Iranian Journal of Numerical Analysis and Optimization Vol. ??, No. ??, ??, pp ?? [https://doi.org/??](https://doi.org/10.22067/ijnao.2024.89204.1491) <https://ijnao.um.ac.ir/>

Research Article

Optimal control of water pollutant transmission by utilizing a combined Jacobi collocation method and mountain Gazelle algorithm

A. Ebrah[i](https://orcid.org/0000-0002-9897-0042)mzadeh^{*, O}, R. Khanduzi, R. Mirabbasi^O and E. Hashemizadeh

Abstract

Water pollution can have many adverse effects on the environment and human health. The study of the transmission of water pollutants over a

*Corresponding author

Received ??? ; revised ??? ; accepted ???

Asiyeh Ebrahimzadeh

Department of Mathematics Education, Farhangian University, P.O. Box 14665-889, Tehran, Iran. e-mail: a.ebrahimzadeh@cfu.ac.ir

Raheleh Khanduzi

Department of Mathematics and Statistics, Gonbad Kavous University, P.O. Box 49717- 99151, Gonbad Kavous, Golestan, Iran. e-mail: raheleh.khanduzi@gmail.com

Rasoul Mirabbasi

Department of Water Engineering, Faculty of Agriculture, Shahrekord University, Shahrekord, Iran. e-mail: mirabbasi@sku.ac.ir

Elham Hashemizadeh

Department of Mathematics, Karaj Branch, Islamic Azad University, Karaj, Iran. email: hashemizadeh@kiau.ac.ir

How to cite this article

Ebrahimzadeh, A., Khanduzi, R., Mirabbasi, R. and Hashemizadeh, E., Optimal control of water pollutant transmission by utilizing a combined Jacobi collocation method and mountain Gazelle algorithm. *Iran. J. Numer. Anal. Optim.*, ??; ??(??): ??-??. ??

finite lifespan is carried out using an optimal control problem (OCP), with the system governed by ordinary differential equations. By utilizing the collocation approach, the OCP is transmuted to a nonlinear programming problem, and then the mountain Gazelle algorithm is applied to determine the optimal control and state solutions. A practical study demonstrates the effect of treatment on reducing water pollutants during a finite time.

AMS subject classifications (2020): 49M25 , 90C30.

Keywords: Optimal control; Jacobi polynomials; Transmission of water pollutant; Collocation method; Mountain Gazelle algorithm.

1 Introduction

Water pollution can result from numerous sources, such as industrial waste, agricultural runoff, sewage treatment plants, oil spills, and more. Some of the most common water pollutants include oxygen depletion, nutrient pollution, groundwater pollution, suspended matter pollution, chemical water pollution, oil spillage, silver pollution, and copper pollution. Water pollution can have several negative effects on the environment. One of the significant problems caused by water pollution is the death of organisms that depend on these water bodies. This can lead to a loss of valuable species and biodiversity. Additionally, polluted water harms communities by destroying underwater life and messing up food chains. polluted water harms communities by destroying underwater life and messing up food chains. Moreover, water pollution can have negatively impacts on human health due to alterations in the food chain and contracting an illness while using contaminated water [[16,](#page-31-0) [10\]](#page-31-1).

We treat water to clean it up and make it safe to human consumption. Water treatment is essential because it removes harmful pollutants from water that can cause illness and disease. Contaminants such as bacteria, viruses, and parasites can be present in untreated water and cause serious health problems. Treating water not only makes it safe to drink, but also removes harmful chemicals that pollute the environment. By treating water before

Iran. J. Numer. Anal. Optim., Vol. ??, No. ??, ??, pp ??

it is released into the environment, we can help to protect aquatic life and preserve our natural resources. There are some ways to treat water, such as Coagulation and flocculation, sedimentation, filtration, disinfection, reverse osmosis, and distillation [[11,](#page-31-2) [26\]](#page-32-0). Mathematical modeling of water pollutant transmission is a low-cost method that can provide valuable information to managers and planners of water resources for quality management of these resources and choosing the appropriate method for water treatment.

A mathematical model is a simplified representation of a real-world system that uses mathematical language to describe the relationships between different variables. Mathematical models are used everywhere, from physics and engineering to economics and biology. They can be utilized to predict the behavior of a system under different conditions and help us understand how different variables interact with each other.

A system of nonlinear ordinary differential equations has been developed as a mathematical model for water pollutants that are soluble and insoluble in [[25\]](#page-32-1). In this paper, converting insoluble water pollutants into soluble water pollutants involves applying control. A discussion of the stability of the water pollutants transmission model is given with numerical data. A value of 0.8373 is computed for the basic reproduction number, indicating that insoluble water pollutants control can lead to an 83*.*73% reduction in water pollutants. In paper [\[21](#page-32-2)] authors used a novel approach in numerical methods such as the finite volume method and artificial neural networks combined as a machine learning method to model pollution transmission in rivers. The modeling of pollution transmission includes numerical solutions of the advection-dispersion equation and estimating the longitudinal dispersion coefficient [[21\]](#page-32-2). In light of ordinary differential equations, the formulation of a mathematical model for soluble and insoluble water pollutants is presented in [[3\]](#page-30-0). This study uses math to predict how different types of pollution move through rivers. Ordinary differential equations were used to formulate the mathematical model, and sensitivity analysis was carried out to test parameters. This research aims to understand how pollution affects oxygen levels in rivers, helping us manage water resources better. Depending on [\[12](#page-31-3)], the paper by Guo and Cheng on mathematical modeling for simulating water pollution accidents, maps categorical variables in a function

