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## Modeling PSA Problems—II: A Cell-to-Cell Transport Theory Approach

P. E. Labeau\*

*Université Libre de Bruxelles (CP165/84)  
Av. F.D. Roosevelt 50, B - 1050 Brussels, Belgium*

and

J. M. Izquierdo

*Consejo de Seguridad Nuclear  
Justo Dorado 11, E - 28040 Madrid, Spain*

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**Abstract**—*In the first paper of this series, we presented an extension of the classical theory of dynamic reliability in which the actual occurrence of an event causing a change in the system dynamics is possibly delayed. The concept of stimulus activation, which triggers the realization of an event after a distributed time delay, was introduced. This gives a new understanding of competing events in the sequence delineation process.*

*In the context of the level-2 probabilistic safety analysis (PSA), the information on stimulus activation mainly consists of regions of the process variables space where the activation can occur with a given probability. The evolution equations of the extended theory of probabilistic dynamics are therefore particularized to a transport process between discrete cells defined in phase-space on this basis. Doing so, an integrated and coherent approach to level-2 PSA problems is propounded. This amounts to including the stimulus concept and the associated stochastic delays discussed in the first paper in the frame of a cell-to-cell transport process.*

*In addition, this discrete model provides a theoretical basis for the definition of appropriate numerical schemes for integrated level-2 PSA applications.*

### I. INTRODUCTION

Integrating the dynamic behavior of a plant in transient conditions in the delineation of accident sequences can be a major concern in the probabilistic safety analysis (PSA) studies of nuclear power plants when hardware–software–process variable–human interaction (or any combination) is involved. Such a circumstance is often met in level-2 analyses. The theory of probabilistic dynamics<sup>1</sup> offers a framework in which the competition between events defining possible PSA headers is driven by the thermohydraulic process evolution in accident de-

velopment. This allows potentially an automatic generation of accident scenarios.<sup>2</sup> Such an approach has been successfully applied to the construction of setpoint-based event trees, characteristic of level-1 PSA studies.<sup>3</sup>

In the first paper of this series,<sup>4</sup> the assumption of instantaneous change in the system dynamics when, e.g., a setpoint is crossed has been released. This has given rise to an extended methodology in which the time to occurrence of an event is seen as the sum of two possibly random times: the time to activation of a stimulus and the elapsing of a delay. The general term of stimulus covers any situation that “triggers” an event, be it the entry in a new system configuration, the crossing of a setpoint, or the satisfaction of combustion criteria.

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\*E-mail: pelabeau@ulb.ac.be

Integral transportlike equations were derived from this assumption in two modeling cases: Either all activated stimuli are deactivated as soon as an event takes place, or some of them can remain activated in the new configuration that the system has entered after the event occurrence. In terms of stochastic processes, the first situation corresponds to a semi-Markov evolution of the branching process, where the system is regenerated at the beginning of a new branch, while the second falls under the umbrella of non-Markov modeling since the past history of the system is likely to affect its future evolution.

Yet, the mathematical problem defined in this way is highly dimensional and hardly tractable when taken to its full extent and applied to industrial cases. However, the full-scale theory developed in the companion paper<sup>4</sup> gives the basis for the deduction of a scheme adapted to the level-2 PSA constraints. The method we present in this paper is inspired by the following observation<sup>5</sup>: Large cells defined in the process variables space naturally arise in the classical PSA approach in the characterization of the undesired, damage situations, like core melt or containment rupture. Moreover, PSA practitioners are not interested in the detailed dependence on the process variables of the probability of a given undesired event but in the probability of this event occurring in specific regions of the process variables space. When considering level-2 PSA problems, stimuli are mainly associated with setpoints and events taking place within regions of the process variables space with known probabilities. The details of the stimulus activation within such regions is either irrelevant or beyond the scope of the analysis. Stimuli provide therefore a problem-related partition of phase-space in cells. The branching process in the continuous event tree, which is driven by the evolution of the continuous process variables along the accident sequence in the full-scale theory,<sup>4</sup> must now be understood in the frame of a dynamic cell-to-cell transport theory.

Before investigating this point, it should be reminded that partitioning phase-space in cells is not an innovative idea in dynamic reliability. Indeed, it was already envisioned to include setpoint-based control devices in the discrete-state Markov methodology<sup>6,7</sup> even before the theory of probabilistic dynamics was formulated. It is therefore worth examining the corresponding techniques, not in their efficiency as numerical schemes but in their ability to model properly the dynamic aspects of the problem.

Section II thus presents an overview of the pros and cons of this pioneer approach in both its time-discrete and continuous versions and raises issues related to the correctness of this discretization method. Section III is dedicated to how the partition in cells can be directly related to the definition of the stimuli and on which basis the cell-to-cell transport process should be considered. Section IV presents the discretized form of the equations

given in Ref. 4 for both semi-Markov and non-Markov cases. A practical implementation of the proposed scheme is propounded in Sec. V. Conclusions and perspectives are finally given.

## II. OVERVIEW OF CELL-TO-CELL MAPPING TECHNIQUES IN SYSTEM RELIABILITY

### II.A. Discretization of Time and Process Variables

Process control systems are an important part of most industrial systems. Yet, when trying to account for their instantaneous solicitation and action in the frame of Markovian reliability, an important problem arises: Only pointwise actions whose agenda could be fixed at the beginning of the analysis (e.g., inspection and maintenance actions at fixed epochs) can be included in a strict Markovian treatment. As for process control systems, the time of their solicitation is defined by the evolution of the process itself, in the configuration the system lies in just before reaching the control setpoint. They cannot be accounted for as such in a Markovian model.

A pioneer paper in dynamic reliability<sup>6</sup> propounded to model the dynamic behavior of the system over a time step as a transition between two cells defined in the process variables space. Doing so, hybrid states are defined by the combination of a cell and a configuration of the system components. While independently developed, this work extended the cell-to-cell mapping concept proposed in Ref. 8 to find the domains of attraction of nonlinear systems to the probabilistic analysis of systems with stochastic configurations. Transition probabilities between cells in a given configuration come from the reinterpretation of the fraction of dynamic evolutions starting from the first cell and reaching the second one after a delay equal to the time step  $\tau$  of the Markov process.

Let us summarize mathematically the main lines of the method. A partition of the safety domain  $D$  in cells  $V_m$ ,  $m = 1 \dots M$ , is first defined

$$\bigcup_{m=1}^M V_m = D, \quad V_m \cap V_n = \emptyset \text{ if } m \neq n. \quad (1)$$

Additional cells cover the outer region of  $D$  in the process variables space. They are supposed to be absorbing and are therefore called sink cells. Control setpoints should be placed at the boundaries of cells, and not inside them, for a better modeling of the corresponding transitions on demand.

The transition probability  $g_{mn}(i, \tau)$  between cells  $V_m$  and  $V_n$  in a configuration  $i$ , in which the dynamic evolution of the process variables  $\bar{x}$  is given by  $\bar{g}_i(t, \bar{x}_o)$  at time  $t$  after entering  $i$  at  $\bar{x}_o$  is written

$$g_{mn}(i, \tau) = \begin{cases} \frac{1}{m(V_m)} \int_{V_m} H_n(\bar{g}_i(\tau, \bar{x})) d\bar{x} & \text{if } V_m \in D \\ \delta_{mn} & \text{if } V_m \notin D \end{cases}, \quad (2)$$

where  $m(V_m)$  is the volume of cell  $V_m$ . Equation (2) makes use of  $H_n(\bar{x})$ , the characteristic function of cell  $V_n$ , defined by

$$H_n(\bar{x}) = \begin{cases} 1 & \text{if } \bar{x} \in V_n \\ 0 & \text{if } \bar{x} \notin V_n \end{cases}. \quad (3)$$

The integral in Eq. (2) over  $V_m$  is in practice approximated by a  $c$ -point quadrature with equal weighting. Then, if  $c'$  out of the  $c$  trajectories  $\bar{g}_i(\tau, \bar{x})$  leaving cell  $V_m$  ends up within cell  $V_n$ ,  $g_{mn}(i, \tau)$  is estimated by the ratio  $c'/c$ . A similar idea will be further explored in Sec. V.

Transitions between system configurations are supposed to occur at the end of the time step, with a probability  $h_{ij}(m \rightarrow n, \tau)$  when leaving state  $i$  for state  $j$ , while the system dynamics has moved from cell  $V_m$  to cell  $V_n$  on the time interval  $\tau$ . Therefore, the transition probability between the hybrid states  $(i, V_m)$  and  $(j, V_n)$  is written

$$\tilde{g}_{im,jn}(\tau) = g_{mn}(i, \tau) \cdot h_{ij}(m \rightarrow n, \tau). \quad (4)$$

Equation (4) defines the elements of a transition matrix  $G$ . Vector  $\bar{\pi}(t)$ , whose components are the probabilities  $\pi_{im}(t)$  to be in the different hybrid states  $(i, V_m)$ , then evolves with time according to

$$\bar{\pi}(k\tau)^T = \bar{\pi}((k-1)\tau)^T \cdot G = \bar{\pi}(0)^T \cdot G^k. \quad (5)$$

The approach sketched above thus succeeds in expressing the continuous process variables evolution by transitions between discrete cells, as the system evolution is represented by a Markov chain between hybrid states. This approach thus appears as a discretization scheme to obtain the probability distribution of the system lying in a cell and in a given configuration, but it does not allow easy identification of the scenarios leading to an undesired situation, with the possible sequence branchings being hidden in the matrix of transition probabilities between hybrid states.

### II.B. Time-Continuous Cell-to-Cell Mapping Technique

Besides the size of the discrete state-space to be handled when using a large number of cells, the discretization method summarized in Sec. II.A suffers from several other drawbacks:

- Though control setpoints are boundaries of cells, the solicitation of process control devices takes place at discrete time intervals  $k\tau$  and not at the exact time the corresponding setpoint is reached. To avoid the discrepancy between the real situation and the time discretization, small values of  $\tau$

are necessary. But, these can lead, in the estimation of the transition probabilities [see Eq. (2)], to a very small (or even nil) probability to leave some cells. Besides the numerical issue of accuracy, a modeling problem thus arises: The dynamics underlying the whole process is incorrectly represented if the size of the cells is not reduced in correspondence to the value of  $\tau$ .

