Preprints of the 21st IFAC World Congress (Virtual)
Berlin, Germany, July 12-17, 2020

Optimal Control of Trajectories Ensemble for a Class of Discrete Dynamic Systems ⋆

Anna Golovkina * **Dmitri Ovsyannikov** **

* *Department of control systems theory for electrophysical facilities, Saint Petersburg State University, Universitetsky pr. 7/9, Saint Petersburg, 199034 Russia (e-mail: a.golovkina@spbu.ru).*
** *Department of control systems theory for electrophysical facilities, Saint Petersburg State University, Universitetsky pr. 7/9, Saint Petersburg, 199034 Russia (e-mail: d.a.ovsyannikov@spbu.ru)*

Abstract: The control problems concerning the manipulation of system trajectories ensembles have received increased attention in recent years. This paper considers a class of nonlinear discrete-time systems with additive control and develops a systematic method to design optimal controls that steer an ensemble from an initial state to a terminal one minimizing the cost functional that estimates ensemble dynamics in average. Necessary optimality condition as well as functional variation are constructed. These allow building different iterative or gradient-based methods to minimize the desired control cost criterion. The motivation for this study originates from the optimization problem of advanced fuel cycle in accelerator driven system. The grand challenge here remains to address the coupled problem over the multiple cycles in the planning horizon taking into account manufacturing and nuclear data uncertainties. A brief description of physical problem and corresponding mathematical model for optimization of advanced fuel cycle in terms of the proposed approach are presented.

Keywords: Optimal control, discrete-time systems, trajectories ensemble, optimization

1. INTRODUCTION

The control problems concerning the manipulation of system trajectories ensembles have received increased attention in recent years. This tendency is caused by the emerging problems arisen from various engineering applications. A special class of such problems are the ones associated with the charged particles beam dynamics optimization in accelerating and focusing structures Ovsyannikov (1980, 1990); Ovsyannikov et al. (2006). The effectiveness of optimization methodology applied for the dynamics of trajectories ensemble is confirmed when solving various problems of electrophysics Golovkina et al. (2018b); Ovsyannikov and Zavadskiy (2018); Ovsyannikov (2000), nuclear medicine Bazhanov et al. (2018), manipulation of spin ensembles in nuclear magnetic resonance Li and Khaneja (2006); Glaser et al. (1998), coordination of the flocks movement in biology Brockett (2010) and so on.

For all described applications the problem statement in terms of trajectories ensemble control originates naturally from the physical aspects of the modeled systems. But additionally to these cases, the problems of dynamical systems control under uncertainties and incompleteness of information generally are reduced to the problems of trajectories ensembles control too. Lots of papers exist devoted to this issue, but we mention several of them Kurzhanski (1977); Kurzhanski and Varaiya (2014); Kurzhanskiy and Varaiya (2011); Panteleev and Pis'mennaya (2018); Bortakovskii and Nemychenkov (2017); Wang and Li (2017).

It is worth to be noted that if system dynamics depends on some parameters which values are uncertain, it can be brought to the problem with uncertainty in the initial data as well. Indeed, the parameter can be replaced by a state coordinate that is constant in time. Adding to the state-space equations a zero derivative of this parameter with respect to time as well as the corresponding indefinite initial condition, we obtain the model without a parameter, but with uncertainty in the initial data.

In practice, smooth and non-smooth functionals are mostly used in solving control problems for trajectories ensembles. Smooth functional can be associated with optimal control in average. This means one should minimize the average value of quality factor for trajectories ensemble. Non-smooth fuctionals in their turn are related to minimizing the quality factor maximum value computed for the whole trajectories ensemble. The paper Mizintseva and Ovsyannikov (2017) develops a method to simultaneously optimize smooth and non-smooth functionals. The mentioned approaches are mainly focused on the mostly studied continuous-time ensemble systems Ovsyannikov (1980, 1990).

In the same time nowadays discrete control processes are gaining more attention both in theory and practice of optimal control. The reason for it in the first turn is the fact that continuous-time systems are controlled by a digital computer. Furthermore, the discrete systems

⋆ This work was supported by a grant from the Russian Science Foundation (project No. 19-71-00074).

are encountered in solving continuous optimal control problems by numerical methods. As a result, in this paper, we consider a class of nonlinear discrete-time systems with additive control and develop a systematic method to design optimal controls that steer an ensemble from an initial state to a terminal one minimizing the cost functional that estimates ensemble dynamics in average.