approximation problem into Euclidean spaces, which are the entity embeddings of the categorical variables. The neural network learns the mapping during the standard supervised training process. The paper also formulates a mathematical model for water pollutant transmission and derives the stability analysis of the transmission model. However, optimal control problems (OCPs) can be utilized to control the transmission of water pollutants. Direct and indirect methods are two numerical methods used to solve OCPs. In an indirect method, the calculus of variations is used to determine the first-order optimality conditions of the OCP. The finer indirect methods use necessary optimality conditions. Direct methods transform the control problem after discretization to an optimization problem. The nonlinear optimization problem can be solved utilizing SQP methods or gradient methods [[8\]](#page-30-1). The direct method has several advantages over the indirect method in OCPs, including no need to derive necessary conditions, more versatility and ease of implementation, and higher accuracy and robustness. Direct methods can handle discontinuities in control functions more effectively and do not require explicit numerical integration, making them more suitable for highly nonlinear dynamics. Additionally, direct methods can handle inequality constraints and interior point constraints more easily and do not require an initial guess for the solution, making them a better choice for many applications [\[22](#page-32-3), [8](#page-30-1)].

In the paper [\[25](#page-32-1)], the authors discussed the OCP for water pollution transmission. The paper presents a mathematical model for the transmission of water pollutants in a system of ordinary differential equation. It proposes an optimal control strategy based on applying Pontryagin's maximum principle to determine the optimal control and minimize the concentration of pollutants in the system. In [\[23](#page-32-4)], the authors also discussed optimal regulation of sudden water pollution. The paper proposes a multi-objective optimization algorithm, the quantifying of pollutant characteristic parameters, and optimization partitioning using three methods, which can meet the emergency regulation and control necessities for various objectives throughout the entire region of a sudden water pollution event.

In this paper, a solution to solve an OCP for the transmission of water pollutants is presented based on the collocation approach. The OCP is converted to nonlinear programming (NLP) by utilizing shifted Jacobi poly-

Iran. J. Numer. Anal. Optim., Vol. ??, No. ??, ??, pp ??

nomials (SJPs) and its derivative operational matrix. So far, the different methods are used to convert the OCP to an NLP problem to get approximate control and to determine the functions that, under definite constraints, converge to the exact solution, and then an appropriate optimization algorithm should be executed to find an optimal solution with high quality. Thus, a productive metaheuristic approach will be utilized based on the mountain gazelle algorithm (MGA) for the OCP of water pollutant transmission.

The MGA was a parameter-free algorithm, thus there were no parameters to determine. The free parameter feature of MGA mean that there was no need to set a fixed parameter before the optimization operation. Since the converted OCP for water pollutant transmission is nonlinear and large scale, we need to survey the impact of local and metaheuristic methods to solve this optimization problem. Among the local approaches, the trust region algorithm is used for solving large-scale nonlinear optimization problems with respect to its efficiency [\[29](#page-32-5), [24\]](#page-32-6). However, it obtains local answers in a high execution time as the problem dimension increases. To prevent this kind of defect, a combined approximate method by a collocation approach based on SJPs and an MGA is developed in this paper. Thus, good performance metaheuristic with high decisions and global search and collocation method is used to solve the OCP for water pollutant transmission. This method combines a collocation approach and an MGA to find the global optimal of the OCP in a more efficient way. The MGA is a nature-inspired metaheuristic algorithm that simulates the social life and hierarchy of wild mountain gazelles (MGs). So, a metaheuristic algorithm with high-quality solutions in terms of high-precision numerical solutions and short computational time should be executed to solve this optimization problem. The MGA finds near-optimal solutions or the global optimal of objective functional in a more efficient way. About the developed MGA, it should be noted that this algorithm is really worthy and proper for the nonlinear optimization problems with the number of more variables and restrictions, especially when solving large-sized examples of the optimization problems [[1\]](#page-29-0). The MGA has derivation-free mechanisms. In contrast to gradient-based optimization methods, this metaheuristic approach optimizes the problems stochastically via the pattern of natural events and social behavior of MGs using the four procedures of Terri-

Iran. J. Numer. Anal. Optim., Vol. ??, No. ??, ??, pp ??

