, we define further the jump distribution in $\mathbb{v}$ as

$$\mu_N(\mathbb{v}, \Gamma) := \mathbb{P}\Big\{\frac{1}{N}\mathbb{V}_N(\tau(\mathbb{v})) \in \Gamma \;\Big|\; \frac{1}{N}\mathbb{V}_N(0) = \mathbb{v}\Big\}.$$

Theorem 2.15 in [17] shows that the sum of all transitions of $\mathbb{V}_N(t)$ which change the number of P's, $\Phi(\mathbb{V}_N(t))_P$, is

$$\begin{aligned}
&\sum_{\alpha\in\mathcal{A}}\Big(\sum_{P'\in\mathcal{B}(M)\setminus\{P\}} p_\alpha(P',P)\mathcal{R}_\alpha(M,\mathbb{V}_N(t),P') - \sum_{P'\in\mathcal{B}(M)\setminus\{P\}} p_\alpha(P,P')\mathcal{R}_\alpha(M,\mathbb{V}_N(t),P)\Big)\\
&=\sum_{\alpha\in\mathcal{A}}\Big(\sum_{P'\in\mathcal{B}(M)} p_\alpha(P',P)\mathcal{R}_\alpha(M,\mathbb{V}_N(t),P') - \sum_{P'\in\mathcal{B}(M)} p_\alpha(P,P')\mathcal{R}_\alpha(M,\mathbb{V}_N(t),P)\Big)\\
&=\sum_{\alpha\in\mathcal{A}}\Big(\sum_{P'\in\mathcal{B}(M)} p_\alpha(P',P)\mathcal{R}_\alpha(M,\mathbb{V}_N(t),P') - \mathcal{R}_\alpha(M,\mathbb{V}_N(t),P)\Big),
\end{aligned}$$

where the last equality sign is due to $\sum_{P'\in\mathcal{B}(M)} p_\alpha(P,P') = 1$. This yields

$$F(M,\mathbb{v}) = \frac{1}{N}\Phi(N\mathbb{v}) = \lambda_N(\mathbb{v})\int_{\mathbb{w}\in E_N}(\mathbb{w}-\mathbb{v})\mu_N(\mathbb{v},d\mathbb{w}).$$

Moreover, it holds that

$$E_N \cap \Big\{\mathbb{v}\in\mathbb{R}^{|\mathcal{B}(M)|} \;\Big|\; \inf_{0\le t\le T}\|\mathbb{v}-v(t)\| \le \frac{1}{2}\Big\} \subseteq E.$$

Together with $\Gamma_N := E_N \cap E$, it holds that

$$\sup_{N\ge 1}\sup_{\mathbb{v}\in\Gamma_N}\lambda_N(\mathbb{v})\int_{\mathbb{w}\in E_N}\|\mathbb{w}-\mathbb{v}\|\mu_N(\mathbb{v},d\mathbb{w}) < \infty.$$

To see this, we first notice that

$$\begin{aligned}
\lambda_N(\mathbb{v})\int_{\mathbb{w}\in E_N}\|\mathbb{w}-\mathbb{v}\|\mu_N(\mathbb{v},d\mathbb{w}) &\le \sqrt{|\mathcal{B}(M)|}\int_{\mathbb{w}\in E_N}\|\mathbb{w}-\mathbb{v}\|_\infty\lambda_N(\mathbb{v})\mu_N(\mathbb{v},d\mathbb{w})\\
&\le \sqrt{|\mathcal{B}(M)|}\frac{1}{N}\int_{\mathbb{w}\in E_N}\lambda_N(\mathbb{v})\mu_N(\mathbb{v},d\mathbb{w})\\
&= \sqrt{|\mathcal{B}(M)|}\frac{\lambda_N(\mathbb{v})}{N}.
\end{aligned}$$

Since the sum of the rates of all outgoing transitions of $\mathbb{V}_N(t)$ is bounded by

$$\sum_{P\in\mathcal{B}(M)}\sum_{\alpha\in\mathcal{A}}\mathcal{R}_\alpha(M,\mathbb{V}_N(t),P)$$

and

$$\sum_{P\in\mathcal{B}(M)}\sum_{\alpha\in\mathcal{A}}\frac{\mathcal{R}_\alpha(M,\mathbb{V}_N(t),P)}{N} = \sum_{P\in\mathcal{B}(M)}\sum_{\alpha\in\mathcal{A}}\mathcal{R}_\alpha\Big(M,\frac{\mathbb{V}_N(t)}{N},P\Big) =: \Theta\Big(M,\frac{\mathbb{V}_N(t)}{N}\Big),$$

we conclude that

$$\lambda_N(\mathbb{v})\int_{\mathbb{w}\in E_N}\|\mathbb{w}-\mathbb{v}\|\mu_N(\mathbb{v},d\mathbb{w}) \le \sqrt{|\mathcal{B}(M)|}\Theta(M,\mathbb{v}).$$