The examined class of controlled discrete systems corresponds to the mathematical model of control for transmutation process in advanced fuel cycle implemented in accelerator driven system (ADS). ADS consists of three major blocks: charged particles accelerator, neutron producing target and subcritical reactor core Nifenecker et al. (2003). Advanced fuel cycle is an important aspect of sustainable nuclear energy, because its implementation leads to resources preservation, significant waste minimization and improved economy Mai (2002); Herczeg (2003). The major challenge for nuclear fuel management optimization remains to address the coupled problem over the multiple cycles in the planning horizon taking into account the manufacturing and nuclear data uncertainties. For advanced fuel cycles, one should make decisions associated with what elements to recycle, in what quantity, and how to physically introduce them into the core Cacuci (2010).

The optimal control problem for advanced fuel cycle is designed to achieve the following goal. This is minimizing the total radioactivity of spent fuel in the long-term storage by successive minimization of waste radioactivity by the end of each cycle. To address it, we build mathematical model of trajectories ensemble control in discrete-time system, where isotope distributions in the reloading fuel at the beginning of each cycle are considered as control parameters. The choice of ensemble model is explained by the necessity to provide a robustness due to the presence of different types of uncertainties encompassing the initial and control data. The solution of discrete-time optimization problem is examined in details, necessary optimality condition as well as functional variation are constructed. These allow building different iterative or gradient-based methods to minimize the desired control cost criterion.

The authors have already successfully utilized the optimal control apparatus for the optimization issue of a single transmutation cycle Golovkina et al. (2018a,b, 2019). The problem there was considered for continuous-time system describing the isotopes concentration dynamics in time. This paper for in the first time formulates the problem of advanced fuel cycle optimization as a discrete-time optimal control problem for trajectories ensemble.

The rest of the paper is organized as follows. In section 2 the optimal control problem for trajectory ensemble of a class of nonlinear discrete system with additive control term is considered. The necessary assumptions are given as well as some notations are introduced. Section 3 is dedicated to the optimal control framework formulation and divided into 2 subsections. The first one among them contains some auxiliary relations and lemmas that are used further in the second subsection, devoted to the derivation of necessary optimality condition and cost functional variation. Section 4 describes a physical example of advanced fuel cycle optimal control served as a motivation for this study.

2. PROBLEM STATEMENT

This paper considers a dynamic system described by the discrete equations of the following type

$$x(k+1) = f(k, x(k)) + u(k), \quad k = 0..N-1, \qquad (1)$$

where $x(k)$ is a n-vector, characterizing the state of the system, $u(k)$ is a n-vector of control actions, $f(k, x(k))$ is a n-dimensional vector function, defining the process dynamics at each step. We suppose that $f(k, x(k))$ is defined and continuous in $\mathbf{\Omega}$ for each k along with its first and second derivatives $\frac{\partial f_l}{\partial x_j}$, $\frac{\partial^2 f_l}{\partial x_i \partial x_j}$, $l, i, j = 1..n$, $u(k) \in \mathbf{U}(k)$. Here $\mathbf{\Omega}$ is a region in $\mathbb{R}^n$, $\mathbf{U}(k)$ is a compact set in $\mathbb{R}^n$. It is assumed also that Jacobian determinant

$$J_k = J(k, x(k)) = |\partial f(k, x(k))/\partial x(k)|$$

is not equal to zero for all possible changes of k and $x(k) \in \mathbf{\Omega}$. Thus, it means that vector $x(k)$ with the fixed vector $u(k)$ uniquely defines the state $x(k+1)$ on the step k and the other way round. Additionally, we suppose that initial values for the system (1) are taken from a compact set $\mathcal{M}_0 \subset \mathbb{R}^n$ of non-zero measure.

The sequence of vectors $\{u(0), u(1), ..., u(N-1)\}$ we will call control and denote u. In the same time the corresponding to this control sequence of vectors $\{x(0), x(1), ..., x(N)\}$ is a trajectory of the system that we denote $x(x_0, u)$. Under the introduced notations, $x(k, x_0, u)$ designates the state of the system at the step k.

Set of trajectories $x(x_0, u)$ corresponding to the control u and different initial conditions $x_0 \in \mathcal{M}_0$ we will call trajectories ensemble.

State of the ensemble at the k-th step is the cross-section of trajectories ensemble denoted as $\mathcal{M}_{k,u} = \{x(k) : x(k) = x(k, x_0, u), x_0 \in \mathcal{M}_0\}$.

Let us introduce a functional

$$I(u) = \sum_{k=1}^{N-1} \int\limits_{\mathcal{M}_{k,u}} \varphi(k, x_k, u(k)) dx_k + \int\limits_{\mathcal{M}_{N,u}} g(x_N) dx_N, \quad (2)$$

characterizing the state of the trajectories ensemble and control quality. Here $x_k = x(k) \in \mathcal{M}_{k,u}$, function $\varphi(k, x, u)$ is defined and continuous in $\mathbf{\Omega} \times \mathbf{U}(k)$ with respect to its arguments for each k along with its partial derivatives with respect to x and u, $g(x)$ is continuously differentiable function defined in $\mathbf{\Omega}$.