torial Alone Males, Maternity Flocks, Bachelor Male Flocks, and Movement to Seek for Food. The optimization mechanism starts with random answer, and there is no need to calculate the derivative of search areas or gradient data of the objective functionals to find the global optimal of the problem. This makes the MGA very useful for the NLP problems with unknown derivative data. Also, the simple structure of the MGA is especially excellence in the presence of nonsmooth objective functionals, for which exact methods may fail to find their global solutions. Reliability of the MGA is evaluated based on some nonsmooth functions and engineering design problems [[19](#page-31-4), [13](#page-31-5), [30,](#page-33-0) [20](#page-32-7), [27](#page-32-8), [2,](#page-30-2) [1](#page-29-0)]. So, the MGA is a good choice and a competitive algorithm when solving nonsmooth and nonlinear functions. For the proposed optimization problem, the values of objective functionals indicate that MGA's performance is suitable and the MGA is a good candidate to solve this problem. The MGA is compared to the most famous and new metaheuristic methods based on best cost, average cost (AVG), corresponding standard deviation (STD), and convergence speed. The comparative results indicated that the MGA obtained very competitive solutions in comparison with other well-known metaheuristic algorithm [\[19](#page-31-4), [13,](#page-31-5) [30,](#page-33-0) [20](#page-32-7), [27](#page-32-8), [2,](#page-30-2) [1\]](#page-29-0). Compared with other metaheuristic algorithms, MGA is preferable based on most of the test mathematical functions' best objective, AVG, and STD values. It had a superior convergence speed as it obtained the global optimal after the first few repetitions, as in test functions. Lastly, considering MGA applied several finite vectors, it had an excellent ability to search all solution regions and a noticeable ability to avoid local optimum solutions. The MGA had been applied for several studies like Magdy et al. [[19\]](#page-31-4), Khodadadi et al. [[13\]](#page-31-5), Zellagui, Belbachir, and El-Sehiemy [[30\]](#page-33-0), Maashi et al. [\[20](#page-32-7)], Utama, Sanjaya, and Nugraha [\[27](#page-32-8)], Aribowo et al. [[2\]](#page-30-2), and Abdelsattar et al. [[1\]](#page-29-0). As to the experiments and numerical results obtained, one can conclude that MGA in this work is a satisfactory and acceptable option for solving real-world OCPs of water pollutant transmission with unknown search regions.

Some benefits of the propounded approach in this paper are as follows:

1. The propounded approach can be applied to other OCP systems, which are governed by nonlinear differential equations.

Iran. J. Numer. Anal. Optim., Vol. ??, No. ??, ??, pp ??

- 2. Although we have no exact solution for this problem, the spectral method in the OCP is convergent according to [\[15](#page-31-6), [4](#page-30-3)].
- 3. The derivative shifted Jacobi operational matrix method can be implemented with ease. One of the main advantages of using derivative operational matrices is that they contain many zero elements and are sparse; hence, they make the present method highly efficient. Another advantage of utilizing these matrices is that they establish an equal relation in equation [\(13](#page-12-0)) for the derivative operational matrix.
- 4. Jacobi polynomials are orthogonal over a finite interval with respect to a weight function, allowing for flexibility in handling various types of boundary conditions in OCPs. This orthogonality simplifies the approximation of functions and reduces numerical errors when transforming differential equations into algebraic equations.

As far as we know, this is the first paper that has used the collocation method and MGA to solve the OCP of water pollutant transmission. This combination is novel and allows for high-precision numerical solutions and efficient handling of complex OCPs. The method developed in the paper effectively handles the nonlinearity and constraints typical of OCPs in environmental systems.

This paper is structured as follows: Section 2 presents an in-depth mathematical model of OCP. In Section 3, we introduce a solution methodology for this problem by utilizing collocation and the MGA. In Section 4, we demonstrate the application of OCP to water pollution transmission and numerical simulations. In Section 5, we give an overview of our conclusions.

2 Model definition

Transmission of water pollutants is a significant environmental issue that directly affects water quality, ecosystem health, and public safety. Contaminants such as industrial chemicals, agricultural runoff, and untreated wastewater can enter water bodies, leading to harmful effects on aquatic life and human health. This problem is particularly challenging because pollu-

Iran. J. Numer. Anal. Optim., Vol. ??, No. ??, ??, pp ??

tants can spread rapidly and accumulate in different parts of the ecosystem, making it difficult to control their impact. From an optimal control perspective, the goal is to develop strategies that minimize the adverse effects of pollutants while optimizing resource use and operational costs. By modeling the transmission of pollutants as an OCP, we can identify the best interventions, such as the optimal timing and intensity of pollutant reduction measures, to achieve desired water quality standards. This approach allows for a systematic examination of different scenarios and policies, providing insights into the most effective ways to mitigate pollution in water bodies. Thus, addressing the transmission of water pollutants as an OCP not only helps in understanding the dynamics and spread of pollutants but also aids in designing efficient and cost-effective strategies for maintaining water quality, protecting ecosystems, and ensuring public heal.

2.1 Notations

The parameters and variables utilized in this mathematical model are depicted in Tables [1](#page-8-0) and [2](#page-8-1).

2.1.1 Variables

The mathematical framework of the OCP for water pollutant transmission is presented as follows in problem *P*.