Moreover, for all $N \geq 1$, it holds that

$$\sup_{\mathbb{v} \in \Gamma_N} \lambda_N(\mathbb{v}) \int_{\|\mathbb{w}-\mathbb{v}\|>\varepsilon_N} \|\mathbb{w}-\mathbb{v}\| \mu_N(\mathbb{v}, d\mathbb{w}) = 0, \qquad \varepsilon_N := \frac{\sqrt{|\mathcal{B}(M)}}{N},$$

because $\varepsilon_N < \|\mathbb{w}-\mathbb{v}\| \leq \sqrt{|\mathcal{B}(M)|}\|\mathbb{w}-\mathbb{v}\|_\infty$ implies $\frac{1}{N} < \|\mathbb{w}-\mathbb{v}\|_\infty$. The claim follows then from Theorem 2.11 in [53]. □

A.2 Proof of Theorem 8

Proof. Let us assume that $\vec{P}^i \sim_{\mathfrak{P}} \vec{P}^j$ is established by the bijections σ_k, $1 \leq k \leq K$, where $K := K_i = K_j$. We will show that the same bijections establish $\vec{P}^i \sim_{\mathfrak{P}^+} \vec{P}^j$. For this, we assume that $\alpha \in L$, since the case $\alpha \notin L$ is easy. Property *ii*) follows then with

$$\begin{aligned} r_\alpha(M \underset{L}{\bowtie} M_0, v) &= \min\big(r_\alpha(M, v), r_\alpha(M_0, v)\big) = \min\big(r_\alpha(M, v^\sigma), r_\alpha(M_0, v^\sigma)\big) \\ &= r_\alpha(M \underset{L}{\bowtie} M_0, v^\sigma) \end{aligned}$$

Then, for any $P \in \mathcal{B}(M \underset{L}{\bowtie} M_0) \setminus \bigcup\{ds(P_k^l) \mid l \in \{i,j\} \wedge 1 \leq k \leq K\}$ and

$$\mathcal{M} := \begin{cases} M & , \ P \in \mathcal{G}(M) \\ M_0 & , \ P \in \mathcal{G}(M_0) \end{cases}$$

it holds that

$$\begin{aligned} \mathcal{R}_\alpha(M \underset{L}{\bowtie} M_0, v, P) &= \mathcal{R}_\alpha(\mathcal{M}, v, P) \frac{\min(r_\alpha(M, v), r_\alpha(M_0, v))}{r_\alpha(\mathcal{M}, v)} \\ &= \mathcal{R}_\alpha(\mathcal{M}, v, P) \frac{\min(r_\alpha(M, v^\sigma), r_\alpha(M_0, v^\sigma))}{r_\alpha(\mathcal{M}, v^\sigma)} \\ &= \mathcal{R}_\alpha(\mathcal{M}, v^\sigma, P) \frac{\min(r_\alpha(M, v^\sigma), r_\alpha(M_0, v^\sigma))}{r_\alpha(\mathcal{M}, v^\sigma)} \\ &= \mathcal{R}_\alpha(M \underset{L}{\bowtie} M_0, v^\sigma, P). \end{aligned}$$

For $P \in ds(P_k^i)$, where $1 \leq k \leq K$, instead, we infer that

$$\begin{aligned} \mathcal{R}_\alpha(M \underset{L}{\bowtie} M_0, v, P) &= \mathcal{R}_\alpha(M, v, P) \frac{\min(r_\alpha(M, v), r_\alpha(M_0, v))}{r_\alpha(M, v)} \\ &= \mathcal{R}_\alpha(M, v, P) \frac{\min(r_\alpha(M, v^\sigma), r_\alpha(M_0, v^\sigma))}{r_\alpha(M, v^\sigma)} \\ &= \mathcal{R}_\alpha(M, v^\sigma, \sigma_k(P)) \frac{\min(r_\alpha(M, v^\sigma), r_\alpha(M_0, v^\sigma))}{r_\alpha(M, v^\sigma)} \\ &= \mathcal{R}_\alpha(M \underset{L}{\bowtie} M_0, v^\sigma, \sigma_k(P)) \end{aligned}$$

