Modelling and control of stochastic hybrid PDP systems

Alfio Borzì

Institut für Mathematik, Universität Würzburg
Lehrstuhl Mathematik IX - Wissenschaftliches Rechnen
and Würzburg - Wroclaw Center for Stochastic Computing (WWCSC)

The Team Scientific Computing - WiReMIX

- Prof. Dr. Alfio Borzì
- Prof. Dr. Roland Griesmaier
- Petra Markert-Autsch
- Dr. Stephan Schmidt
- Tanvir Rahman
- Andreas Schindele
- Suttida Wongkaew
- Martin Sprengel
- Beatrice Gaviraghi
- Gabriele Ciaramella
- Juri Merger
- Duncan Kioi Gathungu
- Christian Schmiedecke

www9.mathematik.uni-wuerzburg.de

Collaboration and projects

- Mario Annunziato (U Salerno)
- Julien Salomon (U Paris-Dauphine)
- Sergio González Andrade (U Quito)
- Marcin Magdziarz, Aleksander Weron (Wroclaw UT)
- Fabio Nobile (EPF Lausanne), Raul Tempone (KAUST Thuwal)
- Kees Oosterlee (CWI Amsterdam, TU Delft)
- Marco Caponigro (CNAM Paris), Krzysztof Kułakowski (AGH Krakow)
- Paola Antonietti, Marco Verani (Politecnico Milano, MOX)

1. EU Project Marie Curie Action 'Multi-ITN STRIKE - Novel Methods in Computational Finance'
2. DFG Project 'Controllability and Optimal Control of Interacting Quantum Dynamical Systems
3. BMBF Project 'Robust energy optimization of fermentation processes for the production of biogas and wine'
4. IZKF Project 'Parallel Multigrid Imaging and Compressed Sensing for Dynamic 3D Magnetic Resonance Imaging'.

Randomness in evolution models

Randomness can be included into modeling evolution equations in two different ways:

Noise is added to deterministic evolution equations to model random perturbations.

Random perturbations are being modeled by jump (point) processes, where a stochastic action affects the deterministic motion only at some instants of time.

In all cases, the state of such processes can be characterized by the shape of the corresponding probability density functions (PDFs).

The evolution of the PDF of a stochastic process is modelled by a Fokker-Planck-Kolmogorov partial differential equation.

Piecewise deterministic processes and all that

Piecewise Deterministic Process (PDP):
A PDP involves a hybrid state space, with both continuous and discrete states. Randomness appears only in the discrete transitions; between two consecutive transitions the continuous state evolves according to a system of ODEs. Transitions occur according to a generalized Poisson process and are driven by a transition matrix. Ex: telegraph process, growth of bacterial populations.

Switching Diffusion Process (SDP):
A SDP involves a hybrid state space, with both continuous and discrete states. The continuous state evolves according to a SDE, while the discrete state that enters in the SDE is a Markov chain. Ex: school of fishes.

Stochastic Hybrid System (SHS):
A SHS involves a hybrid state space, with both continuous and discrete states. The continuous state obeys a SDE/ODE that depends on the hybrid state. Transitions occur when the continuous state hits the boundary of the state space. The value of the discrete state after the transition is determined deterministically by the hybrid state before the transition. The new value of the continuous state is governed by a probability law which depends on the last hybrid state. Ex: bouncing ball with dissipation.

Piecewise deterministic processes

A piecewise-deterministic process is a model governed by a set of differential equations that change their deterministic structure at random points in time.

We consider a PDP model with a d-components state function $X : [t_0, \infty) \to \Omega$, $\Omega \subseteq \mathbb{R}^d$.
The state function satisfies the following evolution equation

$$\dot{X}(t) = A_{\mathcal{S}(t)}(X), \quad t \in [t_0, \infty),$$

where $\mathcal{S}(t) : [t_0, \infty[\to \mathbb{S}$ is a Markov process with discrete states $\mathbb{S} = \{1, \ldots, S\}$.
Given $s \in \mathbb{S}$, we say that the dynamics is in the deterministic state s, driven by the dynamics function

$$A_s : \Omega \to \mathbb{R}^d, \qquad A_s \in \{A_1, \ldots, A_S\}$$

We require that all $A_s(\cdot), s \in \mathbb{S}$, be Lipschitz continuous, so that for fixed s, the solution $X(t)$ exists and is unique and bounded.