Problem *P*

$$
\min J(W, S, I, \mathcal{U}) = \int_{0}^{L} a_1 W(t) + a_2 S(t) + a_3 I(t) + a_4 \mathcal{U}(t) dt, \tag{1}
$$

subject to the following differential equations:

$$
\frac{dW}{dt} = \Lambda - \alpha_1 WS - \alpha_2 WI + \rho \alpha_2 I - \mu W, \quad W \ge 0,
$$

$$
\frac{dS}{dt} = \alpha_1 WS + (\delta + \mathcal{U}(t))I - (\theta_1 + \mu)S, \quad S \ge 0,
$$

Iran. J. Numer. Anal. Optim., Vol. ??, No. ??, ??, pp ??

9 Optimal control of water pollutant transmission by utilizing a combined ...

Table 1: Parameters utilized in the mathematical model

Parameters	Descriptions
Λ	Rate of water pollution
	(amount of pollutants entering the water body per unit time)
α_1	Transportation rate of soluble water contaminants
	(how quickly soluble pollutants move through water)
α_2	Transportation rate of insoluble water contaminants
	(how quickly insoluble pollutants move through water)
ρ	Rate at which insoluble water pollutants
	convert into soluble pollutants
μ	Rate at which water pollutants can be removed or treated
δ	Amount of insoluble water pollutants treated
	and converted into soluble form
θ_1	Treatment capacity for soluble water pollutants
θ_2	Treatment capacity for insoluble water pollutants

Table 2: Variables utilized in the mathematical model

$$
\frac{dI}{dt} = \alpha_2 WI - \rho \alpha_2 I - (\delta + \mathcal{U}(t) + \theta_2 + \mu)I, \quad I \ge 0,
$$

$$
\frac{d\mathcal{T}}{dt} = \theta_1 S + \theta_2 I - \mu \mathcal{T}, \quad \mathcal{T} \ge 0,
$$

with initial conditions

 $W(0) = W_0$, $S(0) = S_0$, $I(0) = I_0$, $\mathcal{T}(0) = \mathcal{T}_0$,

Iran. J. Numer. Anal. Optim., Vol. ??, No. ??, ??, pp ??

Figure 1: Diagram of the mathematical model for the transmission of water pollutants

where W_0 , S_0 , I_0 , and \mathcal{T}_0 are the initial concentrations of the state and control variables. We assume that $0 \leq \mathcal{U}(t) \leq 1$. *L* represents the lifespan of water pollutant transmission, and *a*1, *a*2, *a*3, and *a*⁴ are constants. The diagram of state constraints is given in Figure [1](#page-9-0).

The optimal control model for water pollutant transmission aims to minimize the concentration of insoluble water pollutants by utilizing a control function U . Rivers possess a natural ability to purify themselves through physical, chemical, and biological processes, including sedimentation, oxidation, and biodegradability. This study focuses on the transmission of water pollutants in a river in India $[3, 25]$ $[3, 25]$, specifically examining the dynamics of soluble and insoluble pollutants. The mathematical model developed in this paper is applied to simulate pollutant dispersion in a river, allowing for the assessment of various treatment strategies. By employing numerical simulations, we analyze the effects of different parameters on pollutant concentration and removal rates. The results of this case study provide valuable insights for environmental engineers and policymakers, highlighting the importance of optimizing control measures to effectively manage water quality and reduce pollution levels.

3 Solution methodology

This section describes a clear and concise detailed description of the approach taken to solve the OCP presented in ([1\)](#page-7-0). Firstly, the basic properties of SJPs and its derivative operational matrix are given. In subsection [3.3](#page-12-1), we provide the collocation approach to discretize and transform OCP into an NLP. Finally, in [3.3,](#page-12-1) the MGA is applied to the resulting problem to obtain the solution of OCP in ([1](#page-7-0)).

3.1 Basic features of SJPs

The definition of the set of SJPs ${P}_{L,i}^{(\alpha,\beta)}(t) \}_{i=0}^n$ in $[0,L]$ is given in Doha et al. in $[6]$ is as follows:

$$
P_{L,i}^{(\alpha,\beta)}(t) = \frac{[\alpha + \beta + 2i - 1] \{\alpha^2 - \beta^2 + \left[\frac{2t}{L} - 1\right] [\alpha + \beta + 2i] [\alpha + \beta + 2i - 2]} \} P_{L,i-1}^{(\alpha,\beta)}(t)}{2i [\alpha + \beta + i] [\alpha + \beta + 2i - 2]} - \frac{(\alpha + i - 1)(\beta + i - 1)(\alpha + \beta + 2i)}{i(\alpha + \beta + i)(\alpha + \beta + 2i - 2)} P_{L,i-1}^{(\alpha,\beta)}(t), \qquad i = 2, 3, ..., n,
$$
\n(2)

where $P_{L,0}^{(\alpha,\beta)}$ $L_{L,0}^{(\alpha,\beta)}(t) = 1$ and $P_{L,1}^{(\alpha,\beta)}$ $(L_{L,1}^{(\alpha,\beta)}(t)) = \frac{\alpha+\beta+2}{2}(\frac{2t}{L}-1) + \frac{\alpha-\beta}{2}$. An analytic form for the SJPs $P_{L,i}^{(\alpha,\beta)}(t)$ of degree *i*, is given by the equation below:

$$
P_{L,i}^{(\alpha,\beta)}(t) = \sum_{k=0}^{i} (-1)^{i-k} \frac{\Gamma(i+\beta+1)\Gamma(i+k+\alpha+\beta+1)}{\Gamma(k+\beta+1)\Gamma(i+\alpha+\beta+1)(i-k)!k!T^k} t^k, \quad (3)
$$

where

$$
P_{L,i}^{(\alpha,\beta)}(0) = (-1)^i \frac{\Gamma(i+\beta+1)}{\Gamma(\beta+1)i}.
$$
 (4)