and

$$\begin{aligned}
\sum_{P'} p_\alpha(P',P)\mathcal{R}_\alpha(M \underset{L}{\rtimes} M_0, v, P') &= \\
&= \sum_{P'} p_\alpha(P',P)\mathcal{R}_\alpha(M, v, P')\frac{\min(r_\alpha(M,v), r_\alpha(M_0,v))}{r_\alpha(M,v)} \\
&= \sum_{P'} p_\alpha(P',P)\mathcal{R}_\alpha(M, v, P')\frac{\min(r_\alpha(M,v^\sigma), r_\alpha(M_0,v^\sigma))}{r_\alpha(M,v^\sigma)} \\
&= \sum_{P'} p_\alpha(P',\sigma_k(P))\mathcal{R}_\alpha(M, v^\sigma, P')\frac{\min(r_\alpha(M,v^\sigma), r_\alpha(M_0,v^\sigma))}{r_\alpha(M,v^\sigma)} \\
&= \sum_{P'} p_\alpha(P',\sigma_k(P))\mathcal{R}_\alpha(M \underset{L}{\rtimes} M_0, v^\sigma, P').
\end{aligned}$$

Next, we show that $\sim_{\mathfrak{P}}$ is an equivalence relation on $\mathcal{P}$. The reflexivity $\vec{P}^i \sim_{\mathfrak{P}} \vec{P}^i$ is established by the identity functions on $ds(P^i_k)$, $1 \le k \le K$, and the symmetry by σ_k^{-1}, $1 \le k \le K$, where $\sigma_k : ds(P^i_k) \to ds(P^j_k)$, $1 \le k \le K$, establish $\vec{P}^i \sim_{\mathfrak{P}} \vec{P}^j$. For the proof of transitivity, let us fix $\vec{P}^i, \vec{P}^j, \vec{P}^\nu \in \mathcal{P}$ with $\vec{P}^i \sim_{\mathfrak{P}} \vec{P}^j$ and $\vec{P}^j \sim_{\mathfrak{P}} \vec{P}^\nu$. Clearly, it holds that $\vec{P}^i, \vec{P}^j, \vec{P}^\nu \in \mathfrak{p}$ for some $\mathfrak{p} \in \mathfrak{P}$.

We assume that $\vec{P}^i, \vec{P}^j, \vec{P}^\nu$ are pairwise different, for the other cases are trivial, and that

$$\sigma^i_k : ds(P^i_k) \to ds(P^j_k), \quad \sigma^j_k : ds(P^j_k) \to ds(P^\nu_k), \quad 1 \le k \le K$$

establish $\vec{P}^i \sim_{\mathfrak{P}} \vec{P}^j$, $\vec{P}^j \sim_{\mathfrak{P}} \vec{P}^\nu$, respectively. Using $\sigma^{\mu_1} \circ \sigma^{\mu_2} := (\sigma_1^{\mu_1} \circ \sigma_1^{\mu_2}, \dots$ $\dots, \sigma_K^{\mu_1} \circ \sigma_K^{\mu_2})$, we first observe that

$$\begin{aligned}
r_\alpha(M,v) = r_\alpha(M, v^{\sigma^i}) = r_\alpha\big(M, (v^{\sigma^i})^{\sigma^j}\big) = r_\alpha\big(M, ((v^{\sigma^i})^{\sigma^j})^{\sigma^i}\big) \\
= r_\alpha\big(M, v^{\sigma^j \circ \sigma^i}\big).
\end{aligned}$$

Then, for all $P \in \mathcal{B}(M) \setminus \bigcup\{ds(P^l_k) \mid l \in \{i,j,\nu\} \wedge 1 \le k \le K\}$, it holds that

$$\begin{aligned}
\mathcal{R}_\alpha(M,v,P) = \mathcal{R}_\alpha(M, v^{\sigma^i}, P) = \mathcal{R}_\alpha(M, (v^{\sigma^i})^{\sigma^j}, P) \\
= \mathcal{R}_\alpha(M, ((v^{\sigma^i})^{\sigma^j})^{\sigma^i}, P) = \mathcal{R}_\alpha(M, v^{\sigma^j \circ \sigma^i}, P).
\end{aligned}$$