Let us consider the problem of functional (2) minimization for all admissible controls $u(k) \in \mathbf{U}(k)$, $k = 0..N-1$.

3. OPTIMAL CONTROL FRAMEWORK

3.1 Auxiliary Relations and Lemmas

Let us consider admissible controls u and $\tilde{u}$. The corresponding trajectories are denoted as

$$x(x_0, u) \text{ and } \tilde{x}(x_0, \tilde{u}). \qquad (3)$$

The difference $\Delta u(k) = \tilde{u}(k) - u(k)$ is variation of control u at the step k, the difference $\Delta x(k) = \Delta x(k, x_k) = \tilde{x}(k, x_0, \tilde{u}) - x(k, x_0, u)$ is trajectory $x(x_0, u)$ increment at the step k. Thus, Δu and Δx are variations of control u and trajectory x increments correspondingly. Apparently, due to continuity, $\|\Delta x\| \to 0$ when $\|\Delta u\| \to 0$ uniformly

for $x_0 \in \mathcal{M}_0$, $\|\Delta x\| = \max\limits_{k=0..N} \|\Delta x(k)\|$, the norm of vector Δu is defined in the similar way.

The increment Δx can be substituted with variation δx satisfying the following equation

$$\delta x(k+1) = \frac{\partial f(k, x(k))}{\partial x(k)} \delta x(k) + \Delta u(k), \tag{4}$$

with $\delta x(0) = 0$, $k = 0, .., N-1$.

Let us consider the mapping of set $\mathcal{M}_{k,u}$ to the set $\mathcal{M}_{k,\tilde{u}}$ defined by the trajectories (3) starting at the same points of the set $\mathcal{M}_0$:

$$\tilde{x}_k = \tilde{x}(x_k). \tag{5}$$

Due to assumptions that the right side of the equation (1) is differentiable and Jacobian matrix of mapping (1) is non-singular, we can conclude that mapping (5) is locally bijective and continuously differentiate. Moreover, in view of $\tilde{x}_k = x_k + \Delta x(k, x_k)$, Jacobian determinant of (5) can be written in the form Ovsyannikov (1980)

$$\det(\partial \tilde{x}_k / \partial x_k) = 1 + \operatorname{div} \Delta x(k, x_k) + o\left(\|\Delta x(k, x_k)\|\right), \tag{6}$$

where

$$\operatorname{div} \Delta x(k, x_k) = \sum_{i=1}^{n} \frac{\partial \Delta x_i(k, x(k))}{\partial x_i(k)}.$$

Lemma 1. Let $A(\alpha)$ be a non-singular square matrix with dimension n. Suppose that its elements a_{ij} depend on the parameter α. Then, the following relation takes place

$$\operatorname{tr}\left(A^{-1}(\alpha) \frac{\partial A(\alpha)}{\partial \alpha}\right) = \frac{1}{|A|} \frac{\partial |A(\alpha)|}{\partial \alpha}.$$

Proof. By A_{ij} we denote an algebraic complement for the element a_{ij}. Then, as is known, $A^{-1} = \left((A_{ij})_{i,j=1}^{n}\right)^T / |A|$. Taking this relation into account, we will get

$$\operatorname{tr}\left(A^{-1} \frac{\partial A}{\partial \alpha}\right) = \frac{1}{|A|} \sum_{i=1}^{n} \sum_{j=1}^{n} A_{ij} \frac{\partial a_{ij}}{\partial \alpha} = \frac{1}{|A|} \frac{\partial |A|}{\partial \alpha}. \blacksquare$$

Corollary 2. Due to the fact that the trace of square matrices product does not depend on the order of multiplication and the trace of sum of matrices equals to the sum of these matrices trace, then based on the lemma 1, we can write:

$$\operatorname{tr}\left(\sum_{i=1}^{n} A_i^{-1} \frac{\partial A_i}{\partial \alpha}\right) = \operatorname{tr}\left(\sum_{i=1}^{n} \frac{\partial A_i}{\partial \alpha} A_i^{-1}\right) = \sum_{i=1}^{n} \frac{1}{|A_i|} \frac{\partial |A_i|}{\partial \alpha}. \tag{7}$$

The following lemma is used further during transforming of the considered functional.