Over the interval $[0, L]$, they are orthogonal with respect to the weight function $W_L^{(\alpha,\beta)}$ $L^{(\alpha,\beta)}(t) = t^{\beta}(L-t)^{\alpha}$ and satisfy the following properties for $k = 0, 1, \ldots, n$:

$$
\int_{0}^{L} P_{L,j}^{(\alpha,\beta)}(t) P_{L,k}^{(\alpha,\beta)}(t) W_L^{(\alpha,\beta)}(t) dt = h_k,
$$
\n(5)

in which

Iran. J. Numer. Anal. Optim., Vol. ??, No. ??, ??, pp ??

Ebrahimzadeh, Khanduzi, Mirabbasi and Hashemizadeh 12

$$
h_k = \begin{cases} \frac{T^{\alpha+\beta+1}\Gamma(k+\alpha+1)\Gamma(k+\beta+1)}{(2k+\alpha+\beta+1)k!\Gamma(k+\beta+\alpha+1)}, & i = j, \\ 0, & i \neq j. \end{cases}
$$
 (6)

The SJPs can be used to express a function $f(t) \in L^2(0, L)$ as follows:

$$
f(t) = \sum_{k=0}^{n} a_k P_{L,j}^{\alpha,\beta}(t) = A^T \phi(t),
$$
 (7)

where $A = [a_0, a_1, \dots, a_n]$ and

$$
\phi(t) = [P_{L,0}^{\alpha,\beta}(t), P_{L,1}^{\alpha,\beta}(t), \dots, P_{L,n}^{\alpha,\beta}(t)]^T.
$$
\n(8)

Using the following form, one can obtain the coefficients a_j for $j = 0, 1, \ldots, n$.

$$
a_j = \frac{1}{h_j} \int_0^L W_L^{(\alpha,\beta)(t)} f(t) P_{L,j}^{(\alpha,\beta)}(t) dt.
$$
 (9)

The definition and Lemma below will be required in section [3.3](#page-12-1) from [\[14](#page-31-7)].

Definition 1. The following definition describes the tensor product of vectors $X_{\hat{m}} = [x_i]$ and $Y_{\hat{m}} = [y_i]$:

$$
X \otimes Y = (x_i \times y_i)_{\hat{m}}.\tag{10}
$$

The tensor product of two matrices $M = [m_{i,j}]$ and $N = [n_{i,j}]$ of order $\hat{m} \times \hat{m}$ is expressed as follows:

$$
M \otimes N = (m_{ij} \times y_{ij})_{\hat{m} \times \hat{m}}.
$$
\n(11)

Lemma 1. Let the functions $f(t) = f^T \phi(t)$ and $g(t) = g^T \phi(t)$ belonging to $L^2[0,1]$ be expressed by SJPs. Then,

$$
f(t)g(t) = (f^T \otimes g^T) \phi(t).
$$
 (12)

Proof. We have

$$
f(t)g(t) = f^T \phi(t)\phi^T(t)g = f_1g_1 P_{L,0}^{\alpha,\beta}(t) + f_2g_2 P_{L,1}^{\alpha,\beta}(t) + \dots + f_n g_n P_{L,n}^{\alpha,\beta}(t)
$$

= $f(t)g(t) = (f^T \otimes g^T) \phi(t).$

 \Box

3.2 SJP operational matrix of derivative

The derivative of vector $\phi(t)$ in ([8\)](#page-11-0) can be expressed in the matrix form as shown in [\[7](#page-30-5)]:

$$
\frac{d\phi(t)}{dt} = D^{(1)}\phi(t). \tag{13}
$$

We define the $(n + 1) \times (n + 1)$ derivative operational matrix of SJP as $D^{(1)} = [d_{ij}]$, which is obtained in [[7\]](#page-30-5) and defined as follows:

$$
D^{(1)} = (d_{ij}) = \begin{cases} A_1(i,j), & i > j, \\ 0, & \text{otherwise,} \end{cases}
$$
 (14)

where

$$
A_1(i,j) = \frac{L^{\alpha+\beta}(i+\alpha+\beta+1)(i+\alpha+\beta+2)j(j+\alpha+2)_{i-j-1}\Gamma(j+\alpha+\beta+1)}{(i-j-1)!\Gamma(2j+\alpha+\beta+1)}
$$

$$
\times {}_3F_2\left(\begin{array}{c} -i+1+j, i+j+\alpha+\beta+2 \ j+\alpha+1 \\ j+\alpha+2 \ 2j+\alpha+\beta+2 \end{array} ; 1 \right).
$$
 (15)

In [[7\]](#page-30-5), the proof of obtaining ([15\)](#page-12-2) is provided. Additionally, for the general definition of a generalized hypergeometric series and special ${}_3F_2$, refer to [[17\]](#page-31-8).