- Transitions probabilities between system configurations may depend on the value of some process variables. Whether this dependence must be accounted for in  $V_m$  or in  $V_n$  in determining the probabilities  $h_{ij}(m \rightarrow n, \tau)$  is not obvious.

To tackle these two difficulties related to the discrete nature in time of Eq. (5), a time-continuous version of the cell-to-cell discretization technique was propounded.<sup>9</sup> It is based on the integration over a cell of the Chapman-Kolmogorov equation, which was deduced in Ref. 1 to model dynamic reliability problems:

$$\begin{aligned} \frac{\partial \pi(\bar{x}, i, t)}{\partial t} + \text{div}(\bar{f}_i(\bar{x})\pi(\bar{x}, i, t)) \\ = -\lambda_i(\bar{x})\pi(\bar{x}, i, t) + \sum_{j \neq i} p(j \rightarrow i|\bar{x})\pi(\bar{x}, j, t), \end{aligned} \quad (6)$$

where

$\pi(\bar{x}, i, t) d\bar{x}$  = probability to find the system in  $d\bar{x}$  about  $\bar{x}$ , in configuration  $i$  and at time  $t$

$d\bar{x}/dt = \bar{f}_i(\bar{x})$  = expression of the dynamics in  $i$  in differential form [the solution of this set of ordinary differential equations with the initial condition  $\bar{x}(0) = \bar{x}_0$  gives back  $\bar{x} = \bar{g}_i(t, \bar{x}_0)$ ]

$p(j \rightarrow i|\bar{x})$  = transition rate between  $j$  and  $i$ , given  $\bar{x}$ , with  $\lambda_i(\bar{x}) = \sum_{j \neq i} p(i \rightarrow j|\bar{x}) \equiv -p(i \rightarrow i|\bar{x})$ .

Assuming  $\pi(\bar{x}, i, t)$  is uniformly distributed on each cell, after integrating Eq. (6) on cell  $V_m$ , we obtain

$$\begin{aligned} \frac{d\pi_{im}(t)}{dt} + \oint_{S_m} \bar{f}_i(\bar{x}_s) \cdot \bar{n}(\bar{x}_s) \pi(\bar{x}_s, i, t) d\bar{x}_s \\ = \sum_j L_{ji}^c(m) \pi_{jm}(t). \end{aligned} \quad (7)$$

In Eq. (7),  $S_m$  is the border of cell  $V_m$ , and  $\bar{n}(\bar{x}_s)$  is its exterior normal, while

$$L_{ji}^c(m) = \frac{1}{m(V_m)} \int_{V_m} p(j \rightarrow i|\bar{x}) d\bar{x}. \quad (8)$$

The surface integral in Eq. (7) represents the net probability flux out of cell  $V_m$  due to the dynamic drift in state  $i$ . As we aim at interpreting the process variables evolution as state transitions between discrete cells, we must split this integral between the total flux leaving cell  $V_m$  and the ingoing contributions from neighboring cells. Therefore, we define the transition rate between cells  $V_m$  and  $V_n$  in dynamics  $i$  as

$$L_{mn}^\varphi(i) = \begin{cases} -\frac{1}{m(V_m)} \int_{(S_m)_i^+} \bar{n}(\bar{x}_s) \cdot \bar{f}_i(\bar{x}_s) d\bar{x}_s & \text{if } m = n \\ \frac{1}{m(V_m)} \int_{(S_m \cap S_n)_i^+} \bar{n}(\bar{x}_s) \cdot \bar{f}_i(\bar{x}_s) d\bar{x}_s & \text{if } m \neq n \end{cases}, \quad (9)$$

where  $(S)_i^+$  is the part of  $S$  where  $\bar{n}(\bar{x}_s) \cdot \bar{f}_i(\bar{x}_s) > 0$ . The transition rate between the hybrid states  $(j, V_n)$  and  $(i, V_m)$  then is written

$$L_{jn,im} = L_{ji}^c(n) \delta_{nm} + L_{nm}^\varphi(j) Q_{ji}(n \rightarrow m). \quad (10)$$

In Eq. (10),  $Q_{ji}(n \rightarrow m)$  stands for the probability of moving from state  $j$  to state  $i$  when crossing the control setpoint between cells  $V_n$  and  $V_m$ . This quantity is equal to  $\delta_{ji}$  when the border common to these cells has no physical interpretation.

With these definitions, Eq. (7) becomes

$$\frac{d\pi_{im}(t)}{dt} = \sum_j \sum_n L_{jn,im} \pi_{jn}(t). \quad (11)$$

The original problem of dynamic reliability [see Eq. (6)] is continuous in the evolution of the process variables and discrete in the branchings between system configurations. The cell-to-cell discretization reduces it to a time-continuous Markov problem in a discrete space of hybrid states  $(i, V_m)$ .

### II.C. How Cell-to-Cell Discretization Affects the Problem

At the beginning of Sec. II.B, a discussion was initiated on the potential impact of the time step  $\tau$  on the time discrete cell-to-cell scheme summarized in Sec. II.A: An inappropriately small choice of  $\tau$  could lead not only to slowing down the computation but also to an erroneous representation of the dynamics. Indeed, when  $\tau$  is small compared to the average sojourn time within cells for some dynamics, the estimated probability of leaving the current cell can become very small or even vanish. The error induced by this situation does not relate to the numerical inaccuracy entailed by the discretization, but it comes from an improper modeling of the problem.

The continuous version of the method that we sketched in Sec. II.B turns out to overcome this difficulty. Yet, it does not suppress another intrinsic source of error associated with how the transfer between cells in the way it is modeled actually modifies the problem to be solved, potentially introducing nonphysical situations through a probability ‘‘leakage’’ between cells.

To understand the latter statement, it should first be reminded that accident sequences (or transient scenarios in general) correspond to trajectories in the process variables space, which do not entirely fill the safety domain partitioned in cells, even if the dynamics in the different configurations are defined everywhere. Indeed, once the initial steady-state conditions are left, the system enters a configuration in which the process variables evolve deterministically as long as no branching takes place. In this first section of the transient, the time evolution of  $\bar{x}$  follows a one-dimensional curve in the safety domain. If a branching comes from the solicitation of a control device when crossing a setpoint, this curve will be split into two parts: one of them carrying the failure probability of the control device and the other one carrying the complementary probability. If the next branching is associated with the time distributed occurrence of an event, the set of all possible values of  $\bar{x}$  after the change of configuration becomes a section of a two-dimensional surface since an additional degree of freedom (i.e., the branching time) was introduced. The dimensions of the support of the probability densities  $\pi(\bar{x}, i, t)$  will increase in this way by one unit after each nondeterministic transition between configurations.<sup>10</sup> Because of its singular nature, the support of  $\pi(\bar{x}, i, t)$  does not fully cover the process variables domain partitioned in cells.

For this reason, in the development of a scenario, when the process variables enter a given cell in a given dynamics, they do not necessarily have access to all the neighboring cells; even if the dynamics is well defined and outgoing at some points of each border of the cell, these points could belong to unreachable regions in the continuous evolution process. Yet, in this case, Eq. (9) defines transition rates between all neighboring cells in all configurations, even though the real physical trajectories underlying the accident sequences could never reach their common border in some dynamics. The direct consequence of this incorrect modeling is to obtain a non-zero probability to find the system in a given hybrid state  $(i, V_m)$ , though the physics of the accident transient prevents such a situation.

We must thus conclude that the continuous cell-to-cell mapping technique does not only numerically approximate the actual problem, but it is also likely to modify it, creating additional nonphysical sequences that can be deduced from the connectivity of the transition matrix built according to Eq. (10). The implementation of the cell-to-cell transport approach we purport to do in the case of stimulus-driven branchings should be realized with this possible side effect in mind.



### III. STIMULUS-BASED CELL PARTITIONING OF THE PROCESS VARIABLES SPACE

#### III.A. Definition of Cells

As mentioned in Sec. I, partitioning the process variables space in cells on which the fully dynamic equations of the probability density of accident sequences are integrated is not (only) driven by the numerical necessity to handle the high dimensionality of the problem. It is instead motivated by observations from the PSA practice.

First, although the continuous evolution of process variables drives the delineation process of accident scenarios, the analyst is usually not interested in the detailed information in  $\bar{x}$  contained in the pdf  $\pi(\bar{x}, i, t)$ . The relevant results consist instead of knowing as a function of time the probability that some process variables lie in a given region of phase-space, while evolving in a given dynamics, no matter what their detailed distribution inside this region is.

A second essential motivation of this approach is related to the concept of stimulus that was introduced in the companion paper.<sup>4</sup> This new notion comes from the following observation: An event causing a branching in an accident sequence does not always take place instantaneously once its occurrence has been solicited. This solicitation corresponds to the activation of a stimulus, which “triggers” the event and from which a delay has to elapse before its actual occurrence. Stimuli can take various forms:

- It can correspond to the crossing of a setpoint associated with the actuation of a control/protection device; this threshold divides the process variables space into two regions.
- It can be defined by a safety limit, separating the absorbing failure zone from the safe conditions.
- The entry in a domain where ignition conditions are satisfied is another example of stimulus activation, inducing again a two-region partition of phase-space.
- An operator will diagnose that he/she has a given action to take when process variables lie in specific regions of phase-space.
- another stimulus corresponds to a component failure, taking effect with no delay.
- . . .

All these examples but the last one induce a partition of the process variables space. A process-based definition of cells is thereby obtained by taking the intersection of all these stimuli-dependent regions. This partition can be refined, e.g., to account for criteria used to merge scenarios in plant damage states or accident progression bins.

Besides this natural decomposition in cells, interpreting the dynamic evolution of the plant along an accident sequence as a probabilistic cell-to-cell transfer rests on the practical knowledge on stimulus activations in the level-2 PSA frame. Such an activation takes place with a known probability either when reaching a setpoint or within a given region of phase-space. In the latter case, a detailed description of the activation phenomenon inside the cell is either irrelevant or inaccessible. Stimulus-based cells therefore appear, together with the setpoints corresponding to their respective borders, as the elementary information on the process variables value, which must be accounted for in the sequel of the paper. 11

#### III.B. Path of Cells

The differential nature of Eq. (6) implies it is restricted to a Markovian branching process in the event tree. Releasing the Markovian assumption asks for an integral formulation of the evolution equations of the branching process. This approach, reviewed in our companion paper,<sup>4</sup> was further explored there to account for the stimulus-driven case.