The state function satisfies the initial condition $X(t_0) = X_0 \in \Omega$ being in the initial state $s_0 = \mathcal{S}(t_0)$.

Transition probabilities

The process $\mathcal{S}(t)$ is characterized by a Poisson process PDF given by $\psi_s(t) = \mu_s e^{-\mu_s t}$. It is the PDF for the time the system stays in the state s.

The process $\mathcal{S}(t)$ is modeled by a stochastic transition probability matrix, $\hat{q} := \{q_{ij}\}$, with the following properties

$$0 \leq q_{ij} \leq 1, \quad \sum_{i=1}^{S} q_{ij} = 1, \qquad \forall i, j \in \mathbb{S}.$$

When a transition event occurs, the PDP system switches instantaneously from a state $j \in \mathbb{S}$, with dynamic function A_j, randomly to a new state $i \in \mathbb{S}$, driven by the dynamic function A_i. Virtual transitions from the state j to itself are allowed for this model, this means that we allow $q_{jj} > 0$.

The PDP Fokker-Planck-Kolmogorov equation

The PDP Fokker-Planck-Kolmogorov (FPK) equation for the PDFs of a PDP process is given by

$$\partial_t f_s(x,t) + \nabla \left(A_s(x, u_s)\, f_s(x,t) \right) = \sum_{j=1}^{S} Q_{sj}\, f_j(x,t), \quad s = 1, \dots, S.$$

where $Q_{sj} = \mu_j\, q_{sj}$ if $j \neq s$, and $Q_{ss} = \mu_s\,(q_{ss} - 1)$, $s = 1, \dots, S$, $x \in \Omega \subset \mathbb{R}$, for the scalar process $X(t)$ in the state s. We have $\sum_{j=1}^{S} Q_{sj} = 0$. The initial conditions are given as follows

$$f_s(x,0) = f_s^0(x), \qquad s = 1, \dots, S,$$

where $f_s^0(x) \geq 0$ and $\sum_{s=1}^{S} \int_\Omega f_s^0(x) = 1$.
The solution to the FPK system has the following properties
$\sum_{s=1}^{S} \int_\Omega f_s(x,t) = 1$, $t \geq t_0$: conservativeness of the total probability;
$f_s(x) \geq 0$, $t \geq t_0$: non-negativity of the PDFs;

A FPK framework to control stochastic processes

Consider a controlled stochastic process

$$dX(t) = b(X(t), s, u_s)\, dt + c(X(t), v_s)\, dW(t)$$

Assume that the corresponding FPK system is given by

$$\partial_t f_s + F(b(u_s), c(v_s), f_s, \nabla f_s, \nabla^2 f_s) = 0, \qquad s = 1, \ldots, S.$$

A robust control framework (i.e. independent of the single stochastic realisation) is formulated with an objective depending on the PDFs and the FPK system as follows

$$\min_{f,u,v} J(f, u, v)$$

$$s.t. \quad \partial_t f_s + F(b(u_s), c(v_s), f_s, \nabla f_s, \nabla^2 f_s) = 0, \qquad s = 1, \ldots, S.$$

This strategy has been successfully applied to Itō processes, subdiffusion diffusion processes, PDP processes, ... using quadratic cost functionals.

A FPK optimal control problem with quadratic objective

Consider the following tracking objective

$$J(f,u) = \frac{1}{2}\sum_{s=1}^{S} \|f_s(\cdot,T) - f_s^T(\cdot)\|^2_{L^2(\Omega)} + \frac{\nu}{2}\sum_{s=1}^{S} \|u_s\|^2_{L^2(0,T)}.$$

To be minimized under the constraint given by a PDP model. We obtain the following optimality system.

$$\partial_t f_s(x,t) + \nabla\left(A_s(x,u_s)\, f_s(x,t)\right) = \sum_{j=1}^{S} Q_{sj} f_j(x,t), \quad f_s(x,0) = f_s^0(x)$$

$$-\partial_t p_s(x,t) - A_s(x,u_s)\,\nabla p_s(x,t) = \sum_{j=1}^{S} Q_{js} p_j(x,t),$$

$$p_s(x,T) = -\left(f_s(x,T) - f_s^T(x)\right)$$

$$\nu\, u_s(t) - \int_\Omega \left(\nabla p_s(x,t)\right) \frac{\partial A_s(x,u_s)}{\partial u_s}\, f_s(x,t)\, dx = 0.$$

where $s = 1,\ldots,S$, and $p = (p_s)_{s=1}^S$ is the vector of adjoint var.

