



## Intrinsic common noise in a system of two coupled Brusselators

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### ABSTRACT

We investigate effects of coupling two chemical subsystems through diffusion of chemical species. We consider the Langevin description of the actual microscopic dynamics and show that diffusive coupling gives rise to a common noise term along with the deterministic interaction. As a model example, we study two diffusively coupled Brusselator systems. By numerical Langevin simulations, we inspect the effect of the common noise term on the total correlation between the two Brusselators; we also verify the validity of the Langevin approach by comparison to simulations of the more accurate master equation. The intrinsic common noise has its strongest effect for the Brusselator dynamics operating at a stable fixed point far from the Hopf bifurcation; in this case, the common noise reduces the correlation of the Brusselators significantly. We also show that for specific parameter sets the covariance between the systems is maximized (or minimized) at a finite system size.

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### 1. Introduction

Intrinsic noise is important in chemical reactions that involve only a small number of molecules. This condition is met in many biochemical reactions that occur in cells [1] which are additionally subject to environmental (external) noise [1,2]. Dynamical behaviors that are shaped by these noise sources range from mere steady-state fluctuations [2] to sustained stochastic oscillations [3–6] and transitions between metastable states [7].

Effects of intrinsic noise can be either studied by the master equation for the actual number of reacting molecules [8] or by the chemical Langevin equation (CLE) and its corresponding Fokker–Planck equation [9,10]; the limitations of the latter have been explored by Peter Hänggi in his early work, see, e.g. [11,12]. The CLE basically represents a stochastic version of the well-known rate equations of chemical physics. Therefore, in many cases it is more instructive than the master equation because in the deterministic limit (infinitely many molecules), the CLEs correspond to the standard rate equations. For example, if the rate equations show a limit-cycle solution, it is plausible from the respective Langevin equations that the corresponding finite system displays stochastic oscillations. This behavior would be much harder to predict from the more exact but cumbersome master equation. Numerical studies have shown that the Langevin equation can

approximate the master equation faithfully for sufficiently high number of molecules [10].

The description by a master equation becomes particularly cumbersome for *coupled* chemical systems. Such systems are of special interest because they are capable of *cooperative* behavior. In order to theoretically describe phenomena like synchronization, which are ubiquitous in a wide variety of natural systems [13], coupled rate or Langevin equations are often considered instead of the full master equation (for limitations of the rate-equation approach compared to the master equation in a coupled system, see Ref. [14]). Such mathematical models can describe, for instance, cooperative behavior in coupled biochemical systems, observed across a large population of cells [15,16,4,17–19]. Here, intercell signaling provides the dynamical coupling, for instance, by quorum sensing [20,21] (signaling molecules exchanged between cells regulating their behavior).

Distributed systems can show strong correlations even if its elements are uncoupled but all elements are driven by a common stimulus. This has been studied in detail, for generic limit-cycle oscillators [22,23] and for excitable neural models [24] as well as experimentally in real neurons [25,26].

In this paper we are interested in the effects of intrinsic common noise arising from the coupling of chemical systems. From a theoretical point of view, this brings together the two different origins of cooperative behavior emerging in distributed systems: coupling and common stimulus. As an example, consider two subsystems specified by variables  $\{X\}$  and  $\{Y\}$  and having similar reaction channels. Assume that there is one chemical species, say

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$X_i$  and  $X'_i$  which can freely diffuse between them [27]. The corresponding reaction channels



couple the two subsystems. Depending on the rate of diffusion governed by  $\varepsilon$  and  $\varepsilon'$ , the other variables  $X_j$  and  $X'_j$  (with  $j \neq i$ ) can display correlations. As we will argue in the next section, such coupling via Eq. (1) introduces besides the usually considered deterministic interaction term, a common noise term in the chemical Langevin equation for the coupled system. The specific form of the common noise is multiplicative (it involves the number of molecules of the diffusing species) and anti-correlated between the systems (it enters with different signs into the dynamics of the two subsystems). In order to separate out the effects of the deterministic coupling and the common noise, we artificially set one of them to zero and compare the resulting correlation statistics to those of the full system. We also compare our extensive simulations of the chemical Langevin equations with simulations of the master equation. We aim at a thorough characterization of the effect of intrinsic noise in the system of two coupled Brusselators by looking at the equal-time covariance and the corresponding correlation coefficient [see Eqs. (15) and (16)] for various dynamical regimes of the Brusselator model.

In Section 2, we discuss the effect of coupling two arbitrary chemical systems diffusively, and introduce our methodology of study. In Section 3, we study the equal-time cross-correlation of two coupled Brusselators taking separately into account deterministic coupling and intrinsic common noise. We conclude in Section 4 with a summary and discussion of our results.

## 2. Methodology and coupling mechanism

A chemical process at the microscopic level can be specified by a set of elementary processes which are symbolically written as a set of “reaction” channels



where the  $X$  represent the number of molecules of different chemical species (represented by the subscript), and  $c_m$  is the rate for the  $m$ th such channel. The time evolution of such a system can be treated as a stochastic process where the chemical species  $X_i(t)$  are random variables. Such molecular fluctuations are often referred to as internal noise since their origin is in the very mechanism of the evolution of the state of the system [9]. The strength of the noise depends on the volume of the system and the reaction propensities and is not always small enough to be treated perturbatively.

As is well known, such a system is described by a master equation (ME) [9] for the evolution of configurational probabilities [9], which is written as

$$\frac{d}{dt}P(C, t) = \sum_{C'} P(C', t)W_{C'-C} - \sum_{C'} P(C, t)W_{C-C'}, \quad (3)$$

where  $P(C, t)$  is the probability of configuration  $C$  at time  $t$  and  $\{W\}$  are the transition probabilities.