This requires an adaptation of the way the possible dynamic evolutions of the system can be reinterpreted as a probabilistic transfer between cells. Transition rates between neighboring cells, as propounded in Sec. II.B, are no longer to be computed. They must be replaced by transition probabilities between couples of cells on a finite time interval, which are the fraction of trajectories connecting points inside these two cells, while evolving according to a given dynamics.

In order to perform the integration of the evolution equations deduced in Ref. 4 on the stimulus-based cells in a coherent fashion with the conclusion of Sec. III.A, it must be assumed that the precise value of the process variables inside the cells becomes meaningless. Consequently, we can write<sup>11</sup>

$$\begin{aligned}
 H_m(\bar{u}) & \int H_\ell(\bar{x}) \delta(\bar{x} - \bar{g}_i(t, \bar{u})) d\bar{x} \\
 & = H_m(\bar{u}) H_\ell(\bar{g}_i(t, \bar{u})) \\
 & \simeq H_m(\bar{u}) \int_{V_m} H_\ell(\bar{g}_i(t, \bar{u})) \frac{d\bar{u}}{m(V_m)} \\
 & \equiv H_m(\bar{u}) T_{m\ell}(i, t) . \tag{12}
 \end{aligned}$$

A slight difference between Eq. (12) and Eq. (2) can be observed:  $T_{m\ell}(i, t)$  clearly stands for the fraction of process evolutions in dynamics  $i$ , which are initiated within cell  $V_m$  and end up within cell  $V_\ell$  after a time  $t$ .

Yet, this quantity possibly sums up contributions from different situations. To understand this point, one can look at Fig. 1.

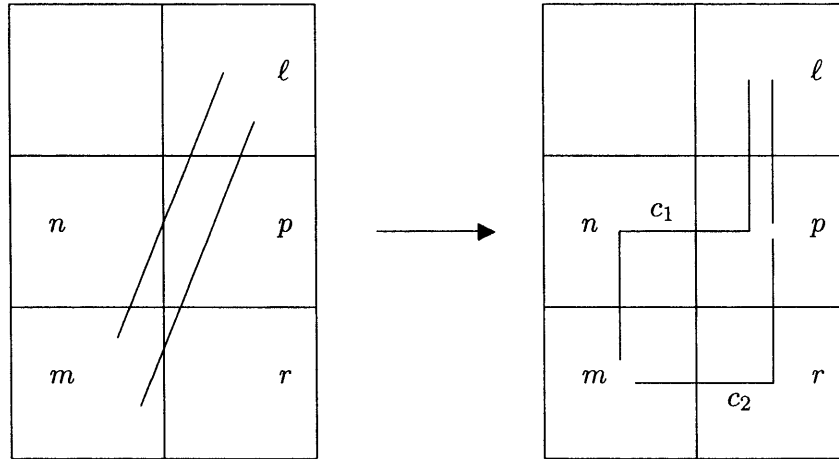


Fig. 1. Examples of paths of cells.

Two evolutions in the current dynamics  $i$  and on the same time interval  $t$  are represented. Both originate in cell  $V_m$  and reach cell  $V_\ell$ . Yet, if these evolutions are now considered in terms of transitions between cells, one of them follows a path  $c_1$ , made up of cells  $V_m$ ,  $V_n$ ,  $V_p$ , and  $V_\ell$ , while the second one is discretized along path  $c_2 = \{V_m, V_r, V_p, V_\ell\}$ . If stimuli can be activated at each border between cells or inside each cell visited, the possibilities for the system to branch out of  $i$  are different, depending on which path will be actually followed. Indeed, assuming stimuli can be activated within cells or at their borders, the way events associated with these stimuli are in competition is totally different along paths  $c_1$  and  $c_2$ . Therefore, the total fraction  $T_{m\ell}(i, t)$  of deterministic trajectories in dynamics  $i$  connecting cells  $V_m$  and  $V_\ell$  in a time  $t$  should not be used globally. This fraction should instead be particularized to each path of cells  $c$  along which the system can evolve between these two cells in this time interval; the corresponding quantity, denoted  $T_{m\ell}^c(i, t)$ , is such that

$$T_{m\ell}(i, t) = \sum_c T_{m\ell}^c(i, t) . \quad (13)$$

We can also notice that the different paths  $c$  correspond to mutually exclusive situations, which can therefore be treated independently. The so-interpreted probabilities

$T_{m\ell}^c(i, t)$  can thus be used to weigh the different scenarios, which appear more naturally in this discretization while they were absent in the schemes presented in Sec. II. The actual estimation of  $T_{m\ell}^c(i, t)$ , which is of course not performed based on Eq. (12), is explained in Sec. V.

#### IV. CELL-TO-CELL SCHEMES FOR STIMULUS-DRIVEN BRANCHING PROCESSES

##### IV.A. Semi-Markov Case

##### IV.A.1. Continuous Model

Accounting for stimulus activations and delays in the equations modeling the possible branchings between different dynamics can be done first with the following assumption: Once an event takes place and a new dynamics is entered, all stimuli that had been activated but whose delays were not fully elapsed are deactivated. In terms of the stochastic process, this amounts to saying that the entry in a new dynamics is a regeneration point and the branching process is semi-Markovian.

We showed in our companion paper that with this assumption, the ingoing density  $\varphi(\bar{x}, i, t)$  in configuration  $i$  at point  $\bar{x}$  is the solution of

$$\varphi(\bar{x}, i, t) = \sum_F \sum_{j \neq i} \int_0^t d\tau \int d\bar{u} [\pi(\bar{u}, j, \tau) \delta(\tau) + \varphi(\bar{u}, j, \tau)] \delta(\bar{x} - \bar{g}_j(t - \tau, \bar{u})) q_{ji}^F(t - \tau; \bar{u}) , \quad (14)$$

where  $q_{ji}^F(t; \bar{u})$  is the probability per unit time that the event induced by stimulus  $F$  will cause a change of dynamics from  $j$  to  $i$ , at time  $t$  after entering dynamics  $j$  at point  $\bar{u}$ . It can be expressed according to

$$q_{ij}^F(t; \bar{u}) = \int_0^t f_i^F(\tau; \bar{u}) h_{ij}^F(t - \tau; \bar{g}_i(\tau, \bar{u})) d\tau \prod_{G \neq F} \left[ 1 - \int_0^t dt' \int_0^{t'} d\tau f_i^G(\tau; \bar{u}) h_i^G(t' - \tau; \bar{g}_i(\tau, \bar{u})) \right] , \quad (15)$$



where  $f_i^F(t; \bar{u})$  is the probability density function (pdf) of the activation time of stimulus  $F$  in dynamics  $i$  entered at  $\bar{u}$  and  $h_{ij}^F(t; \bar{u})$  is the probability per unit time of a delay  $t$  between the activation of  $F$  at point  $\bar{u}$  and the occurrence of the event causing the transition  $i \rightarrow j$  [the pdf of the delay associated with the  $F$ -induced event out of  $i$  being  $h_i^F(t; \bar{u}) = \sum_j h_{ij}^F(t; \bar{u})$ ].

The ingoing density is related to the probability density through

$$\begin{aligned} \pi(\bar{x}, i, t) &= \int_0^t d\tau \int d\bar{u} [\pi(\bar{u}, i, \tau) \delta(\tau) + \varphi(\bar{u}, i, \tau)] \\ &\times \delta(\bar{x} - \bar{g}_i(t - \tau, \bar{u})) \cdot (1 - P_i(t - \tau; \bar{u})) , \end{aligned} \quad (16)$$

where the probability  $1 - P_i(t; \bar{u})$  to survive a time  $t$  in dynamics  $i$  entered at  $\bar{u}$  is written

$$P_i(t; \bar{u}) \equiv \sum_F \sum_{j \neq i} \int_0^t q_{ij}^F(\tau; \bar{u}) d\tau . \quad (17)$$

A backward formulation of the problem, based on conditional probability densities, can also be used. Its discrete cell-to-cell counterpart is provided in the Appendix.

#### IV.A.2. Cell-to-Cell Transport Approach

Let us introduce the following quantities:

$$\varphi_\ell(i, t) = \int H_\ell(\bar{x}) \varphi(\bar{x}, i, t) d\bar{x} \quad (18)$$

and

$$\pi_\ell(i, t) = \int H_\ell(\bar{x}) \pi(\bar{x}, i, t) d\bar{x} . \quad (19)$$

In order to perform the integration of Eqs. (14) and (16) on cell  $V_\ell$ , we replace  $\int \dots d\bar{u}$  with  $\sum_m \int \dots H_m(\bar{u}) d\bar{u}$ . We then obtain for the integration of the Dirac peaks on cell  $V_\ell$  the result expressed in Eq. (12). Moreover, taking into account the different paths between two cells, we obtain from Eq. (14)

$$\begin{aligned} \varphi_\ell(i, t) &= \sum_F \sum_{j \neq i} \sum_m \sum_{c \in \mathcal{C}_j\{m, \ell\}} \int_0^t d\tau T_{m\ell}^c(j, t - \tau) \\ &\times [\pi_m(j, \tau) \delta(\tau) + \varphi_m(j, \tau)] q_{ji}^{F,c}(t - \tau, m) , \end{aligned} \quad (20)$$

where

$$\begin{aligned} \mathcal{C}_j\{m, \ell\} &= \text{set of all paths of cells between } V_m \text{ and } \\ &V_\ell \text{ in dynamics } j \\ q_{ji}^{F,c}(t, m) &= \text{probability per unit time that the transi-} \\ &\text{tion } j \rightarrow i \text{ will follow the activation of } \\ &F \text{ along path } c \text{ given dynamics } j \text{ was} \\ &\text{entered inside cell } V_m . \end{aligned}$$

As for Eq. (16), after integration on cell  $V_\ell$ , it becomes

$$\begin{aligned} \pi_\ell(i, t) &= \int_0^t d\tau \sum_m [\pi_m(i, \tau) \delta(\tau) + \varphi_m(i, \tau)] \\ &\times \sum_{c \in \mathcal{C}_j\{m, \ell\}} T_{m\ell}^c(i, t - \tau) \mathcal{P}_{m\ell}^c(i, t - \tau) , \end{aligned} \quad (21)$$

where  $\mathcal{P}_{m\ell}^c(i, t)$  is the survival probability in dynamics  $i$  for a system evolution between cells  $V_m$  and  $V_\ell$  alongside path  $c$ . Since this implies that the system has ‘‘survived’’ all stimulus-based events, we can write

$$\mathcal{P}_{m\ell}^c(i, t) = \prod_F \mathcal{P}_{m\ell}^{F,c}(i, t) . \quad (22)$$

The expression of each factor in the latter probability can be built by examining on a step-by-step basis along path  $c$  the different possibilities of activation of  $F$ . We will treat the example of the path  $c = \{V_m, V_n, V_p, V_\ell, V_s\}$  given above (see Fig. 1), as these particular results can be generalized to any path. Note that we have added a cell  $V_s$  to the path given in Fig. 1 in order to model the competition between the occurrence of the  $F$ -induced event inside cell  $V_\ell$  and the dynamic drift toward the next cell  $V_s$  in configuration  $i$  along path  $c$ .