3.3 Collocation method

Firstly, we can express our unknown functions in terms of SJPs as an approximation

$$
W(t) \approx C_1^T \phi(t), \quad I(t) \approx C_2^T \phi(t), \quad S(t) \approx C_3^T \phi(t),
$$

$$
\mathcal{T}(t) \approx C_4^T \phi(t), \quad \mathcal{U}(t) \approx C_5^T \phi(t), \tag{16}
$$

where ϕ is defined in equation ([8\)](#page-11-0). Vectors $C_i : i = 1, ..., 4$ are defined as follows:

$$
C_1 = [c_0, \dots, c_n]^T, \ C_2 = [c_{n+1}, \dots, c_{2n+1}]^T, \ C_3 = [c_{2n+2}, \dots, c_{3n+2}]^T,
$$
\n
$$
C_4 = [c_{3n+3}, \dots, c_{4n+3}]^T, \ C_5 = [c_{4n+4}, \dots, c_{5n+4}]^T.
$$
\n(18)

By utilizing (13) and (16) (16) , we possess

Ebrahimzadeh, Khanduzi, Mirabbasi and Hashemizadeh 14

$$
\frac{dW}{dt} = C_1^T \phi'(t) = C_1^T D^{(1)} \phi(t) \qquad \frac{dS}{dt} = C_2^T \phi'(t) = C_2^T D^{(1)} \phi(t),
$$

$$
\frac{dI}{dt} = C_3^T \phi'(t) = C_3^T D^{(1)} \phi(t), \qquad \frac{d\mathcal{T}}{dt} = C_4^T \phi'(t) = C_4^T D^{(1)} \phi(t). \tag{19}
$$

By substituting equations (16) (16) and (19) (19) in system dynamics (1) (1) (1) , we have

$$
C_1^T D^{(1)} \phi(t) = \Lambda - \alpha_1 \left(C_1^T \otimes C_2^T \right) \phi(t) - \alpha_2 \left(C_1^T \otimes C_3^T \right) \phi(t)
$$

$$
+ \rho \alpha_2 C_3^T \phi(t) - \mu C_1^T \phi(t),
$$

$$
C_2^T D^{(1)} \phi(t) = \alpha_1 \left(C_1^T \otimes C_2^T \right) \phi(t) + \left(\delta + C_5^T \phi(t) \right) C_3^T \phi(t) - \left(\theta_1 + \mu \right) C_2^T \phi(t),
$$

\n
$$
C_3^T D^{(1)} \phi(t) = \alpha_2 \left(C_1^T \otimes C_3^T \right) \phi(t) - \rho \alpha_2 C_3^T \phi(t) - \left(\delta + C_5^T \phi(t) + \theta_2 + \mu \right) C_3^T \phi(t),
$$

\n
$$
C_4^T D^{(1)} \phi(t) = \theta_1 C_2^T \phi(t) + \theta_2 C_3^T \phi(t) - \mu C_4^T \phi(t).
$$
\n(20)

This essay aim is to determine $(4n+4)$ unknowns of a_i for $i = 0, 1, \ldots, 4n+3$. We can obtain four linear equations by substituting the initial conditions in equations [\(16](#page-12-3)).

$$
W_0 = C_1^T \phi(0) \quad (0), S_0 = C_2^T \phi(0), \quad I_0 = C_3^T \phi(0), \quad \mathcal{T}_0 = C_4^T \phi(0). \quad (21)
$$

We can determine $\phi(0)$ from [\(4](#page-10-0)). By replacing a set of (n) points $\tau_i = \frac{2i-1}{2(n+1)}$ for $i = 1, 2, \ldots, n$, we possess

$$
C_1^T D^{(1)} \phi(\tau_i) = \Lambda - \alpha_1 \left(C_1^T \otimes C_2^T \right) \phi(\tau_i) - \alpha_2 \left(C_1^T \otimes C_3^T \right) \phi(\tau_i)
$$

$$
+ \rho \alpha_2 C_3^T \phi(\tau_i) - \mu C_1^T \phi(\tau_i),
$$

 $C_2^T D^{(1)} \phi(\tau_i) = \alpha_1 \left(C_1^T \otimes C_2^T \right) \phi(\tau_i) + (\delta + C_5^T \phi(\tau_i)) C_3^T \phi(\tau_i) - (\theta_1 + \mu) C_2^T \phi(\tau_i),$

$$
C_3^T D^{(1)} \phi(\tau_i) = \alpha_2 \left(C_1^T \otimes C_3^T \right) \phi(\tau_i) - \rho \alpha_2 \ C_3^T \phi(\tau_i) - (\delta + C_5^T \phi(\tau_i) + \theta_2 + \mu) C_3^T \phi(\tau_i), C_4^T D^{(1)} \phi(\tau_i) = \theta_1 C_2^T \phi(\tau_i) + \theta_2 C_3^T \phi(\tau_i) - \mu C_4^T \phi(\tau_i).
$$
(22)