One way to study such a system is by using stochastic simulation techniques [8]. The Gillespie algorithm [8] is consistent with the master equation formalism and gives a numerical method to study the time evolution of different chemical species. Alternatively, one can obtain the chemical Langevin equation (CLE) for the system, which provides an approximate description for sufficiently large system size [10]. In general, these will have the form

$$\frac{dX_i(t)}{dt} = \sum_{j=1}^M v_{ji} a_j(\mathbf{X}(t)) + \sum_{j=1}^M v_{ji} a_j^{1/2}(\mathbf{X}(t)) \xi_j(t), \quad (4)$$

where  $v_{ji}$  is the change in  $X_i$  produced by the  $j$ th reaction (typically, an integer number),  $a_j(\mathbf{X}(t))$  is the propensity of  $j$ th reaction and  $\xi_j(t)$  are

temporally uncorrelated, statistically independent Gaussian white noises with  $\langle \xi_i(t) \rangle = 0$  and  $\langle \xi_i(t) \xi_j(t') \rangle = \delta_{ij} \delta(t - t')$ . Note that the  $X_i$ 's are treated as continuous rather than discrete variables and that the equations have to be interpreted in the sense of Ito [9]. This equation can be solved numerically by the simple Euler scheme:

$$X_i(t + dt) = X_i(t) + \sum_{j=1}^M v_{ji} a_j(\mathbf{X}(t)) dt + \sum_{j=1}^M v_{ji} a_j^{1/2}(\mathbf{X}(t)) N_j(t) (dt)^{1/2}, \quad (5)$$

where  $N_j(t)$  are normally distributed variables with zero mean and unit variance. Instead of considering the number of molecules, we use in the following the concentrations  $x_i = X_i/V$  ( $V$  is the volume) and their corresponding Langevin equations. Because the propensities  $a_i$  scale with the volume, the deterministic parts of the Langevin equations for the concentrations will be (largely) independent of the volume, whereas the stochastic force scales like  $V^{-1/2}$ .

Let us consider two uncoupled chemical systems with species denoted by  $X$  and  $X'$  and corresponding concentrations  $x$  and  $x'$ , with identical reaction schemes and the same chemical rates. The Langevin equations for the two uncoupled systems will have the general form:

$$\dot{x} = f(x) + g(x, V) \xi_x(t), \quad (6)$$

$$\dot{x}' = f(x') + g(x', V) \xi_{x'}(t), \quad (7)$$

where  $\xi_x(t)$  and  $\xi_{x'}(t)$  are uncorrelated Gaussian white noises. The functional form of  $f$  and  $g$  depends on the actual reaction schemes and is given by Eq. (4). If we now couple the two systems diffusively via Eq. (1), following the prescription of Eq. (4), we obtain an additional deterministic interaction term in the drift term of the Langevin equation and an additional common noise term in the fluctuating driving force:

$$\dot{x} = f(x) + \varepsilon(x' - x) + g(x, V) \xi_x(t) - \sqrt{\frac{\varepsilon X}{V}} \xi_c^{(1)}(t) + \sqrt{\frac{\varepsilon X'}{V}} \xi_c^{(2)}(t), \quad (8)$$

$$\dot{x}' = f(x') + \varepsilon(x - x') + g(x', V) \xi_{x'}(t) + \sqrt{\frac{\varepsilon X}{V}} \xi_c^{(1)}(t) - \sqrt{\frac{\varepsilon X'}{V}} \xi_c^{(2)}(t). \quad (9)$$

Since  $\xi_c^{(1)}(t)$  and  $\xi_c^{(2)}(t)$  are independent noise sources (with  $\langle \xi_c^{(i)}(t) \xi_c^{(j)}(t') \rangle = \delta_{(ij)} \delta(t - t')$ ) appearing due to the coupling, we can write,

$$\sqrt{\frac{\varepsilon X}{V}} \xi_c^{(1)}(t) - \sqrt{\frac{\varepsilon X'}{V}} \xi_c^{(2)}(t) = \sqrt{\frac{\varepsilon(x + x')}{V}} \xi_c(t). \quad (10)$$

where  $\xi_c(t)$  is an uncorrelated Gaussian white noise. Eqs. (8) and (9) is then written as,

$$\dot{x} = f(x) + \varepsilon(x' - x) + g(x, V) \xi_x(t) - \sqrt{\frac{\varepsilon(x + x')}{V}} \xi_c(t), \quad (11)$$

$$\dot{x}' = f(x') + \varepsilon(x - x') + g(x', V) \xi_{x'}(t) + \sqrt{\frac{\varepsilon(x + x')}{V}} \xi_c(t). \quad (12)$$

The deterministic interaction term has the usual form of Hookean spring and will be also referred in the following as the deterministic coupling. This term will typically lead to positive correlations between  $x$  and  $x'$ . The common noise term (the last one in both equations) is special in several respects. First, it enters both equations with opposite signs, i.e., the common noise terms affecting  $x$  and  $x'$  are actually anti-correlated. So, it is plausible that this term may lead to negative correlations or at least reduce positive correlations (which are due to the deterministic coupling). Secondly, the amplitude of the common noise is determined by the sum of  $x$  and  $x'$ . A sudden increase in either of the variables will lead to a sudden increase of the noise level in both systems. Below we will see an example where such an increase can also lead to positive correlations.

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