Lemma 3. The following equality takes place

$$\operatorname{div} \delta x(k+1, x(k+1)) = \operatorname{div} \delta x(k, x(k)) + \\ + \frac{\partial J_k}{\partial x(k)} \delta x(k, x(k)) J_k^{-1}. \tag{8}$$

Proof. Taking into account the definition of divergence

$$\operatorname{div} \delta x(k+1, x(k+1)) = \sum_{i=1}^{n} \frac{\partial \delta x_i(k+1, x(k+1))}{\partial x_i(k+1)}$$

and equation in variations (4), we can conclude that

$$\operatorname{div} \delta x(k+1, x(k+1)) = \operatorname{tr}\left[\frac{\partial}{\partial x(k)} \right. \\ \left. \left(\frac{\partial f(k, x(k))}{\partial x(k)} \delta x(k, x(k)) + \Delta u(k)\right) \frac{\partial x(k)}{\partial x(k+1)}\right]. \tag{9}$$

From equation (1) follows that

$$\frac{\partial x(k)}{\partial x(k+1)} = \left[\frac{\partial f(k, x(k))}{\partial x(k)}\right]^{-1}.$$

Besides

$$\frac{\partial}{\partial x(k)} \left(\frac{\partial f(k, x(k))}{\partial x(k)} \delta x(k, x(k)) + \Delta u(k)\right) = \\ = \sum_{i=1}^{n} \frac{\partial}{\partial x_i(k)} \frac{f(k, x(k))}{\partial x(k)} \delta x_i(k, x(k)) + \\ + \frac{\partial f(k, x(k))}{\partial x(k)} \frac{\partial \delta x(k, x(k))}{\partial x(k)}. \tag{10}$$

Using lemma 1 along with the obtained relations (9) and (10), we can get the desired expression

$$\operatorname{div} \delta x(k+1, x(k+1)) = J_k^{-1} \frac{\partial J_k}{\partial x(k)} \delta x(k, x(k)) + \\ + \operatorname{div} \delta x(k, x(k)). \blacksquare$$

Corollary 4. The iterative formula for divergence calculation can be derived from the expression (8) and the fact that $\operatorname{div}(\delta x(0, x(0))) = 0$

$$\operatorname{div} \delta x(k+1, x(k+1)) = \sum_{s=0}^{k} J_s^{-1} \frac{\partial J_s}{\partial x(s)} \delta x(s, x(s)).$$

3.2 The Necessary Optimality Conditions

Let us find the functional (2) increment between admissible controls u and $\tilde{u}$:

$$\Delta I = I(\tilde{u}) - I(u) = \sum_{k=1}^{N-1} \left[\int\limits_{\mathcal{M}_{k,\tilde{u}}} \varphi(k, \tilde{x}_k, \tilde{u}(k)) d\tilde{x}_k - \right. \\ \left. - \int\limits_{\mathcal{M}_{k,u}} \varphi(k, x_k, u(k)) dx_k \right] + \\ + \int\limits_{\mathcal{M}_{N,\tilde{u}}} g(\tilde{x}_N) d\tilde{x}_N - \int\limits_{\mathcal{M}_{N,u}} g(x_N) dx_N. \tag{11}$$

Using the mapping (5) from $\mathcal{M}_{k,u}$ set to the $\mathcal{M}_{k,\tilde{u}}$, we carry out the change of variables under the integrals with respect to the trajectories cross-section $\mathcal{M}_{k,\tilde{u}}$. After then we get

$$\Delta I = \sum_{k=1}^{N-1} \int\limits_{\mathcal{M}_{k,u}} [\varphi(k, x_k + \Delta x(k, x_k), u(k) + \Delta u(k)) \cdot \\ \cdot \left|\frac{\partial \tilde{x}(x_k)}{\partial x_k}\right| - \varphi(k, x_k, u(k))] dx_k + \\ \int\limits_{\mathcal{M}_{N,u}} \left[g(x_N + \Delta x(N, x_N)) \cdot \left|\frac{\partial \tilde{x}(x_k)}{\partial x_k}\right| - g(x_N)\right] dx_N. \tag{12}$$

Dividing out the linear terms in (12) with respect to $\Delta x(k, x(k))$, $\operatorname{div} \Delta x(k, x(k))$ and $\Delta u(k)$ and taking into account that $\|\Delta x(k, x(k)) - \delta x(k, x(k))\|$ and

$\|\operatorname{div}\Delta x(k,x(k)) - \operatorname{div}\delta x(k,x(k))\|$ are infinitesimals of higher order than $\|\Delta u\|$ uniformly in $x \in \mathcal{M}_0$ and $k = 1,2,..,N$, we can represent (12) in the following way

$$\Delta I = \delta I + o(\|\Delta u\|), \tag{13}$$

where

$$\delta I = \sum_{k=1}^{N-1} \int\limits_{\mathcal{M}_{k,u}} \left[\operatorname{div}\left(\varphi(k,x_k,u(k))\right)\delta x(k,x_k) + \right. \\ \left. + \frac{\partial\varphi(k,x_k,u(k))}{\partial u(k)}\Delta u(k)\right] dx_k + \\ + \int\limits_{\mathcal{M}_{N,u}} \operatorname{div}\left(g(x_N)\delta x(N,x_N)\right) dx_N. \tag{14}$$