A PDP process with dichotomic noise

Consider the case of a dissipative process subject to dichotomic noise. Let $X(t)$ be a process whose evolution is described by the following equation

$$\dot{X} = -X + (1+u)\,\xi$$

where the noised input $\xi(t)$ represents a dichotomic noise (random telegraph signal), that takes values ± 1, with Poisson statistics of the switching time.

We have the following (controlled) dynamics

$$A_1(x,u_1) = 1 - x + u_1, \qquad A_2(x,u_2) = -(1 + x + u_2).$$

The adjoint equations are as follows

$$\begin{aligned} -\partial_t p_1(x,t) - (1 - x + u_1)\,\partial_x p_1(x,t) &= -\mu\, p_1(x,t) + \mu\, p_2(x,t) \\ -\partial_t p_2(x,t) + (1 + x + u_2)\,\partial_x p_2(x,t) &= +\mu\, p_1(x,t) - \mu\, p_2(x,t) \end{aligned}$$

with terminal condition given as follows

$$p_s(x,T) = -\left(f_s(x,T) - f_s^T(x)\right), \qquad s = 1,2.$$

Numerical experiments with dichotomic noise

The initial PDF is given by two narrow Gauss distributions centered in $x = 0$ and variance $\sigma = 0.1$. The Poisson parameter of the underling Markov process is $\mu = 0.8$ (singular case).

We define a PDF target given by two Gauss densities traveling in opposite directions and with increasing variances as follows

$$f_1^d(x,t) = \frac{1}{2\sqrt{2\pi\sigma(t)}} e^{-\frac{(x-\mu_1(t))^2}{2\sigma(t)}}$$
$$f_2^d(x,t) = \frac{1}{2\sqrt{2\pi\sigma(t)}} e^{-\frac{(x-\mu_2(t))^2}{2\sigma(t)}}.$$

where $\sigma(t) = 0.1\sqrt{(1+t)}$ and we take an asymmetric pair of Gaussian densities with different velocities for the distribution mean as follows, $\mu_1(t) = 1 - e^{-t}$ and $\mu_2(t) = -\mu_1(t)/3$.

Results of numerical experiments with dichotomic noise

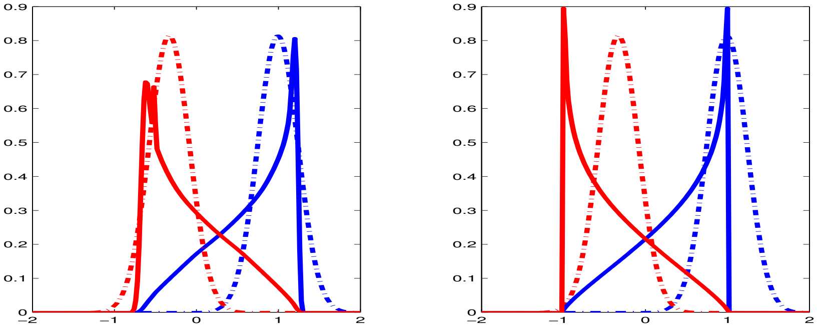
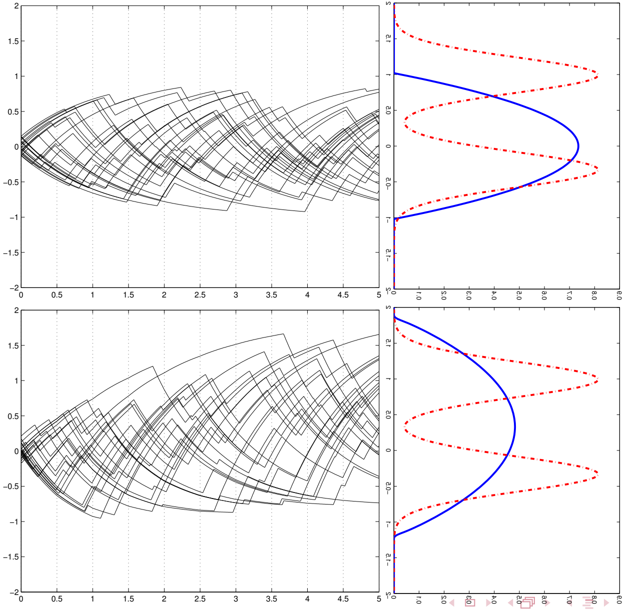


Figure : Results obtained with the PDP process with Poisson rate $\mu = 0.8$. Dotted lines denote the desired PDF target. Solid lines represent the PDFs resulting from the FP evolution. Left is for the controlled process; right the uncontrolled process.