For approximating the cost function given in [\(1](#page-7-0)), the Gauss Legendre (GL) quadrature has been applied after the appropriate interval transformation as follows:

$$
J(W, S, I, U) = \int_0^L a_1 W(t) + a_2 S(t) + a_3 I(t) + a_4 U(t) dt
$$

Iran. J. Numer. Anal. Optim., Vol. ??, No. ??, ??, pp ??

15 Optimal control of water pollutant transmission by utilizing a combined ...

$$
= \frac{L}{2} \int_{-1}^{1} a_1 W(\frac{L(\tau + 1)}{2}) + a_2 S(\frac{L(\tau + 1)}{2}) + a_3 I(\frac{L(\tau + 1)}{2})
$$

+ $a_4 U(\frac{L(\tau + 1)}{2}) d\tau$

$$
\approx \frac{L}{2} \sum_{j=1}^{N} w_j \left(a_1 W(\frac{L(\tau_j + 1)}{2}) + a_2 S(\frac{L(\tau_j + 1)}{2}) + a_3 I(\frac{L(\tau_j + 1)}{2}) + a_4 U(\frac{L(\tau_j + 1)}{2}) \right).
$$
(23)

By substituting (16) (16) in (23) (23) , we have

$$
J(W, S, I, U) \approx \sum_{j=1}^{N} w_j' \left(a_1 C_1^T \phi(\tau_j') + a_2 C_2^T \phi(\tau_j') + a_3 C_3^T \phi(\tau_j') + a_4 C_5^T \phi(\tau_j') \right)
$$

= $\bar{\mathcal{J}}(W, S, I, U)$ (24)

The GL nodes τ_j 's are zeros of Legendre polynomials $L_N(t)$ in [−1, 1], where $w'_{j} = \frac{T}{2}w_{j}$ and $\tau'_{j} = \frac{L(\tau_{j+1})}{2}$. The corresponding weights w_{j} can be obtained using the following relation [\[18](#page-31-9)]:

$$
w_j = \frac{2}{(1 - \tau_j^2)[L'_N(\tau_j)]^2}.
$$
\n(25)

The primary OCP in ([1\)](#page-7-0) is converted to an NLP problem with [\(24](#page-14-1)) as the cost functional and equation [\(22](#page-13-1)) as the constraints. This leads to following problem P_N , where N is the number of basis.

Problem P_N :

$$
\min \quad \bar{\mathcal{J}}(W,S,I,\mathcal{U})
$$

subject to

$$
C_1^T D^{(1)} \phi(\tau_i) = \Lambda - \alpha_1 \left(C_1^T \otimes C_2^T \right) \phi(\tau_i) - \alpha_2 \left(C_1^T \otimes C_3^T \right) \phi(\tau_i) + \rho \alpha_2 C_3^T \phi(\tau_i) - \mu C_1^T \phi(\tau_i), C_2^T D^{(1)} \phi(\tau_i) = \alpha_1 \left(C_1^T \otimes C_2^T \right) \phi(\tau_i) + (\delta + C_5^T \phi(\tau_i)) C_3^T \phi(\tau_i) - (\theta_1 + \mu) C_2^T \phi(\tau_i), C_3^T D^{(1)} \phi(\tau_i) = \alpha_2 \left(C_1^T \otimes C_3^T \right) \phi(\tau_i) - \rho \alpha_2 C_3^T \phi(\tau_i) - (\delta + C_5^T \phi(\tau_i) + \theta_2 + \mu) C_3^T \phi(\tau_i),
$$

Iran. J. Numer. Anal. Optim., Vol. ??, No. ??, ??, pp ??

Ebrahimzadeh, Khanduzi, Mirabbasi and Hashemizadeh 16

$$
C_4^T D^{(1)} \phi(\tau_i) = \theta_1 C_2^T \phi(\tau_i) + \theta_2 C_3^T \phi(\tau_i) - \mu C_4^T \phi(\tau_i).
$$

\n
$$
W_0 = C_1^T \phi(0), \qquad S_0 = C_2^T \phi(0), \qquad I_0 = C_3^T \phi(0), \qquad \mathcal{T}_0 = C_4^T \phi(0).
$$

After solving the problem P_N , the unknown vectors C_1 , C_2 , C_3 , C_4 , and C_5 are obtained. By substituting these values in (16) (16) , the unknown functions $W(t)$, $I(t)$, $S(t)$, $\mathcal{T}(t)$, and $\mathcal{U}(t)$ can be obtained. In section [3.4,](#page-15-0) the MGA [[1\]](#page-29-0) can be utilized to solve this NLP.