Let us transform the functional variation (14) in the convenient form. It is necessary for the further calculation and construction of optimization algorithm. For this reason, we introduce the auxiliary variables satisfying the following difference system:

$$q(k-1) = \varphi(k-1,x(k-1),u(k-1)) + J_{k-1}q(k), \tag{15}$$

$$p(k-1) = J_{k-1}\left(\frac{\partial f(k-1,x(k-1))}{\partial x(k-1)}\right)^T p(k) + \\ q(k)\left(\frac{\partial J_{k-1}}{\partial x(k-1)}\right)^T + \left(\frac{\partial\varphi(k-1,x(k-1),u(k-1))}{\partial x(k-1)}\right)^T, \tag{16}$$

where $k = N-1, N-2, .., 1$ and conditions at the end of the interval are given:

$$q(N) = g(x(N)),\ \ p(N) = \left(\frac{\partial g(x(N))}{\partial x(N)}\right)^T. \tag{17}$$

Here $p(k)$ is a n-vector, $q(k)$ is a scalar.

After that, let us rewrite the last integral in variation (14) using the newly introduced variables (15) and (16). To accomplish this, we do the change of variables due to the system (1) and by this switching to integrating with respect to x_{N-1}. In this case we get

$$\int\limits_{\mathcal{M}_{N,u}} \operatorname{div}\left(g(x_N)\delta x(N,x_N)\right) dx_N = \tag{18}$$

$$\int\limits_{\mathcal{M}_{N-1,u}} \left(p(N)\delta x(N,x_N) + q(N)\operatorname{div}\delta x(N,x_N)\right) J_{N-1}dx_{N-1}.$$

Substituting here $\delta x(N,x_N)$ using formula (4) and taking into account the relation (8) for $\operatorname{div}\delta x(N,x_N)$ obtained in lemma 3, we get

$$\int\limits_{\mathcal{M}_{N,u}} \operatorname{div}\left(g(x_N\delta x(N,x_N))\right) dx_N = \\ \int\limits_{\mathcal{M}_{N-1,u}} \left[\left(\left(p(N), \frac{\partial f(N-1,x_{N-1})}{\partial x(N-1)}\delta x(N-1,x_{N-1})\right)\right) + \right. \\ \left. (p(N),\Delta u(N-1)) + q(N)\operatorname{div}\delta x(N-1,x_{N-1}))\, J_{N-1} + \right. \\ \left. q(N)\frac{\partial J_{N-1}}{\partial x(N-1)}\delta x(N-1,x_{N-1})\right] dx_{N-1}. \tag{19}$$

Let us sum the expression (19) with the integral with respect to the cross section $\mathcal{M}_{N-1,u}$ in variation (14). Gathering terms next to $\delta x(N-1)$ and $\operatorname{div}\delta x(N-1)$, taking into account formulas (15) and (16), we write this sum in the following way

$$\int\limits_{\mathcal{M}_{N-1,u}} \left[(p(N),\Delta u(N-1))\, J_{N-1} + \right. \\ \left. + \frac{\partial\varphi(N-1,x_{N-1},u(N-1))}{\partial u(N-1)}\Delta u(N-1)\right] dx_{N-1} + \\ + \int\limits_{\mathcal{M}_{N-1,u}} (p(N-1),\delta x(N-1,x_{N-1}) + \\ + q(N-1)\operatorname{div}\delta x(N-1,x_{N-1}))\, dx_{N-1}. \tag{20}$$

If in the second integral in (20) we change integration with respect to x_{N-1} into x_{N-2}, taking into account (1), we get the expression similar to (19) distinguishing only in the step number. Thus, the expression (20) allows one to switch to the integration with respect to the previous cross sections in the integrals of type (18). Repeat this procedure until the integration over the trajectories ensemble cross sections is brought to the integration over the initial values set $\mathcal{M}_0$, where $\delta x(0,x_0) = 0$ and $\operatorname{div}\delta x(0,x_0) = 0$. This let us get the following expression for the functional (2) variation:

$$\delta I = \sum_{k=0}^{N-1}\left(\int\limits_{\mathcal{M}_{k,u}} \left[J_k p(k+1) + \left(\frac{\partial\varphi(k,x_k,u(k))}{\partial u(k)}\right)^T\right] dx_k, \Delta u(k)\right) \tag{21}$$