Dichotomic noise: Monte Carlo simulations



From open to closed loop control

An alternative PDP FPK control setting

Consider the following PDP FPK system for the PDFs of a PDP process

$$\partial_t f_s(x,t) + \nabla \left(A_s(x, u_s)\, f_s(x,t) \right) = \sum_{j=1}^{S} Q_{sj}\, f_j(x,t), \quad s = 1, \ldots, S,$$

with controls $u_s = u_s(x,t)$, $s = 1, \ldots, S$.
Now, we chose the following expectation objective

$$J(f,u) = \sum_{s=1}^{S} \int_{\mathbb{R}} g_s(x) f_s(x,T)\, dx + \frac{\nu}{2} \sum_{s=1}^{S} \int_0^T \int_{\mathbb{R}} |u_s(x,t)|^2\, f_s(x,t)\, dx\, dt.$$

We focus on the optimal control problem of finding u_s, $s \in \mathbb{S}$, such that this objective is minimized subject to the constraint given by the PDP FPK system.

The PDP FPK optimality system with expectation objective

The solution of our new PDP FPK optimal control problem is characterized by the solution of the optimality system consisting of the PDP FPK equation and the following

$$
\begin{aligned}
\partial_t p_s(x,t) + A_s(x,u_s)\,\nabla p_s(x,t) + \frac{1}{2}(u_s)^2 &= -\sum_{j=1}^{S} Q_{sj}\, p_j(x,t) \\
p_s(x,T) &= g_s(x) \\
u_s(x,t) + \left(\frac{\partial A_s}{\partial u_s}\right)\nabla p_s(x,t) &= 0,
\end{aligned}
$$

where $s = 1,\ldots,S$. Notice this adjoint problem is decoupled from the FPK system.

Equivalence to the HJB equation

The HJB optimal control of our PDP model was considered in Moresino et al.. In this work, the following Hamiltonian is derived

$$H_s(t, x, \{q_j\}_{j=1}^S, \nabla q_s) := \min_{u_s} \left[A_s(x, u_s) \nabla q_s + \frac{1}{2} u_s^2 + \sum_{j=1}^S Q_{js} q_j \right].$$

It is also proved that the corresponding HJB problem

$$\begin{cases} \partial_t q_s + H_s(t, x, \{q_j\}_{j=1}^S, \nabla q_s) = 0 \\ q_s(x, T) = g_s(x) \end{cases}$$

admits a unique viscosity solution that is also the classical solution to the adjoint FPK equation including the optimality condition.
The adjoint variable p_s corresponds to the value function q_s.

Modelling and control of Subtilin production

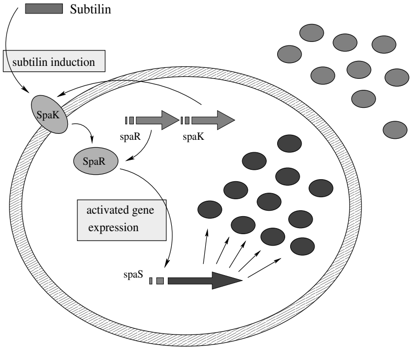


Figure : A schematic representation of the Subtilin production mechanism.

Subtilin production

We discuss PDP systems for modelling the production of the antibiotic Subtilin that is synthesized by the Bacillus Subtilis to eliminate competing microbial species in the same ecosystem.

Whenever the amount of nutrients is sufficient, the B. Subtilis population grows without changing the Subtilin concentration.
When the amount of nutrients falls under a threshold, Subtilin production starts, thus the dynamics of the model changes. The Bacillus Subtilis produces Subtilin to eliminate competing species and other B. Subtilis cells, with the purpose of reducing the demand for nutrients while the decomposition of the killed cells also releases additional nutrients in the environment.

The biological mechanism of Subtilin production

The mechanism of Subtilin production can be sketched as follows. If the amount of nutrients is scarce the composition of SigH, a sigma factor that regulates gene expressions, is turned on. This sigma factor enables the production of SpaRK (SpaR and SpaK) proteins by binding the promoter regions of their genes. The SpaRK ensamble directs the production of the Subtilin structural peptide SpaS, the biosynthesis complex SpaBTC and the immunity machinery SpaIFEG. The complex SpaBTC modifies SpaS to yield the final product Subtilin.