We first assume that average sojourn times in the different cells belonging to path  $c$  can be considered. Let  $t_{mn}$  be the average time spent in cell  $V_m$  before reaching its border with cell  $V_n$ , along path  $c$  in dynamics  $i$  (this double dependence has been skipped in the notation for the sake of clarity). We also introduce  $t_{mp}$ ,  $t_{m\ell}$ , and  $t_{ms}$ , total sojourn times along path  $c$  between the borders of the cells referenced as indexes. We must have  $t_{m\ell} < t$  and  $t < t_{ms}$  to ensure a positive value of  $\mathcal{P}_{m\ell}^{F,c}(i, t)$ . This should be implicitly accounted for in the definition of  $T_{m\ell}^c(i, t)$ .

Let  $v_{i,m}^F$  denote the probability of activation of stimulus  $F$  within cell  $V_m$  in configuration  $i$ . The activation time of  $F$  within a cell is assumed uniformly distributed on the sojourn time in this cell. In order to account for the possibility of activation at a setpoint, we also define  $w_{i,mn}^F$  as the probability of activating  $F$  in dynamics  $i$  while crossing the border between cells  $V_m$  and  $V_n$ .

The expression of  $\mathcal{P}_{m\ell}^{F,c}(i, t)$  is established as follows. If  $F$  is activated in the first cell, the system survives in configuration  $i$  only if the corresponding change of dynamics is delayed after  $t$ . If it is not activated in the first cell, it can be activated at the first setpoint, but the delay up to the occurrence of the transition must prevent a change of dynamics to occur before  $t$ , and so on. Therefore,

$$\begin{aligned} \mathcal{P}_{m\ell}^{F,c}(i, t) &= v_{i,m}^F \int_0^{t_{mn}} \frac{1}{t_{mn}} (1 - H_i^F(t - \tau; m)) d\tau \\ &+ (1 - v_{i,m}^F) [w_{i,mn}^F (1 - H_i^F(t - t_{mn}; mn)) \\ &+ (1 - w_{i,mn}^F) \cdot \alpha] , \end{aligned} \quad (23)$$

where  $H_i^F(t; m)$  is the cumulative density function of the delay if stimulus  $F$  is activated in cell  $V_m$  in dynamics  $i$ , while  $H_i^F(t; mn)$  corresponds to the same probability, given the activation occurring at the border between cells  $V_m$  and  $V_n$ . Factor  $\alpha$  appearing in Eq. (23) stands for the survival probability in dynamics  $i$  once stimulus  $F$  has not been activated in cell  $V_m$  nor at its border with cell  $V_n$ . In the particular case we treat, it is written by recurrence as follows:

$$\begin{aligned} \alpha = & v_{i,n}^F \int_{t_{mn}}^{t_{mp}} \frac{1}{t_{mp} - t_{mn}} (1 - H_i^F(t - \tau; n)) d\tau \\ & + (1 - v_{i,n}^F) [w_{i,np}^F (1 - H_i^F(t - t_{mp}; np)) + (1 - w_{i,np}^F) \cdot \beta] , \end{aligned} \quad (24)$$

$$\begin{aligned} \beta = & v_{i,p}^F \int_{t_{mp}}^{t_{m\ell}} \frac{1}{t_{m\ell} - t_{mp}} (1 - H_i^F(t - \tau; p)) d\tau \\ & + (1 - v_{i,p}^F) [w_{i,p\ell}^F (1 - H_i^F(t - t_{m\ell}; p\ell)) + (1 - w_{i,p\ell}^F) \cdot \gamma] , \end{aligned} \quad (25)$$

and

$$\gamma = v_{i,\ell}^F \int_{t_{m\ell}}^t \frac{1}{t_{ms} - t_{m\ell}} (1 - H_i^F(t - \tau; \ell)) d\tau + \left( 1 - v_{i,\ell}^F \cdot \frac{t - t_{m\ell}}{t_{ms} - t_{m\ell}} \right) . \quad (26)$$

It must be underlined that in practice, the expression of  $\mathcal{P}_{m\ell}^{F,c}(i, t)$  is likely to reduce to a much more compact form because of the physical impossibility of having stimulus  $F$  activated in some cells and at some setpoints. Indeed, a stimulus will correspond in general to one setpoint or several cells.

The developments above rest on the assumption that average values of  $t_{mn}$ ,  $t_{mp}$ ,  $t_{m\ell}$ , and  $t_{ms}$  can be used. Actually, this might not be appropriate as it reduces the possible evolutions of the system along path  $c$  to one single deterministic time sequence. Considering that these sojourn times are distributed according to a four-variate distribution  $g_i^c$  (since these times are not independent), we must understand Eq. (23) as being conditional to  $t_{mn}$ ,  $t_{mp}$ ,  $t_{m\ell}$ , and  $t_{ms}$ . The same is true for  $T_{m\ell}^c(i, t)$ . Equation (21) should then make use of

$$\begin{aligned} T_{m\ell}^c(i, t) \mathcal{P}_{m\ell}^c(i, t) = & \int \dots \int_{\substack{t_{m\ell} < t < t_{ms} \\ t_{mn} < t_{mp} < t_{m\ell}}} g_i^c(t_{mn}, t_{mp}, t_{m\ell}, t_{ms}) T_{m\ell}^c(i, t; t_{mn}, t_{mp}, t_{m\ell}, t_{ms}) \\ & \times \prod_F \mathcal{P}_{m\ell}^{F,c}(i, t; t_{mn}, t_{mp}, t_{m\ell}, t_{ms}) dt_{mn} dt_{mp} dt_{m\ell} dt_{ms} . \end{aligned} \quad (27)$$

We will discuss in Sec. V how to practically determine and use these distributions  $g_i^c$ .

Let us express now the probability per unit time of a transition between dynamics  $i$  and  $j$  after a time  $t$ , while having been transported from cell  $V_m$  to cell  $V_n$ , following an event triggered by stimulus  $F$ . From Eqs. (15) and (17), we can write

$$q_{ij}^{F,c}(t, m) = p_{m\ell}^{F,c}(i \rightarrow j, t) \prod_{G \neq F} \mathcal{P}_{m\ell}^{G,c}(i, t) , \quad (28)$$

where  $p_{m\ell}^{F,c}(i \rightarrow j, t)$  denotes the same probability per unit time as  $q_{ij}^{F,c}(t, m)$  but when considering only stimulus  $F$ . It is built on Eq. (23) by deriving it and selecting the transition to dynamics  $j$ :

$$\begin{aligned} p_{m\ell}^{F,c}(i \rightarrow j, t) = & v_{i,m}^F \int_0^{t_{mn}} \frac{1}{t_{mn}} h_{ij}^F(t - \tau; m) d\tau \\ & + (1 - v_{i,m}^F) [w_{i,mn}^F h_{ij}^F(t - t_{mn}; mn) + (1 - w_{i,mn}^F) \cdot (-\dot{\alpha})] , \end{aligned} \quad (29)$$

where along the particular path  $c$  taken as example, we have

$$\begin{aligned} (-\dot{\alpha}) = & v_{i,n}^F \int_{t_{mn}}^{t_{mp}} \frac{1}{t_{mp} - t_{mn}} h_{ij}^F(t - \tau; n) d\tau \\ & + (1 - v_{i,n}^F) [w_{i,np}^F h_{ij}^F(t - t_{mp}; np) + (1 - w_{i,np}^F) \cdot (-\dot{\beta})] , \end{aligned} \quad (30)$$

$$\begin{aligned} (-\dot{\beta}) = & v_{i,p}^F \int_{t_{mp}}^{t_{m\ell}} \frac{1}{t_{m\ell} - t_{mp}} h_{ij}^F(t - \tau; p) d\tau \\ & + (1 - v_{i,p}^F) [w_{i,p\ell}^F h_{ij}^F(t - t_{m\ell}; p\ell) + (1 - w_{i,p\ell}^F) \cdot (-\dot{\gamma})] , \end{aligned} \quad (31)$$

and

$$(-\dot{\gamma}) = v_{i,\ell}^F \int_{t_{m\ell}}^t \frac{1}{t_{ms} - t_{m\ell}} h_{ij}^F(t - \tau; \ell) d\tau. \quad (32)$$

The distribution of  $t_{mm}$ ,  $t_{mp}$ ,  $t_{m\ell}$ , and  $t_{ms}$  can be accounted for just as before.

It is easily seen that the adaptation of Eqs. (23) through (26), and (29) through (32), respectively, to a general path  $c \equiv \{V_m \equiv V_{n_1}, V_{n_2} \dots V_{n_{r-1}}, V_\ell \equiv V_{n_r}, V_s\}$  is straightforward.

#### IV.B. General Non-Markov Case

##### IV.B.1. Continuous Model

Releasing the assumption of disactivation of all activated stimuli once a change of dynamics occurs leads to a non-Markov modeling based on two ingoing densities<sup>4</sup>:

- $\varphi_{in}(\bar{x}, j, t, \vec{\tau}_A, \mathcal{A})$ : density of entering dynamics  $j$  at point  $\bar{x}$  and time  $t$ , with a set  $\mathcal{A}$  of stimuli remaining activated;  $\vec{\tau}_A$  denotes the activation times of the stimuli belonging to  $\mathcal{A}$
- $\varphi_F(\bar{x}, j, t, \tau, \vec{\tau}_A, \mathcal{A})$ : density of activating stimulus  $F$  in dynamics  $j$  at  $(\bar{x}, t)$ , this configuration  $j$  being entered at  $\tau$ , this activation resulting in a set  $\mathcal{A}$  of activated stimuli (this density is nonzero if  $\tau_F \equiv t$ ).