Let us introduce a special control variation, namely $\Delta u(k) = 0, k = 1,2,..,N-1,\ k \neq j,\ \Delta u(j) \neq 0$. Variation is called admissible for admissible control u if $\bar\varepsilon > 0$ exists, such that when $0 \leq \varepsilon \leq \bar\varepsilon$

$$u(j) + \varepsilon\Delta u(j) \in \mathbf{U}(j).$$

Theorem 5. So that control $u^0 = (u^0(0), u^0(1), .., u^0(N-1))$ becomes optimal, it is necessary that the following inequality holds for all admissible variations of control u^0

$$\int\limits_{\mathcal{M}_{k,u^0}} \left[J(k,x_k,u^0(k))p^T(k+1,x_k) + \frac{\partial\varphi(k,x_k,u(k))}{\partial u(k)}\right] \\ dx_k\Delta u(k) \geq 0,\ \ k = 0,1,..,N-1. \tag{22}$$

Here $p(k+1)$ satisfies relations (16) in the optimal process, i.e. for the optimal control u^0 and optimal trajectories $x(x_0,u^0)$ corresponding to it.

Proof. The proof follows from the representation of functional variation (21), expression (13) and the definition of a special variation. ■

Taking into account the representation of functional variation (21) as well as necessary optimality condition (22), one can build different iterative and gradient-based optimization methods.

Let us consider method of possible directions applied for the introduced problem using the results of Theorem 5. Inequality (22) can be simply written as

$$\omega_k\Delta u_k \geq 0,\ \ k = 0,1,..,N-1, \tag{23}$$

Suppose, there is m, where the optimality condition (23) does not hold. This means u_m and Δu_m exist such that $\omega_m\Delta u_m < 0$, the minimizing sequence of controls $\{u_m^{(j)}\}$,

$j = 0, 1...$ should be built $u_m^{(j+1)} = u_m^{(j)} - \mu_j \omega_m(u^{(j)})$. Here $\mu_j = \underset{\mu \geq 0}{\operatorname{argmin}}\, I(u_m^{(j)} - \mu_j \omega_m(u^{(j)}))$. If there are several m violating (23), step-wise descent method is applied subsequently for each of them using the procedure described above.

4. MATHEMATICAL MODEL OF ADVANCED FUEL CYCLE

The "transmutation" concept in advanced fuel cycle is related to the physical process that transforms a fresh fuel into an irradiated fuel. Mathematical description of such phenomena in one cycle is obtained by the solution of Bateman equations (24) from which the vector of the nuclei densities $\mathbf{N}_{\text{end}}$ at the end of the cycle $t = t_{\text{end}}$, starting from the initial value (25), is obtained Salvatores and Palmiotti (2011):

$$\frac{dN_i}{dt} = -\left(\sum_d \lambda_{di} - \sum_x \langle \sigma_{xi}, \varphi \rangle\right) N_i + \\ + \sum_{j \neg i} \left(\gamma_d^{i \leftarrow j} \lambda_{dj} + \gamma_x^{i \leftarrow j} \langle \sigma_{xj}, \varphi \rangle\right) N_j, \quad (24)$$

$$N_i(t_0) = N_0^i \quad (25)$$

where $i = \overline{1..l}$ — total number of nuclei considered in the system, $\mathbf{N} = [N_1, N_2, \ldots, N_l]^T$. Some coefficients of equation (24) depend on $\mathbf{N}$(we use here bold font to show vector notation), some are constants characterizing the transitions between nuclei.

Let us rewrite equations (24) in the matrix form, carrying out decomposition of the right part according to its coefficient properties Wieselquist (2015):

$$\frac{d\mathbf{N}}{dt} = \left(A_\varphi(\mathbf{N}) + A_\lambda\right)\mathbf{N}, \quad (26)$$

where

$$A_\lambda = \begin{bmatrix} -\sum_d \lambda_{d1} & \gamma_d^{1\leftarrow 2}\lambda_{d2} & \ldots & \gamma_d^{1\leftarrow n}\lambda_{dl} \\ \gamma_d^{2\leftarrow 1}\lambda_{d1} & -\sum_d \lambda_{d2} & \ldots & \gamma_d^{2\leftarrow n}\lambda_{dl} \\ \vdots & \vdots & \ddots & \vdots \\ \gamma_d^{n\leftarrow 1}\lambda_{d1} & \gamma_d^{n\leftarrow 2}\lambda_{d2} & \ldots & -\sum_d \lambda_{dl} \end{bmatrix},$$

$$A_\varphi = \begin{bmatrix} -\sum_x \langle \sigma_{x1}, \varphi \rangle & \gamma_x^{1\leftarrow 2} \langle \sigma_{x2}, \varphi \rangle & \ldots & \gamma_x^{1\leftarrow n} \langle \sigma_{xl}, \varphi \rangle \\ \gamma_x^{2\leftarrow 1} \langle \sigma_{x1}, \varphi \rangle & -\sum_x \langle \sigma_{x2}, \varphi \rangle & \ldots & \gamma_x^{2\leftarrow n} \langle \sigma_{xl}, \varphi \rangle \\ \vdots & \vdots & \ddots & \vdots \\ \gamma_x^{n\leftarrow 1} \langle \sigma_{x1}, \varphi \rangle & \gamma_x^{l\leftarrow 2} \langle \sigma_{x2}, \varphi \rangle & \ldots & -\sum_x \langle \sigma_{xl}, \varphi \rangle \end{bmatrix}.$$