In the Subtilin production model presented in Hu et al., the complexes SpaBTC and SpaIFEG are not taken into account and the proteins SpaK and SpaR are considered as one protein SpaRK. This model comprises 5 dependent variables: the normalized population of Bacillus Subtilis, y_1, the concentration of the nutrients, y_2, and the concentrations of the molecules SigH, SpaRK, and SpaS that are denoted with y_3, y_4, and y_5, respectively.

A PDP model of Subtilin production (I)

The growth of the Bacillus Subtilis population can be modeled by the logistic equation

$$\frac{d}{dt}y_1 = r\, y_1 \left(1 - \frac{y_1}{D_\infty(y_2)}\right),$$

where $D_\infty(y_2)$ represents the equilibrium population size depending on the amount of nutrients y_2. It is given by

$$D_\infty(y_2) = \min\{\frac{y_2}{Y_0}, D_{max}\},$$

where Y_0 and D_{max} are constants (constraints due to space limitation and competition).

The dynamics of the nutrients y_2 is given by

$$\frac{d}{dt}y_2 = -k_1 y_1 + k_2 y_5,$$

where k_1 and k_2 are constants describing the rate of nutrient consumption and the rate of nutrient production, respectively. The second term describes a nutrient increase due to the concentration of SpaS protein, y_5, that eliminates the competitors in the environment.

A PDP model of Subtilin production (II)

The sigma factor SigH, y_3, is produced if and only if the amount of nutrients y_2 falls below a certain threshold ηD_{max} for some $\eta > 0$.
The dynamics of y_3 can be modeled as follows

$$\frac{d}{dt} y_3 = k_3 \, \chi_{(-\infty,\, \eta D_{\boldsymbol{max}})}(y_2) - \lambda_1 y_3,$$

where k_3 represents the production rate of SigH and λ_1 represents its natural decaying rate. We use the indicator function
$\chi_M(y) := \{1 \text{ if } y \in M,\ 0 \text{ if } y \notin M\}$.
Notice that y_3 decreases exponentially towards zero whenever $y_2 \geq \eta D_{max}$ and tends exponentially towards k_3/λ_1 whenever $y_2 < \eta D_{max}$.

A PDP model of Subtilin production (III)

The production of the protein SpaRK, y_4, is controlled by a binary switch S_1. The ensamble SpaRK is produced if and only if S_1 is ON. Therefore the dynamics of y_4 is as follows

$$\frac{d}{dt} y_4 = \begin{cases} -\lambda_2 y_4 & \text{if } S_1 \text{ is OFF,} \\ k_4 - \lambda_2 y_4 & \text{if } S_1 \text{ is ON,} \end{cases}$$

where k_4 represents the SpaRK production rate and λ_2 represents its natural decaying rate.

The production of the protein SpaS is also controlled by a binary switch denoted by S_2. Its dynamics is similar to the dynamics of y_4. We have

$$\frac{d}{dt} y_5 = \begin{cases} -\lambda_3 y_5 & \text{if } S_2 \text{ is OFF,} \\ k_5 - \lambda_3 y_5 & \text{if } S_2 \text{ is ON.} \end{cases}$$

The parameter k_5 represents the production rate and λ_3 represents the natural decaying rate of SpaS.

A PDP model of Subtilin production (IV)

The Subtilin production model can be in four different dynamical states given by $(S_1, S_2) \in \{(0,0),(1,0),(0,1),(1,0)\}$ where ON$=1$ and OFF$=0$.

The switch S_1 is modeled by a 2-states continuous time Markov chain with transition probabilities $a_0(y_3)$ and $a_1(y_3)$, depending on the concentration of SigH and at random exponentially distributed times. We assume the following

$$a_0(y_3) = \frac{e^{-\Delta G_{\boldsymbol{rk}}/RT} y_3}{1 + e^{-\Delta G_{\boldsymbol{rk}}/RT} y_3} \quad \text{and} \quad a_1(y_3) = \frac{1}{1 + e^{-\Delta G_{\boldsymbol{rk}}/RT} y_3},$$

where ΔG_{rk} is the Gibbs free energy of the molecular configuration when the switch S_1 in ON, T is the temperature in Kelvin and $R = 1.99$ cal/mol/K is the gas constant.