They were shown to obey the following evolution equations:

$$\begin{aligned} & \varphi_{in}(\bar{x}, j, t, \vec{\tau}_A, \mathcal{A}) \\ &= \sum_{A' \supset \mathcal{A}} \sum_{F \in A'} \sum_{i \neq j} \int d\bar{u} \int_0^t d\tau \\ & \times \int_0^\tau \dots \int_0^\tau d\vec{\tau}_{A'/A} \delta(\bar{x} - \bar{g}_i(t - \tau, \bar{u})) \\ & \times p_{ij}^F(t; \tau, \tau, \bar{u}, \vec{\tau}_{A'}, \mathcal{A}') \cdot \varphi_{in}(\bar{u}, i, \tau, \vec{\tau}_{A'}, \mathcal{A}') \\ & \times \delta_{ij}^F(\mathcal{A}' \rightarrow \mathcal{A}) \\ & + \sum_{A' \supset \mathcal{A}} \sum_{F \in A'} \sum_{i \neq j} \sum_{G \in A'} \int d\bar{u} \int_0^t d\tau^* \int_0^{\tau^*} d\tau \\ & \times \int_0^{\tau^*} \dots \int_0^{\tau^*} d\vec{\tau}_{A'/A} \delta(\bar{x} - \bar{g}_i(t - \tau_G, \bar{u})) \\ & \times p_{ij}^F(t; \tau_G, \tau, \bar{u}, \vec{\tau}_{A'}, \mathcal{A}') \cdot \varphi_G(\bar{u}, i, \tau_G, \tau, \vec{\tau}_{A'}, \mathcal{A}') \\ & \times \delta_{ij}^F(\mathcal{A}' \rightarrow \mathcal{A}) \delta(\tau^* - \tau_G) \end{aligned} \quad (33)$$

and

$$\begin{aligned} & \varphi_F(\bar{x}, j, t, \tau, \vec{\tau}_{A+\{F\}}, \mathcal{A} + \{F\}) \\ &= \int d\bar{u} \delta(\bar{x} - \bar{g}_j(t - \tau, \bar{u})) p_j^{F*}(t; \tau, \tau, \bar{u}, \vec{\tau}_A, \mathcal{A}) \\ & \times [\pi(\bar{u}, j, \tau) \delta(\tau) \delta_{\mathcal{A}, \emptyset} + \varphi_{in}(\bar{u}, j, \tau, \vec{\tau}_A, \mathcal{A})] \\ & + \sum_{G \in \mathcal{A}} \int d\bar{u} \delta(\bar{x} - \bar{g}_j(t - \tau_G, \bar{u})) \\ & \times p_j^{F*}(t; \tau_G, \tau, \bar{u}, \vec{\tau}_A, \mathcal{A}) \cdot \varphi_G(\bar{u}, j, \tau_G, \tau, \vec{\tau}_A, \mathcal{A}). \end{aligned} \quad (34)$$

Note that in the second term on the right side of Eq. (33), a Dirac peak on  $\tau^*$ , taken equal to the last activation time  $\tau_G$ , is not directly integrated. Indeed, stimulus  $G$  may or may not belong to set  $\mathcal{A}$ . Only in the negative case will  $\tau_G$  be a dummy variable for integration (accounted for in  $\vec{\tau}_{A'/A}$ ).

In these expressions, we have made use of the following quantities:

- $\delta_{ij}^F(\mathcal{A}' \rightarrow \mathcal{A})$  embodies the rules of disactivation of the stimuli belonging to  $\mathcal{A}'$  due to the  $F$ -induced transition  $i \rightarrow j$ , with only those in  $\mathcal{A}$  remaining activated in the new dynamics.
- $p_{ij}^F(t; \tau^*, \tau, \bar{u}^*, \vec{\tau}_A, \mathcal{A}) dt$  is the probability that the  $F$ -induced transition  $i \rightarrow j$  takes place in  $[t, t + dt]$ , given dynamics  $i$  was entered at  $\tau$  and the last event occurred at  $(\bar{u}^*, \tau^*)$ , with a set  $\mathcal{A}$  of stimuli activated at  $\vec{\tau}_A$  resulting from it:

$$\begin{aligned} & p_{ij}^F(t; \tau^*, \tau, \bar{u}^*, \vec{\tau}_A, \mathcal{A}) dt \\ &= \frac{\tilde{h}_{ij}^F(t - \tau; \bar{u} | \tau - \tau_F) dt}{1 - \tilde{H}_i^F(\tau^* - \tau; \bar{u} | \tau - \tau_F)} \\ & \times \prod_{\substack{G \in \mathcal{A} \\ G \neq F}} \frac{1 - \tilde{H}_i^G(t - \tau; \bar{u} | \tau - \tau_G)}{1 - \tilde{H}_i^G(\tau^* - \tau; \bar{u} | \tau - \tau_G)} \\ & \times \prod_{H \notin \mathcal{A}} \frac{1 - F_i^H(t - \tau; \bar{u})}{1 - F_i^H(\tau^* - \tau; \bar{u})}, \end{aligned} \quad (35)$$

where  $\bar{u}^* = \bar{g}_i(\tau^* - \tau, \bar{u})$ .

- $p_i^{F*}(t; \tau^*, \tau, \bar{u}^*, \vec{\tau}_A, \mathcal{A}) dt$  is the probability of activating  $F$  in dynamics  $i$  in  $[t, t + dt]$ , given the same conditions as before:

$$\begin{aligned} & p_i^{F*}(t; \tau^*, \tau, \bar{u}^*, \vec{\tau}_A, \mathcal{A}) dt \\ &= \frac{f_i^F(t - \tau; \bar{u}) dt}{1 - F_i^F(\tau^* - \tau; \bar{u})} \cdot \prod_{\substack{H \notin \mathcal{A} \\ H \neq F}} \frac{1 - F_i^H(t - \tau; \bar{u})}{1 - F_i^H(\tau^* - \tau; \bar{u})} \\ & \times \prod_{G \in \mathcal{A}} \frac{1 - \tilde{H}_i^G(t - \tau; \bar{u} | \tau - \tau_G)}{1 - \tilde{H}_i^G(\tau^* - \tau; \bar{u} | \tau - \tau_G)}. \end{aligned} \quad (36)$$

Tilded distributions  $\tilde{H}_i^F(t; \bar{u} | \tau - \tau_F)$  for the delays were introduced. They are conditioned by the probability of a delay larger than  $\tau - \tau_F$  if  $F$  was activated at  $\tau_F < \tau$ , the time of entry in configuration  $i$ .

The probability density then is written

$$\begin{aligned} \pi(\bar{x}, i, t; \mathcal{A}) &= \int d\bar{u}^* \int_0^t d\tau^* \int_0^{\tau^*} d\tau \int_0^{\tau} \dots \int_0^{\tau^*} d\vec{\tau}_A \delta(\bar{x} - \bar{g}_i(t - \tau^*, \bar{u}^*)) (1 - P_i(t; \tau^*, \tau, \bar{u}^*, \vec{\tau}_A, \mathcal{A})) \\ &\times \left[ \pi(\bar{u}, j, \tau) \delta(\tau) \delta_{\mathcal{A}, \emptyset} + \varphi_{in}(\bar{u}^*, i, \tau^*, \vec{\tau}_A, \mathcal{A}) \delta(\tau^* - \tau) + \sum_{F \in \mathcal{A}} \varphi_F(\bar{u}^*, i, \tau^*, \tau, \vec{\tau}_A, \mathcal{A}) \delta(\tau^* - \tau_F) \right] \end{aligned} \quad (37)$$

with

$$1 - P_i(t; \tau^*, \tau, \bar{u}^*, \vec{\tau}_A, \mathcal{A}) = \prod_{G \in \mathcal{A}} \frac{1 - \tilde{H}_i^G(t - \tau; \bar{u} | \tau - \tau_G)}{1 - \tilde{H}_i^G(\tau^* - \tau; \bar{u} | \tau - \tau_G)} \times \prod_{H \in \mathcal{A}} \frac{1 - F_i^H(t - \tau; \bar{u})}{1 - F_i^H(\tau^* - \tau; \bar{u})}. \quad (38)$$

#### IV.B.2. Cell-to-Cell Transport Approach

The discrete forms of Eqs. (33) and (34) rest on the definition of the following densities:

- $\varphi_{in}(\ell, j, t, \vec{\tau}_A, \mathcal{A})$ : density of entering dynamics  $j$  in cell  $V_\ell$  and time  $t$ , with a set  $\mathcal{A}$  of stimuli activated at times  $\vec{\tau}_A$
- $\varphi_F(L, j, t, m, \tau, \vec{\tau}_A, \vec{m}_A, \mathcal{A})$ : density of activating stimulus  $F$  in dynamics  $j$  at “place”  $L$  and time  $t$ , given this configuration  $j$  was entered in cell  $V_m$  and at time  $\tau$ , this activation resulting in a set  $\mathcal{A}$  of stimuli activated at times  $\vec{\tau}_A$  and places  $\vec{m}_A$ . This density will be nonzero if  $\tau_F \equiv t$  and  $m_F \equiv L$ .

Note that if the first quantity directly comes from the integration on cell  $V_\ell$  of its correspondent in the continuous process variables space, the situation is slightly different for the second one. Indeed, in the definition of the discrete  $\varphi_F$ , we have added to the entry time  $\tau$  in the current configuration  $j$  the cell  $V_m$  in which this event took place. This information is essential to restrict the paths of cells reaching  $L$  to those originating in  $V_m$ , thereby avoiding nonphysical scenarios (see Sec. II.C). Moreover, the concept of “place” was introduced in the foregoing second bulleted item. As we assume a stimulus can be activated at a border between cells or inside a cell, we must account for these two kinds of situations in the ingoing density of stimulus activation. Any of this case is then re-

ferred to as a place. This now forces us to understand a path of cells in a broader way, including their common borders as well. Therefore, the fraction of dynamic trajectories  $T_{m\ell}^c(i, t)$  connecting  $V_m$  and  $V_\ell$  along path  $c$  in dynamics  $i$  has to be seen between places, and not cells only.