- Here A_λ is a decay part with d indicating a decay mode, the off-diagonal elements representing gains of nuclide i due to the decay mode d and the diagonal elements representing the loss of nuclide i due to all decay modes, λ_{di} is the decay (d) constant for nuclide i, $\gamma_d^{i\leftarrow j}$ is a coefficient characterizing "yield" of nuclide i from j in decay d. Decay part is independent of $\mathbf{N}$.
- A_φ is a reaction part with x indicating a nuclear reaction type, off-diagonal elements representing gains of nuclide i due to the reaction type x and the diagonal elements representing the loss of nuclide i due to all reaction mechanisms. $\gamma_x^{i\leftarrow j}$ is a coefficient characterizing "yield" of nuclide i from j in nuclear reaction x, σ_{xi} is a reaction x cross section for nuclide i, φ represents a neutron spectrum in the reactor core.

Isotopic depletion modeling capability is well developed. Its major limitation originates not so much from the mathematical limitations of solving the Bateman equation (24)–(26), but from the quality of the input data provided Cacuci (2010). Nuclear data for certain isotopes and reaction types are not sufficiently accurate to support the needs of nuclear fuel management, particularly for some advanced nuclear systems under consideration, e.g., ADS.

Nuclear fuel management practices are very well established for nuclear power plant types that have wide deployment. For the promising nuclear power plant types not yet widely deployed, like ADS, there is considerable opportunity to consider more creative nuclear fuel management practices. The big challenge for nuclear fuel management optimization remains to address the coupled problem over the multiple cycles in the planning horizon. For advanced fuel cycles, one can add additional decisions associated with what elements to recycle, in what quantity, and how to physically introduce them into the core.

However, the uncertainties associated with advanced fuel cycle are of great importance. This involves not only the methods introduced uncertainties, but also all the other sources, e.g., manufacturing and nuclear data. Thus, the further development of adaptive simulation capability may play an important role complementary to refinement of optimization and models as well as numerical methods.

Let us consider the discrete formulation of the depletion model (26) which we extend to the multi-cycle level. It is well known, that by integrating ODEs are in fact reduced to a discrete-time system. Taking into account that the integration step in (26) is relatively large due to slow dynamics change and the fact that control action are discrete in time, we can conclude that building control models for discrete-time system is more reasonable.

Discrete system can be built in different ways, not only by choosing the integrating method, but also by choice of the model, describing the fuel depletion. According to the assumption for neutron flux during one cycle to change slightly, we can neglect the dependence of A_φ on $\mathbf{N}$ and come to an autonomous system in (26). Then, we can choose the discretization step corresponding to the intervals of fuel reloading:

$$\mathbf{N}(k+1) = A(k, \mathbf{N}(k))\mathbf{N}(k) + \mathbf{N}^u(k), \quad (27)$$

where $\mathbf{N}^u$ is a control action at each step k representing the nuclear densities of additive fuel, $A(k, \mathbf{N}(k))$ is a matrix of coefficients, obtained by combining and discretizing A_φ and A_λ.

For out problem statement, functions φ and g in the cost functional (2) are defined in the following way:

$$\varphi(k, \mathbf{N}(k), \mathbf{N}^u(k)) = (\mathbf{DF}, \mathbf{N}(k) + \mathbf{N}^u(k)), \\ g(\mathbf{N}(N)) = (\mathbf{DF}, \mathbf{N}(N)). \quad (28)$$

Here **DF** is a vector of size l representing the doze factors for the considered isotopic vector **N**.

The introduced in section 3 approach can be used for solving of optimal control problem for advanced fuel cycle (27)–(28).

5. CONCLUSION

Optimal control problem of trajectories ensemble for a class of discrete dynamic systems with additive control term is considered in this paper. Such system arises naturally in optimization problem of advanced fuel cycle. The necessary optimality condition as well as variation of the cost functional estimating the ensemble dynamics in average are constructed. Based on it one can build different iterative or gradient-based methods for cost criterion minimization. The corresponding discrete-time model for advanced fuel cycle control is shown.

ACKNOWLEDGEMENTS

Anna Golovkina acknowledges Russian Science Foundation for grant (project No. 19-71-00074).

REFERENCES

(2002). Accelerator-driven systems (ads) and fast reactors (fr) in advanced nuclear fuel cycles. Technical report, OECD Nuclear Energy Agency.