Likewise, the switch S_2 is also modeled according to a Markov chain, with $b_0(y_4)$ and $b_1(y_4)$ denoting the probabilities that S_2 switches from OFF to ON and from ON to OFF, respectively. As above, we assume the following

$$b_0(y_4) = \frac{e^{-\Delta G_{\boldsymbol{s}}/RT} y_4}{1 + e^{-\Delta G_{\boldsymbol{s}}/RT} y_4} \quad \text{and} \quad b_1(y_4) = \frac{1}{1 + e^{-\Delta G_{\boldsymbol{s}}/RT} y_4}.$$

A reduced PDP model of Subtilin production

We assume that the variable y_1 is very slowly varying. We obtain $y_1 = D_\infty(y_2) \approx y_2/Y_0$ provided that D_{max} is large enough. Next, we have

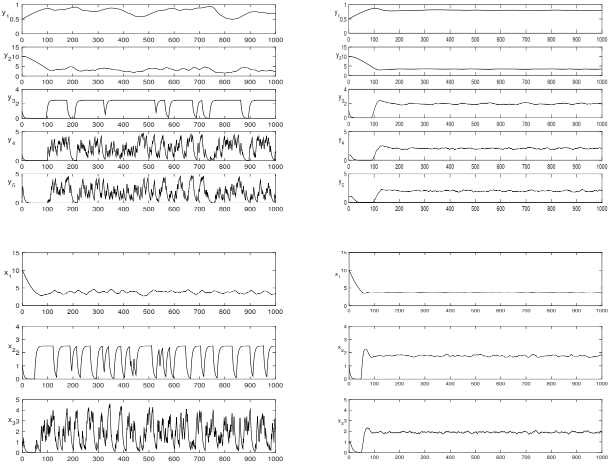
$$\frac{d}{dt} y_2 \approx -k_1 \frac{y_2}{Y_0} + k_2 y_5 .$$

Monte Carlo simulations: SpaRK and SpaS have similar behaviour
Reduced model with (x_1, x_2, x_3), where $x_1 = y_2$ (amount of nutrients), $x_2 = y_3$ (concentration of SigH), and $x_3 = y_5$ (concentration of SpaS). We obtain the following reduced Subtilin production PDP model

$$\begin{aligned} \tfrac{d}{dt} x_1 &= -\tilde{k}_1 x_1 + k_2 x_3 \\ \tfrac{d}{dt} x_2 &= \chi_{(-\infty,\, \eta D_{max})}(x_1)\, k_3 - \lambda_1 x_2 \\ \tfrac{d}{dt} x_3 &= \begin{cases} -\lambda_3 x_3 & \text{if } S_2 \text{ is OFF,} \\ k_5 - \lambda_3 x_3 & \text{if } S_2 \text{ is ON.} \end{cases} \end{aligned}$$

where we set $\tilde{k}_1 \approx k_1/Y_0$.
The transition probabilities for the switch S_2 are given by $b_0(x_2)$ and $b_1(x_2)$.

A comparison of the Subtilin production models



Compare $x_1 \to y_2$, $x_2 \to y_3$, and $x_3 \to y_5$. Top: full model; bottom: reduced model. Left: A run of the Subtilin production model; Right: Evolution of the average variables values corresponding to 200 runs of the reduced Subtilin production model.

The parameter setting is as follows: $\tilde{k}_1 = 0.02$, $k_2 = 0.4$, $k_3 = 0.5$, $k_5 = 1$, $\xi = 0.1$, $\lambda_1 = 0.2$, $\lambda_3 = 0.2$, $\eta = 4$, $D_{max} = 1$, $e^{-\Delta G_s/RT} = 0.4$, and $T = 1000$. The initial values are $y_1(0) = 0.5$, $y_2(0) = 10$, $y_3(0) = 1$, $y_4(0) = 1$, and $y_5(0) = 1$ (full model), and $x_1(0) = 10$, $x_2(0) = 1$ and $x_3(0) = 1$ (reduced