An additional dependence of  $\varphi_F$  on  $\vec{m}_A$ , a vector containing the activation places of all stimuli  $G \in \mathcal{A}$  and such that  $\tau_G > \tau$ , has been introduced. Indeed, if stimulus  $G$  was activated at time  $\tau_G < \tau$ , the time of entry in dynamics  $i$ , the place where  $G$  was activated has no direct influence after  $\tau$  because of the change of dynamics that occurred there. There is therefore no dependence on  $\vec{m}_A$  in  $\varphi_{in}$ . When  $\tau_G > \tau$ , however, the corresponding activation place is a constraint for the *path of places* that can be followed in dynamics  $i$ . These places should then be kept in memory together with the activation times. When considering the probability of a next event, either a change of dynamics or an additional stimulus activation, the places of activation of these stimuli define which path of cells can be followed in a coherent way with the chronological series of activation times. Vectors  $\vec{m}_A$  and  $\vec{\tau}_A$  will thus be used to limit the study to those paths of cells  $c$  that are relevant in modeling the possible discrete dynamic evolutions of the system in a given state. We will then denote the dependence of the delay distributions on the process variables as a dependence on the current path  $c$ .

The cell-to-cell transport equation associated with Eq. (33) then is written

$$\begin{aligned} \varphi_{in}(\ell, j, t; \vec{\tau}_A, \mathcal{A}) &= \sum_{\mathcal{A}' \supset \mathcal{A}, i \neq j} \int_0^t d\tau^* \int_0^{\tau^*} \dots \int_0^{\tau^*} d\vec{\tau}_{\mathcal{A}'/\mathcal{A}} \sum_m \varphi_{in}(m, i, \tau^*, \vec{\tau}_{\mathcal{A}'}, \mathcal{A}') \sum_{c \in \mathcal{C}_i\{m, \ell\}} T_{m\ell}^c(i, t - \tau^*) \\ &\times \sum_{F \in \mathcal{A}'} \tilde{h}_{ij}^F(t - \tau^*, c | \tau^* - \tau_F) \cdot \prod_{\substack{G \in \mathcal{A}' \\ G \neq F}} (1 - \tilde{H}_i^G(t - \tau^*, c | \tau^* - \tau_G)) \cdot \prod_{H \in \mathcal{A}'} \mathcal{R}_{m\ell}^{H,c}(i, t | \tau^*, m, \tau^*) \cdot \delta_{ij}^F(\mathcal{A} \rightarrow \mathcal{A}') \\ &+ \sum_{\mathcal{A}' \supset \mathcal{A}, i \neq j} \sum_{J \in \mathcal{A}'} \int_0^t d\tau_J \int_0^{\tau_J} d\tau \int_0^{\tau} \dots \int_0^{\tau_J} d\vec{\tau}_{\mathcal{A}'/(\mathcal{A} + \{J\})} \sum_m \sum_{\vec{m}_A} \varphi_J(m_J, i, \tau_J, m, \tau, \vec{\tau}_{\mathcal{A}'}, \vec{m}_{\mathcal{A}'}, \mathcal{A}') \\ &\times \sum_{c \in \mathcal{C}_i\{m, \vec{m}_{\mathcal{A}'}, \vec{\tau}_{\mathcal{A}'}, \ell\}} T_{m_J \ell}^c(i, t - \tau_J) \sum_{F \in \mathcal{A}'} \frac{\tilde{h}_{ij}^F(t - \tau, c | \tau - \tau_F)}{1 - \tilde{H}_i^F(\tau_J - \tau, c | \tau - \tau_F)} \\ &\times \prod_{\substack{G \in \mathcal{A}' \\ G \neq F}} \frac{1 - \tilde{H}_i^G(t - \tau, c | \tau - \tau_G)}{1 - \tilde{H}_i^G(\tau_J - \tau, c | \tau - \tau_G)} \cdot \prod_{H \in \mathcal{A}'} \mathcal{R}_{m_J \ell}^{H,c}(i, t | \tau, m, \tau_J) \cdot \delta_{ij}^F(\mathcal{A}' \rightarrow \mathcal{A}). \end{aligned} \quad (39)$$

Let us comment on Eq. (39).

It should be observed that this time,  $\mathcal{C}_i\{m, \vec{m}_A, \vec{\tau}_A, \ell\}$  still denotes the set of all paths of cells connecting  $V_m$  and  $V_\ell$  in dynamics  $i$ , but with the additional condition of including places  $\vec{m}_A$ , where the previous activations took place, in the chronological order given by  $\vec{\tau}_A$ . Following the remark above Eq. (39), the possible paths are thus restricted to those containing the places of activation of stimuli having been activated between the entry in configuration  $i$  and the last activation that took place at  $V_{m_j}$ . Doing so, we avoid considering paths that, despite connecting  $V_{m_j}$  and  $V_\ell$ , could not have originated in cell  $V_m$ . This strongly limits the number of terms to be considered in practice when dealing with the multiple sum  $\sum_{\vec{m}_A}$  on all components of this vector.

Equation (39) also makes use of  $\mathcal{R}_{L\ell}^{G,c}(i, t|\tau, m, \tau^*)$ , the conditional probability that stimulus  $G$  is not activated before time  $t$ , on the section of path  $c$  between place  $L$  and cell  $V_\ell$ , in dynamics  $i$ , provided the latter was entered in cell  $V_m$  at time  $\tau$ , given  $G$  was not activated when the last event took place at  $\tau^*$ . Before developing this expression, we introduce the corresponding pdf of activation

$$r_{L\ell}^{G,c}(i, t|\tau, m, \tau^*) = -\frac{d\mathcal{R}_{L\ell}^{G,c}(i, t|\tau, m, \tau^*)}{dt}$$

in order to write the cell-to-cell process associated with Eq. (34):

$$\begin{aligned} & \varphi_F(\ell, j, t, m, \tau, \vec{\tau}_{A+\{F\}}, \vec{m}_{A+\{F\}}, \mathcal{A} + \{F\}) \\ &= [\delta_{\mathcal{A}, \emptyset} \delta(\tau) \pi_m(j, \tau) + \varphi_{in}(m, j, \tau, \vec{\tau}_A, \mathcal{A})] \\ & \times \sum_{c \in \mathcal{C}_j\{m, \ell\}} T_{m\ell}^c(j, t - \tau) \cdot r_{m\ell}^{F,c}(j, t|\tau, m, \tau) \\ & \times \prod_{\substack{H \notin \mathcal{A} \\ H \neq F}} \mathcal{R}_{m\ell}^{H,c}(j, t|\tau, m, \tau) \\ & \times \prod_{G \in \mathcal{A}} (1 - \tilde{H}_i^G(t - \tau, c|\tau - \tau_G)) \\ & + \sum_{J \in \mathcal{A}} \varphi_J(m_J, j, \tau_J, m, \tau, \vec{\tau}_A, \vec{m}_A, \mathcal{A}) \\ & \times \sum_{c \in \mathcal{C}_j\{m, \vec{m}_A, \vec{\tau}_A, \ell\}} T_{m_j\ell}^c(j, t - \tau_J) \\ & \times r_{m_j\ell}^{F,c}(j, t|\tau, m, \tau_J) \prod_{\substack{H \notin \mathcal{A} \\ H \neq F}} \mathcal{R}_{m_j\ell}^{H,c}(j, t|\tau, m, \tau_J) \\ & \times \prod_{G \in \mathcal{A}} \frac{1 - \tilde{H}_i^G(t - \tau, c|\tau - \tau_G)}{1 - \tilde{H}_i^G(\tau_J - \tau, c|\tau - \tau_G)}. \end{aligned} \quad (40)$$

When  $F$  is activated, vector  $\vec{m}_A$  is updated with  $m_F \equiv \ell$ , and vector  $\vec{\tau}_A$  is updated with  $\tau_F \equiv t$ .

As for the probability to find the system in cell  $V_\ell$  and dynamics  $i$ , it is easily obtained in terms of ingoing densities according to

$$\begin{aligned} \pi_\ell(i, t; \mathcal{A}) &= \int_0^t d\tau^* \int_0^{\tau^*} \dots \int_0^{\tau^*} d\vec{\tau}_A \\ & \times \sum_m [\delta_{\mathcal{A}, \emptyset} \delta(\vec{\tau}_A - \vec{0}) \delta(\tau^*) \pi_m(i, \tau^*) \\ & \quad + \varphi_{in}(m, i, \tau^*, \vec{\tau}_A, \mathcal{A})] \\ & \times \sum_{c \in \mathcal{C}_i\{m, \ell\}} T_{m\ell}^c(i, t - \tau^*) \\ & \times \prod_{G \in \mathcal{A}} (1 - \tilde{H}_i^G(t - \tau^*, c|\tau^* - \tau_G)) \\ & \times \prod_{H \notin \mathcal{A}} \mathcal{R}_{m\ell}^{H,c}(i, t|\tau^*, m, \tau^*) \\ & + \sum_{F \in \mathcal{A}} \int_0^t d\tau_F \int_0^{\tau_F} d\tau \int_0^{\tau_F} \dots \int_0^{\tau_F} d\vec{\tau}_{A \setminus \{F\}} \\ & \times \sum_m \sum_{\vec{m}_A} \varphi_F(m_F, i, \tau_F, m, \tau, \vec{\tau}_A, \vec{m}_A, \mathcal{A}) \\ & \times \sum_{c \in \mathcal{C}_i\{m, \vec{m}_A, \vec{\tau}_A, \ell\}} T_{m_F\ell}^c(i, t - \tau_F) \\ & \times \prod_{G \in \mathcal{A}} \frac{1 - \tilde{H}_i^G(t - \tau, c|\tau - \tau_G)}{1 - \tilde{H}_i^G(\tau_F - \tau, c|\tau - \tau_G)} \\ & \times \prod_{H \notin \mathcal{A}} \mathcal{R}_{m_F\ell}^{H,c}(i, t|\tau, m, \tau_F). \end{aligned} \quad (41)$$

Let us now give the expression of  $\mathcal{R}_{L\ell}^{G,c}(i, t|\tau, m, \tau^*)$  and  $r_{L\ell}^{G,c}(i, t|\tau, m, \tau^*)$  using the same notations as in Sec. IV.A. Assume thus that  $c \equiv \{V_m \equiv V_{n_1}, V_{n_2} \dots L \dots V_{n_{r-1}}, V_\ell \equiv V_{n_r}, V_s\}$  is the full path between  $V_m$  and  $V_\ell$ , which is as before completed by cell  $V_s$ . We should first observe that our results will depend on the nature of  $L$  and  $\ell$ , i.e., if they correspond to cells or borders.