Bazhanov, P., Kotina, E., Ovsyannikov, D., and Ploskikh, V. (2018). Optimization algorithm of the velocity field determining in image processing. *Cybernetics and Physics*, 7(4), 174–181.

Bortakovskii, A. and Nemychenkov, G. (2017). Suboptimal control of bunches of trajectories of discrete deterministic automaton time-invariant systems. *Journal of Computer and Systems Sciences International*, 56(6), 914–929.

Brockett, R.W. (2010). On the control of a flock by a leader. *Proceedings of the Steklov Institute of Mathematics*, 268(1), 49–57. doi:10.1134/S0081543810010050.

Cacuci, D.G. (ed.) (2010). *Handbook of Nuclear Engineering*, volume I. Springer.

Glaser, S.J., Schedletzky, O., and Griesinger, C. (1998). Unitary control in quantum ensembles: maximizing signal intensity in coherent spectroscopy. *Science*, 280(5362), 421–424.

Golovkina, A., Kudinovich, I., and Ovsyannikov, D. (2018a). Optimization model for radioactive waste transmutation in advanced fuel cycle. In *17th IFAC Workshop on Control Applications of Optimization*, 179–183. Yekaterinburg, Russia.

Golovkina, A., Olaru, S., and Ovsyannikov, D. (2019). A robust optimization model for the radioactive waste transmutation in ads. In *6th International Conference on Control, Decision and Information Technologies (CoDIT)*, 703–708. IEEE, Paris, France.

Golovkina, A., Ovsyannikov, D., and Olaru, S. (2018b). Performance optimization of radioactive waste transmutation in accelerator driven system. *Cybernetics and Physics*, 7(4), 210–215.

Herczeg, J.W. (2003). The advanced fuel cycle initiative: the future path for advanced spent fuel treatment and transmutation research in the united states. Technical report, Nuclear Energy Agency of the OECD (NEA).

Kurzhanski, A.B. (1977). *Control and surveillance in the presence of uncertainty*. Science, Moscow. (in Russian).

Kurzhanski, A.B. and Varaiya, P. (2014). *Dynamics and Control of Trajectory Tubes*, volume 85. Birkhauser Basel.

Kurzhanskiy, A.A. and Varaiya, P. (2011). Theory and computational techniques for analysis of discrete-time control systems with disturbances. *Optimization Methods and Software*, 26(4-5), 719–746. URL `https://doi.org/10.1080/10556788.2010.548867`.

Li, J.S. and Khaneja, N. (2006). Control of inhomogeneous quantum ensembles. *Phys. Rev. A*, 73, 030302. doi: 10.1103/PhysRevA.73.030302.

Mizintseva, M. and Ovsyannikov, D. (2017). Minimax problem of simultaneous optimization of smooth and non-smooth functionals.

Nifenecker, H., Meplan, O., and David, S. (2003). *Accelerator Driven Subcritical Reactors*. Institute of Physics Publishing Bristol and Philadelphia.

Ovsyannikov, A.D. (2000). New approach to beam dynamics optimization problem. In *Proc. of the 6th International Computational Accelerator Physics Conference*.

Ovsyannikov, D. and Zavadskiy, S. (2018). Pareto-optimal choice of controller dimension for plasma stabilization system. *IFAC-PapersOnLine*, 51(32), 175 – 178. 17th IFAC Workshop on Control Applications of Optimization CAO 2018.

Ovsyannikov, D.A. (1980). *Mathematical methods of beam control*. Leningrad University. (in Russian).

Ovsyannikov, D.A. (1990). *Modeling and optimization of charged particle beam dynamics*. Leningrad University, Leningrad. (in Russian).

Ovsyannikov, D., Ovsyannikov, A., Vorogushin, M., Svistunov, Y., and Durkin, A. (2006). Beam dynamics optimization: Models, methods and applications. *Nuclear Instruments and Methods in Physics Research Section A*, 558(1), 11 – 19.

Panteleev, A. and Pis'mennaya, V. (2018). Application of a memetic algorithm for the optimal control of bunches of trajectories of nonlinear deterministic systems with incomplete feedback. *Journal of Computer and Systems Sciences International*, 57(1), 25–36.

Salvatores, M. and Palmiotti, G. (2011). Radioactive waste partitioning and transmutation within advanced fuel cycles: Achievements and challenges. *Progress in Particle and Nuclear Physics*, 66(1), 123–126.

Wang, S. and Li, J.S. (2017). Fixed-endpoint optimal control of bilinear ensemble systems. *SIAM Journal on Control and Optimization*, 55(5), 3039–3065. doi: 10.1137/15m1044151.

Wieselquist, W.A. (2015). The scale 6.2 origen api for high performance depletion. techreport CASL-U-2015-0165-000, Oak Ridge National Laboratory, Nashville, TN, USA.