Julius-Maximilians-UNIVERSITÄT WÜRZBURG

PDP dynamics and control functions

We write our reduced PDP model of Subtilin production in the general form $\dot{x}(t) = A_{\mathcal{S}(t)}(x, u_{\mathcal{S}(t)})$. The dynamics-control functions $A_s : \Omega \times U \to \mathbb{R}^3$, $s = 1, 2$, are as follows

$$A_1(x, u_1) = \begin{pmatrix} -\tilde{k}_1\, x_1 + k_2\, x_3 + u_1 \\ \chi_{(-\infty,\, \eta D_{\boldsymbol{max}})}(x_1)\; k_3 - \lambda_1 x_2 \\ -\lambda_3 x_3 \end{pmatrix},$$

and

$$A_2(x, u_2) = \begin{pmatrix} -\tilde{k}_1\, x_1 + k_2\, x_3 + u_2 \\ \chi_{(-\infty,\, \eta D_{\boldsymbol{max}})}(x_1)\; k_3 - \lambda_1 x_2 \\ k_5 - \lambda_3 x_3 \end{pmatrix},$$

where $u_s \in U \subset \mathbb{R}$ denotes the value of the control acting on the Subtilin PDP model in the state s. Notice that the controls model an increase or decrease of concentration of the nutrients.

Stochastic validation

In our model, the stochastic probability transition matrix results in the following ($\mu = \mu_1 = \mu_2$)

$$Q(x_2) = \mu \begin{pmatrix} -b_0(x_2) & b_0(x_2) \\ b_1(x_2) & -b_1(x_2) \end{pmatrix}.$$

We use results of Monte Carlo simulation to compare the PDFs obtained solving the FPK system with the trajectories of the PDP model. This procedure allows to determine Ω such that $Pr(x(t) \in \Omega : t \in (0, T)) = 1$.

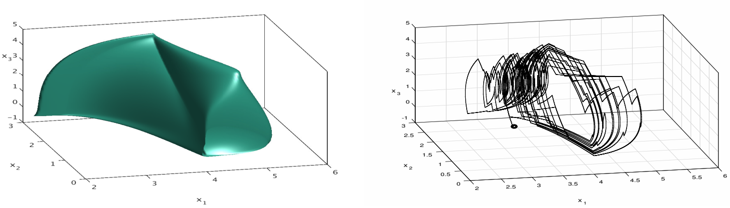


Figure : Representation of the probability density function in the 3 dimensional space. Surface level of the PDFs with value 0.01 (left); a trajectory of the PDP model (right).

Control's objective

We consider the following objective functional

$$J(f,u) = \frac{1}{2}\sum_{s=1}^{2}\int_0^T\int_\Omega |u_s(x,t)|^2\, f_s(x,t)\,\mathrm{d}x\,\mathrm{d}t + \sum_{s=1}^{2}\int_\Omega g_s(x) f_s(x,T)\mathrm{d}x.$$

The first term represents the mean nutrition effort of the control $u = (u_1, u_2)$.
The function g_s models an attractive potential for the final configuration: we require that the mean quantity of SpaS (antibiotics) reaches a desired value given by d_3.
We choose the following attracting potential

$$g(x) = -\frac{\alpha}{2\sigma\sqrt{2\pi}}\, e^{-\dfrac{(x_3-d_3)^2}{2\sigma^2}},$$

where $\sigma > 0$. We take $g_1(x) = g(x)$ and $g_2(x) = g(x)$.

The adjoint FPK system and the optimal controls

With our optimal control setting, we obtain the following

$$u_s(x,t) + \partial_1 \, p_s(x,t) = 0, \qquad s = 1,2.$$

We insert this result in the adjoint FPK equations:

$$\partial_t p_s(x,t) + \sum_{i=1}^{3} A_s^i(x) \partial_1 \, p_s(x,t) - \frac{1}{2}\big(\partial_1 p_s(x,t)\big)^2 = -\sum_{l=1}^{2} Q_{sl}(x) p_l(x,t)$$

$$p_s(x,T) = g_s(x), \qquad s = 1,2.$$

The resulting (p_1, p_2) are inserted in the optimality condition above to obtain the controls.

We derive an appropriate discretization of the transformed adjoint FPK equations using a first-discretize-than-optimize approach where the FPK system is approximated by a first-order accurate, positive preserving, conservative scheme!

Results of numerical experiments: uncontrolled PDP model

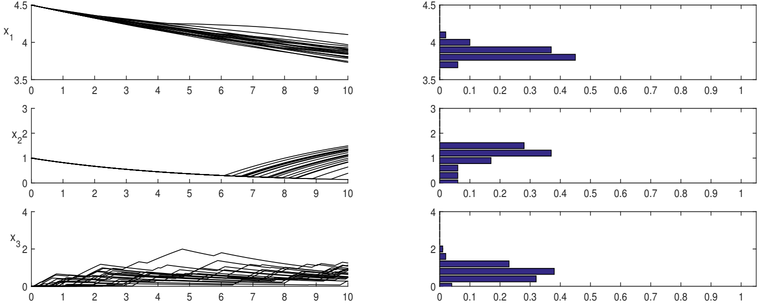
We show results of Monte-Carlo simulation with our PDP Subtilin production model with zero controls.