The probability of nonactivation of stimulus  $G$  at time  $t$  is the product of the individual probabilities of nonactivation in the cells belonging to path  $c$  and at their borders. The same is true for the conditioning probability of not being activated up to place  $L$  at time  $\tau^*$ . Therefore, all factors of these probabilities up to  $L$  will disappear in the conditional probability  $\mathcal{R}_{L\ell}^{G,c}(i, t|\tau, m, \tau^*)$ , possibly but the one corresponding to  $L$  if it is a cell. Indeed, in this case ( $L \equiv V_{n_a}$ ), the probability of not being activated in this cell before  $\tau^*$  is  $(1 - v_{i, n_a}^G \cdot [(\tau^* - \tau) - t_{mn_a}]) / (t_{mn_{a+1}} - t_{mn_a})$  since we have  $\tau + t_{mn_a} \leq \tau^* \leq \tau + t_{mn_{a+1}}$ .



Then, if  $L \neq \ell$ , we can write

$$\begin{aligned} \mathcal{R}_{L\ell}^{G,c}(i, t | \tau, m, \tau^*) &= \frac{1 - v_{i,n_a}^G}{1 - v_{i,n_a}^G \cdot \frac{(\tau^* - \tau) - t_{mn_a}}{t_{mn_{a+1}} - t_{mn_a}}} \\ &\times (1 - w_{i,n_a n_{a+1}}^G) \\ &\times \left[ \prod_{j=a+1}^{r-1} (1 - v_{i,n_j}^G) \cdot (1 - w_{i,n_j n_{j+1}}^G) \right] \\ &\times \left( 1 - v_{i,\ell}^G \cdot \frac{t - (\tau + t_{m\ell})}{t_{ms} - t_{m\ell}} \right) \quad (42) \end{aligned}$$

iff  $V_\ell$  is a cell and  $\tau + t_{m\ell} < t < \tau + t_{ms}$ . If index  $\ell$  denotes the border  $L_\ell$  between cells  $V_{n_{r-1}}$  and  $V_{n_r}$ , the last factor after the brackets in Eq. (42) must be skipped. If  $L = \ell$ , Eq. (42) reduces to

$$\mathcal{R}_{LL}^{G,c}(i, t | \tau, m, \tau^*) = \frac{1 - v_{i,n_a}^G \cdot \frac{(t - \tau) - t_{mn_a}}{t_{mn_{a+1}} - t_{mn_a}}}{1 - v_{i,n_a}^G \cdot \frac{(\tau^* - \tau) - t_{mn_a}}{t_{mn_{a+1}} - t_{mn_a}}} \quad (43)$$

Now, let us consider the second case where  $L$  is the border between cells  $V_{n_a}$  and  $V_{n_{a+1}}$ ; we have

$$\begin{aligned} \mathcal{R}_{L\ell}^{G,c}(i, t | \tau, m, \tau^*) &= \left[ \prod_{j=a+1}^{r-1} (1 - v_{i,n_j}^G) \cdot (1 - w_{i,n_j n_{j+1}}^G) \right] \\ &\times \left( 1 - v_{i,n_a}^G \cdot \frac{t - (\tau + t_{m\ell})}{t_{ms} - t_{m\ell}} \right) \quad (44) \end{aligned}$$

if  $\ell$  stands for the cell  $V_\ell \equiv V_{n_r}$ , and

$$\mathcal{R}_{L\ell}^{G,c}(i, t | \tau, m, \tau^*) = \left[ \prod_{j=a+1}^{r-1} (1 - v_{i,n_j}^G) \cdot (1 - w_{i,n_j n_{j+1}}^G) \right] \quad (45)$$

if  $\ell$  denotes the border  $L_\ell$  between  $V_{n_{r-1}}$  and  $V_{n_r}$ .

Finally, we give the expression of  $r_{L\ell}^{G,c}(i, t | \tau, m, \tau^*)$  in the different possible cases. If  $\ell$  stands for the cell  $V_{n_r}$ , we have

$$\begin{aligned} r_{L\ell}^{G,c}(i, t | \tau, m, \tau^*) &= \mathcal{R}_{LL_r}^{G,c}(i, \tau + t_{m\ell} | \tau, m, \tau^*) \\ &\times H(t - \tau - t_{m\ell}) H(\tau + t_{ms} - t) \\ &\times \frac{v_{i,\ell}^G}{t_{ms} - t_{m\ell}}, \quad (46) \end{aligned}$$

where  $L_r$  is the border between  $V_{n_{r-1}}$  and  $V_{n_r}$ .

If  $\ell$  denotes the border  $L_\ell \equiv L_r$ , we obtain

$$\begin{aligned} r_{L\ell}^{G,c}(i, t | \tau, m, \tau^*) &= \mathcal{R}_{L_{n_{r-1}}}^{G,c}(i, t | \tau, m, \tau^*) w_{i,n_{r-1} n_r}^G \\ &\times \delta(t - \tau - t_{m\ell}) \quad (47) \end{aligned}$$

The Dirac peak in Eq. (47) actually comes from the derivation of the implicit Heaviside stepfunction on  $t$  in the expression of  $\mathcal{R}$ .

#### IV.C. Accounting for Random Shocks

In the first paper of this series,<sup>4</sup> we have modeled the possibility of an instantaneous modification of some process variables value when a change of dynamics occurs. Such a situation can for instance correspond to the modeling of a combustion, which has a much smaller duration than the other characteristic times of the transient and which can therefore be considered instantaneous.

The magnitude of such a jump in the process variables is random; the value  $\bar{x}^+$  of the process variables after a transition between dynamics  $j$  and  $i$  is written

$$\bar{x}^+ = \bar{y}_{ji}(\bar{x}^-, \bar{z}), \quad (48)$$

where  $\bar{x}^-$  are the process variables before the transition and  $\bar{z}$  is a vector of shock variables, distributed according to the pdf  $\phi_{ji}(\bar{z})$ . Going back to the combustion example mentioned above, a possible shock variable is the burn completeness.

In order to integrate this feature in our cell-to-cell framework and to obtain the adaptation of Eq. (20) [or Eq. (39) in the non-Markov case], we introduce the probability  $J_{ji}(n \rightarrow \ell | \bar{z})$  that the transition  $j \rightarrow i$  will be associated with a jump between cells  $V_n$  and  $V_\ell$ , given  $\bar{z}$  is the value of the shock variables. We observe therefore that the deterministic jump (given  $\bar{z}$ ) determined by Eq. (48) in the continuous model is again interpreted in the cell-to-cell transport theory as a transfer probability between cells.

Equation (20) then becomes

$$\begin{aligned} \varphi_\ell(i, t) &= \sum_F \sum_j \sum_m \sum_n \sum_{c \in \mathcal{C}_j\{m, n\}} \int_0^t d\tau T_{mn}^c(j, t - \tau) \\ &\times \left( \int J_{ji}(n \rightarrow \ell | \bar{z}) \phi_{ji}(\bar{z}) d\bar{z} \right) \\ &\times [\pi_m(j, \tau) \delta(\tau) + \varphi_m(j, \tau)] q_{ji}^{F,c}(t - \tau, m) \quad (49) \end{aligned}$$

Of course, the integration on  $\bar{z}$  could easily be replaced with a sum on  $\bar{z}$  cells on which these shock variables would be discretized as well.

The same kind of adaptation is straightforward in Eqs. (39) and (40) in the non-Markov case.



## V. PRACTICAL IMPLEMENTATION

Considering the evolution equations between hybrid states that were deduced in Sec. IV.B.2, we observe the following:

- The activation probabilities of stimuli within cells and at setpoints are data for the problem.
- The distributions of the time delays between a stimulus activation and the occurrence of the event should not be more difficult to assess in the discrete cell-to-cell scheme than in the continuous case.
- Transfer probabilities  $T_{m\ell}^c(i, t)$  in dynamics  $i$  along path  $c$  cannot be computed as such from Eq. (12); they have to be approximated from a limited number of dynamic runs. The same conclusion is true for the pdf  $g_i^c$  of the sojourn times in the different cells of the path.

In order to estimate these two sets of quantities, we define, such as in the first time discrete cell-to-cell technique (see Sec. II.A), a finer grid inside each cell. Yet, the way we suggest to use it is somehow different.

The stimulus-based theory developed in Ref. 4 aims at dealing with level-2 PSA scenarios. Therefore, the corresponding accident sequences are not likely to display cycles of transitions between configurations; rather, they present a one-directional evolution toward an end state, be it a failure event or a safe situation. For this reason, there is no need to preprocess transfer probabilities for each and every couple of cells, in all possible dynamics, since some regions of phase-space will never be visited in some dynamics. Moreover, the risk of creating nonphysical scenarios through the discretization process, which was mentioned in Sec. II.C, should be reduced as much as possible.

In order to account for these characteristics of the problem, the following scheme is propounded, starting only from those cells  $V_m$  in which the system can initially lie and in those dynamics  $i$  that can be entered at the beginning of the transient:

- From the center of each subcell belonging to the fine grid within cell  $V_m$ , the continuous process variables evolution in dynamics  $i$  is computed.
- Each cell  $V_\ell$  crossed by this trajectory is checked to belong to or not belong to an already identified path of cells  $c$ . The time interval during which the system lies in cell  $V_\ell$  leads to a crenellation-shaped estimation of  $T_{m\ell}^c(i, t)$  for this run; these individual estimations will be averaged on all runs initiated in subcells of  $V_m$  to provide the approximated value of  $T_{m\ell}^c(i, t)$ .
- The subcells of  $V_\ell$  visited by the current trajectory are marked; only those subcells that are marked

after completing all the runs originating in cell  $V_m$  are to be considered when estimating the transfer probabilities of type  $T_{m\ell}^c(j, t)$  at a second stage of preprocessing; only those dynamics  $j$  where the system can undergo a transition to from dynamics  $i$  in cell  $V_\ell$  are then to be investigated.