Similarly, for all $P \in ds(P^j_k)$, it holds that

$$\begin{aligned}
\mathcal{R}_\alpha(M,v,P) = \mathcal{R}_\alpha(M, v^{\sigma^i}, (\sigma^i_k)^{-1}(P)) = \mathcal{R}_\alpha(M, (v^{\sigma^i})^{\sigma^j}, (\sigma^i_k)^{-1}(P)) \\
= \mathcal{R}_\alpha(M, ((v^{\sigma^i})^{\sigma^j})^{\sigma^i}, \sigma^i_k((\sigma^i_k)^{-1}(P))) = \mathcal{R}_\alpha(M, v^{\sigma^j \circ \sigma^i}, P).
\end{aligned}$$

On the other hand, we infer for all $P \in ds(P^i_k)$

$$\begin{aligned}
\mathcal{R}_\alpha(M,v,P) = \mathcal{R}_\alpha(M, v^{\sigma^i}, \sigma^i_k(P)) = \mathcal{R}_\alpha(M, (v^{\sigma^i})^{\sigma^j}, \sigma^j_k(\sigma^i_k(P))) = \\
= \mathcal{R}_\alpha(M, ((v^{\sigma^i})^{\sigma^j})^{\sigma^i}, \sigma^j_k(\sigma^i_k(P))) = \mathcal{R}_\alpha(M, v^{\sigma^j \circ \sigma^i}, (\sigma^j_k \circ \sigma^i_k)(P))
\end{aligned}$$

and

$$\begin{aligned}\sum_{P'} p_\alpha(P',P)\mathcal{R}_\alpha(M,v,P') &= \sum_{P'} p_\alpha(P',\sigma_k^i(P))\mathcal{R}_\alpha(M,v^{\sigma^i},P')\\ &= \sum_{P'} p_\alpha(P',\sigma_k^j(\sigma_k^i(P)))\mathcal{R}_\alpha(M,(v^{\sigma^i})^{\sigma^j},P')\\ &= \sum_{P'} p_\alpha(P',\sigma_k^j(\sigma_k^i(P)))\mathcal{R}_\alpha(M,((v^{\sigma^i})^{\sigma^j})^{\sigma^i},P')\\ &= \sum_{P'} p_\alpha(P',(\sigma_k^j\circ\sigma_k^i)(P))\mathcal{R}_\alpha(M,v^{\sigma^j\circ\sigma^i},P').\end{aligned}$$

Thus, $(\sigma^j\circ\sigma^i)_k : ds(P_k^i)\to ds(P_k^\nu)$, $1\le k\le K$, establishes $\vec{P}^i\sim_{\mathfrak{P}}\vec{P}^\nu$. □

A.3 Proof of Proposition 3

Proposition 3. The first claim follows from Lemma B.1 in [54]. 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 $A_1,\dots,A_I$ such that for a given $1\le\iota\le I$, 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 $D\ge 1$ and $a_1,b_1,\dots,a_n,b_n$ are apparent rates which satisfy

$$a_n(\xi,v)\ge b_n(\xi,v)\quad\wedge\quad a_n(\xi,v)\ge v_Q r_\alpha(Q)(\xi)\prod_{m=1}^{n-1}\frac{b_m(\xi,v)}{a_m(\xi,v)}$$

for all $1\le n\le D$. As $r_\alpha(Q)(\xi)=\sum_{k\in S}\xi_k$ for some set $S\subseteq\{1,\dots,|\nu(M)|\}$, 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

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

for some $S'\subseteq\{1,\dots,|\nu(M)|\}$, 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 $\mathbb{R}_{>0}^{|\nu(M)|} \setminus A_i \subseteq \cup_{\iota\neq i} A_\iota$ which converges to ξ. As $\cup_{\iota\neq i} A_\iota$ is closed, it follows that $\xi \in \cup_{\iota\neq i} A_\iota$, meaning that $\cup_{\iota\neq i} A_\iota$ 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

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

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

$$\begin{aligned} \Big|\partial_{\xi_j} F[n](\xi,v)\Big(v_Q \sum_{k\in S} \xi_k\Big)\Big| \leq{}& |\partial_{\xi_j} b_n(\xi,v)| + |\partial_{\xi_j} a_n(\xi,v)| \\ &+ \Big|\partial_{\xi_j} F[n-1](\xi,v)\Big(v_Q \sum_{k\in S} \xi_k\Big)\Big| \end{aligned}$$

and we conclude

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

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 [54]. □