The initial conditions are given by

$$x_1(0) = 4.5, \qquad x_2(0) = 1.0, \qquad x_3(0) = 0.$$

The obtained mean values at terminal time are given by

$$\bar{x}_1 = 3.861, \qquad \bar{x}_2 = 1.083, \qquad \bar{x}_3 = 0.759.$$



Results of numerical experiments: controlled PDP model

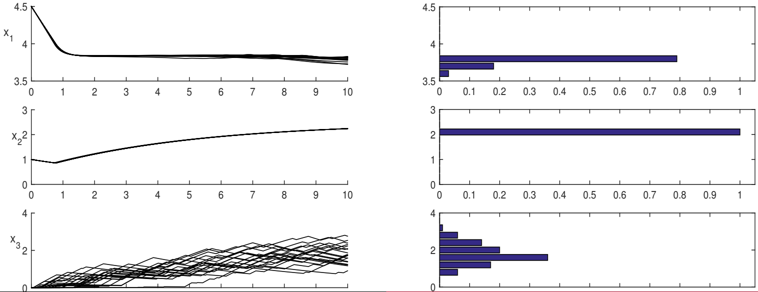
We solve the transmormed adjoint FPK problem to determine the optimal controls u_1 and u_2, that are inserted in the PDP model for a new set of Monte Carlo simulations.

The initial conditions are given by (equal to the uncontrolled case)

$$x_1(0) = 4.5, \qquad x_2(0) = 1.0, \qquad x_3(0) = 0.$$

The obtained mean values at terminal time are given by

$$\overline{x}_1 = 3.783, \qquad \overline{x}_2 = 2.242, \qquad \overline{x}_3 = 1.743.$$



References

- M. Annunziato and A. Borzì, Optimal control of probability density functions of stochastic processes, *Mathematical Modelling and Analysis* **15** (2010) 393–407.
- M. Annunziato and A. Borzì, A Fokker-Planck control framework for multidimensional stochastic processes, *Journal of Computational and Applied Mathematics* **237** (2013) 487–507.
- M. Annunziato and A. Borzì, Fokker-Planck-Based Control of a Two-Level Open Quantum System, *Mathematical Models and Methods in Applied Sciences (M3AS)*, 23 (2013), 2039.
- M. Annunziato and A. Borzì, Optimal Control of Piecewise Deterministic Processes, European Journal of Applied Mathematics, 25 (2014), 1–25.
- M. Annunziato, A. Borzì, F. Nobile, and R. Tempone, *On the connection between the Hamilton-Jacobi-Bellman and the Fokker-Planck control frameworks*, Applied Mathematics, 5 (2014), 2476-2484.
- M. Annunziato, A. Borzì, M. Magdziarz, A. Weron, *A fractional Fokker-Planck control framework for subdiffusion processes*, Optimal Control, Applications and Methods (2015).
- A. Borzì and V. Schulz, *Computational Optimization of Systems Governed by Partial Differential Equations*, (SIAM book series on CSE 08, SIAM, Philadelphia, PA, 2012).
- G. Carlier and J. Salomon, *A monotonic algorithm for the optimal control of the Fokker-Planck equation*, CDC, (2008) 269–273.
- D.R. Cox and H.D. Miller, *The Theory of Stochastic Processes* (Chapman & Hall CRC, 2001).
- M. H. A. Davis, Piecewise-deterministic Markov processes: A general class of non-diffusion stochastic models, *Journal of the Royal Statistical Society. Series B*, **46** (1984) 353–388.
- J. Hu, W.C. Wu, S. Sastry, *Modeling Subtilin Production in Bacillus subtilis Using Stochastic Hybrid Systems.*, Hybrid Systems: Computation and Control, Lecture Notes in Computer Science, Ed.: R. Alur, G.J. Pappas, Springer (2004) 417–431.
- F. Moresino, O. Pourtallier, M. Tidball, *Using Viscosity Solution for Approximations in Piecewise Deterministic Control Systems*, Report RR-3687 - HAL - INRIA, Sophia-Antipolis, 1988.
- R. Risken, *The Fokker-Planck Equation: Methods of Solution and Applications*, (Springer, Berlin, 1996).