As for the pdf  $g_i^c$ , it can be assessed from the runs we have to perform to obtain the transfer probabilities  $T_{mv}^c(i, t)$ . Indeed, in each run,  $t_{mv}$  is the time at which cell  $V_v$  is entered. Collecting this information in all runs performed from the hybrid state  $(i, V_m)$  provides a histogram from which the distribution  $g_i^c(t_{mv})$  can be obtained after proper normalization. It can be noticed that using such a normalized histogram is more appropriate than choosing a specific type of distribution, such as a simple uniform law. Indeed, we have for instance  $t_{mp} = t_{mn} + \tau_{np}$ , where  $\tau_{np}$  is the sojourn time in cell  $V_n$  up to the border of  $V_p$  and  $g_i^c(t_{mp})$  is the convolution of  $g_i^c(t_{mn})$  and the pdf of  $\tau_{np}$ . Yet, uniform densities are not conjugate, and this choice of distribution would imply a strong assumption on the nature of the distribution of  $\tau_{np}$ .

We can also note that such a histogram, before normalization, can be used in the non-Markov case as well. It must then be averaged to provide the transfer probability between cell  $V_m$  and the setpoint at the border before entering  $V_v$ .

## VI. CONCLUSIONS

In this second paper, the issue of practically implementing the concept of stimulus-driven branchings in the construction of an accident progression event tree was addressed. We propounded to resort to an interpretation of the dynamic evolution of the plant in the different configurations in which it can lie as a probabilistic transfer between cells based on the partition of the process variables space entailed by the definition of the stimuli.

First, previous works on cell-to-cell mapping applied to dynamic reliability problems were reviewed. This allowed us to pinpoint new challenges to be taken up in our case, namely, the discretization of integral equations instead of partial differential equations and the need to release the Markovian assumption. Above this, a deeper look at these works highlighted how the discretization of the dynamics could affect the problem itself by creating nonphysical situations with a nonzero probability.

The notion of path of cells helped us to bring a first solution to the abovementioned drawback. These mutually exclusive paths along which two cells can be connected alongside the same dynamics are an essential part of the modeling of competing events, as stimuli are activated in a possibly different order depending on the path considered. This concept was included in the

discrete form of both semi-Markov and non-Markov sets of evolution equations for the ingoing and probability densities describing the branching process. As a result, a sound methodological approach to level-2 PSA applications, including the effect of the dynamics on the generation of scenarios, is thus propounded. Considerations on how to implement practically the discrete cell-to-cell scheme were then given.

Ongoing work devoted to the application of this method to large-sized applications is now needed. Its use as a basis for devising numerical schemes to solve the quantitative problem of estimating the frequency of accident sequences should also be considered. Accordingly, future developments should also investigate if the present partition in cells based on the regions defined by the stimuli in phase-space is sufficiently refined in practice.

## APPENDIX

### BACKWARD TREATMENT

One of the drawbacks of the forward treatment presented in Sec. IV is the need to resort to a coupled system of equations (for the ingoing density and for the probability density) to model the problem and to give allowance to the entry in a new dynamics in a semi-Markovian assumption. The backward formulation of the problem, which refers to the conditional probability density, contains similar information in one equation, provided the conditioning coordinates correspond to the entry in a new dynamics.

We therefore present in this Appendix the cell-to-cell form of the backward equations that were also given in our companion paper.

#### A.I. SEMI-MARKOV CASE

Using Eqs. (15) and (17), we obtain for the conditional probability density

$$\begin{aligned} \pi(\bar{x}, i, t | \bar{x}_o, k, t_o) &= \delta_{ik}(1 - P_i(t - t_o; \bar{x}_o))\delta(\bar{x} - \bar{g}_i(t - t_o, \bar{x}_o)) \\ &+ \sum_{j \neq k} \sum_F \int_{t_o}^t q_{kj}^F(\tau - t_o; \bar{x}_o) \pi(\bar{x}, i, t | \bar{g}_k(\tau - t_o, \bar{x}_o), j, \tau) d\tau . \end{aligned} \quad (\text{A.1})$$

Let  $\pi_\ell(i, t | m, k)$  be the probability that the system lies in cell  $V_\ell$  while evolving according to dynamics  $i$ , a time  $t$  after entering dynamics  $k$  in cell  $V_m$ . Using the notations introduced in Eqs. (20), (21), and (22), we obtain as the result of the discretization

$$\pi_\ell(i, t | m, k) = \delta_{ik} \mathcal{P}_{m\ell}(i, t) + \sum_n \sum_{j \neq k} \sum_F \sum_{c \in C_k\{m, n\}} \int_o^t T_{mn}^c(k, \tau) q_{kj}^{F,c}(\tau, m) \pi_\ell(i, t - \tau | n, j) d\tau , \quad (\text{A.2})$$

where

$$\mathcal{P}_{m\ell}(i, t) = \sum_{c \in C_i\{m, \ell\}} T_{m\ell}^c(i, t) \mathcal{P}_{m\ell}^c(i, t) . \quad (\text{A.3})$$

#### A.II. GENERAL NON-MARKOV CASE

This time, the probability density is taken conditional to a last event having taken place at  $(\bar{u}^*, \tau^*)$  and having resulted in a set  $\mathcal{A}$  of activated stimuli in dynamics  $k$  entered at  $\tau$ . We have

$$\begin{aligned} \pi(\bar{x}, i, t | \bar{u}^*, k, \tau^*, \tau, \vec{\tau}_A, \mathcal{A}) &= \delta_{ik} \cdot \delta(\bar{x} - \bar{g}_i(t - \tau^*, \bar{u}^*)) (1 - P_i(t; \tau^*, \tau, \bar{u}^*, \vec{\tau}_A, \mathcal{A})) \\ &+ \sum_{G \notin \mathcal{A}} \int_{\tau^*}^t d\tau_G \pi(\bar{x}, i, t | \bar{g}_k(\tau_G - \tau^*, \bar{u}^*), k, \tau_G, \tau, \vec{\tau}_{\mathcal{A} + \{G\}}, \mathcal{A} + \{G\}) \cdot p_k^G(\tau_G; \tau^*, \tau, \bar{u}^*, \vec{\tau}_A, \mathcal{A}) \\ &+ \sum_{\mathcal{A}'} \sum_j \int_{\tau^*}^t ds \pi(\bar{x}, i, t | \bar{g}_k(s - \tau^*, \bar{u}^*), j, s, s, \vec{\tau}_{\mathcal{A}'}, \mathcal{A}') \sum_{G \in \mathcal{A}} p_{kj}^G(s; \tau^*, \tau, \bar{u}^*, \vec{\tau}_A, \mathcal{A}) \delta_{kj}^G(\mathcal{A} \rightarrow \mathcal{A}') . \end{aligned} \quad (\text{A.4})$$

In order to discard nonphysical system evolutions, the conditional probability associated with the cell-to-cell transfer process refers to the cell  $V_m$  where dynamics  $k$  was entered, as well as to places  $\vec{m}_A$  where the activations took place. Then, using the notations defined in Sec. IV.B,

$$\begin{aligned}
& \pi_\ell(i, t | L, k, \tau^*, \tau, m, \vec{\tau}_A, \vec{m}_A, \mathcal{A}) \\
&= \delta_{ik} \cdot \sum_{c \in \mathcal{C}_i\{m, \vec{m}_A, \vec{\tau}_A, \ell\}} T_{L\ell}^c(i, t - \tau^*) \prod_{G \in \mathcal{A}} \mathcal{R}_{L\ell}^{G,c}(i, t | \tau, m, \tau^*) \cdot \prod_{F \in \mathcal{A}} \frac{1 - \tilde{H}_i^F(t - \tau; c | \tau - \tau_F)}{1 - \tilde{H}_i^F(\tau^* - \tau; c | \tau - \tau_F)} \\
&+ \sum_{G \notin \mathcal{A}} \sum_{m_G} \int_{\tau^*}^t d\tau_G \sum_{c \in \mathcal{C}_k\{m, \vec{m}_A, \vec{\tau}_A, m_G\}} T_{Lm_G}^c(k, \tau_G - \tau^*) \sum_{G \in \mathcal{A}} r_{Lm_G}^{G,c}(k, \tau_G | \tau, m, \tau^*) \cdot \prod_{\substack{H \notin \mathcal{A} \\ H \neq G}} \mathcal{R}_{Lm_G}^{H,c}(k, \tau_G | \tau, m, \tau^*) \\
&\times \prod_{F \in \mathcal{A}} \frac{1 - \tilde{H}_k^F(s^* - \tau; c | \tau - \tau_F)}{1 - \tilde{H}_k^F(\tau^* - \tau; c | \tau - \tau_F)} \cdot \pi_\ell(i, t | m_G, k, \tau_G, \tau, m, \vec{\tau}_{A+\{G\}}, \vec{m}_{A+\{G\}}, \mathcal{A} + \{G\}) \\
&+ \int_{\tau^*}^t ds \sum_n \sum_{c \in \mathcal{C}_k\{m, \vec{m}_A, \vec{\tau}_A, n\}} T_{Ln}^c(k, s - \tau^*) \cdot \prod_{F \notin \mathcal{A}} \mathcal{R}_{Ln}^{F,c}(k, s | \tau, m, \tau^*) \\
&\times \sum_j \sum_{G \in \mathcal{A}} \frac{\tilde{h}_{kj}^G(s - \tau; c | \tau - \tau_G)}{1 - \tilde{H}_k^G(\tau^* - \tau; c | \tau - \tau_G)} \cdot \prod_{\substack{H \in \mathcal{A} \\ H \neq G}} \frac{1 - \tilde{H}_k^H(s - \tau; c | \tau - \tau_H)}{1 - \tilde{H}_k^H(\tau^* - \tau; c | \tau - \tau_H)} \\
&\times \sum_{A'} \delta_{kj}^G(\mathcal{A} \rightarrow A') \cdot \pi_\ell(i, t | n, j, s, n, \vec{\tau}_{A'}, \vec{0}, A') . \tag{A.5}
\end{aligned}$$

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