3.4 Mountain Gazelle Algorithm (MGA)

In this subsection, an innovative optimization approach released in 2022 with respect to social behaviors among MGs is introduced. The main contexts of collective and gregarious habitancy of MGs had been applied to design a mathematical formulation of the MGA [[1](#page-29-0)]. The MGA execute strategies based on four fundamental components in the habitancy of MGs: Young male flocks, maternal flocks, alone, territorial males, and movement to seek for food.

Each MG (C_i) is one of the flocks of maternal flocks, young male flocks, or alone, territorial males through the MGA. A child MG is born out by one of three flocks. MGA's best global answer is mature male MG in the flock zone. The MGs in the male young flocks are young and not powerful to generate or conduct the female MG. So, 1/3 of the population in the total MGs is evaluated to get the smallest objective value in comparison to other parameters for mathematical formulation.

Besides, other feasible answers to the total population take into account MGs in maternal flocks. Powerful MGs with high quality answers are considered in the end of each iteration. Other answers that adjoined to the total MGs and had a much smaller objective value are acknowledged as old and sick MGs and are deleted from the whole MGs. Subsequently, the techniques in MGA to execute strategies are modeled and defined mathematically. Furthermore, based on the nature of the MGA, exploitation and exploration processes are executed in parallel with respect to four methods. Indeed, it is possible for an answer to proceed toward the best answer and also exe17 Optimal control of water pollutant transmission by utilizing a combined ...

cute the exploration strategy using the four procedures of the mathematical formulation.

3.4.1 Territorial alone males

When male MGs grew up and became powerful, an alone zone was generated that was vastly territorial, and long distances divided the zones. The combat between mature male MGs occurred over the zone for ownership of the females. The young males endeavor to grab the zone or the female; furthermore, the mature males endeavor to keep their surroundings. The following relation [\(26](#page-16-0)) had been applied to formulate the mature male zone:

$$
TAM = m_g - |(ei_1 \times BF - ei_2 \times C(t)) \times F| \times Cof_e.
$$
 (26)

In relation (26) (26) , m_g is the location of the best global answer (mature male). The inputs ei_1 and ei_2 are random integer numbers 1 or 2. Also, BF is the coefficient vector of the young male flock, computed based on the relation (27) (27) , and *F* is also calculated according to (28) (28) . Moreover, Cof_e is a randomly chosen coefficient vector changed in each repetition and applied for increasing the search ability, computed based on the relation [\(29](#page-17-0)). Therefore,

$$
BF = C_{ea} \times \lfloor e_1 \rfloor + M_{pe} \times \lceil e_2 \rceil, \qquad ea = \{\lceil \frac{N}{3} \rceil \cdots N\}.
$$
 (27)

In relation ([27\)](#page-16-1), *Cea* is a random answer (young male) in the interval of *ea*, and M_{pe} is the mean of search operatives $\lceil \frac{N}{3} \rceil$ that are randomly chosen. In addition to, N is the whole number of MGs, and e_1 and e_2 are random numbers from the interval [0*,* 1]. Then

$$
F = N_1(D) \times \exp(2 - I \cdot \left(\frac{2}{MaxIter})\right). \tag{28}
$$

In relation (28) (28) , in the dimensions of the NLP, N_1 is a random value from the standard distribution. The Exponential function is also known as exp, *M axIter* is the total number of repetitions, and *Iter* is the current number of repetitions. Also,

Iran. J. Numer. Anal. Optim., Vol. ??, No. ??, ??, pp ??

Ebrahimzadeh, Khanduzi, Mirabbasi and Hashemizadeh 18

$$
Cof_e = \begin{cases} (a+1) + e_3, \\ a \times N_2(D), \\ e_4(D), \\ N_3(D) \times N_4(D)^2 \times \cos((e_4 \times 2) \times N_3(D)) \end{cases}
$$
 (29)

In relation (29) (29) , *a* is computed based on relation (30) (30) . In addition to, e_3 , e_4 , and *rand* are random values in the interval $[0, 1]$. In addition, N_2 , N_3 , and *N*⁴ are random values in the normal interval and the dimensions of the NLP. Now,

$$
a = -1 + Iter \times \frac{-1}{MaxIter}.
$$
\n(30)

At last, in relation ([30\)](#page-17-1), *M axIter* describes the whole repetitions, and *Iter* illustrates the current number of repetitions.

3.4.2 Maternity flocks

Maternity flocks had a pivotal performance in the habitancy process of MGs, as they gave birth to strong male MGs. Male MGs could had a pivotal performance in the transfer of MGs and young males attempting to occupy females. The action is modeled based on the relation (31) (31) as follows:

$$
MF = (BF + Cof_{1,e}) + (ei_3 \times m_g - ei_4 \times C_{rand}) \times Cof_{1,e}. \tag{31}
$$

In relation (31) (31) , *BF* is the vector of the affect coefficient of young males, which is computed based on relation [\(27](#page-16-1)). Also, $Cof_{2,e}$ and $Cof_{3,e}$ are randomly chosen factors, which are computed according to relation (29) (29) . Moreover, ei_3 and ei_4 are integer and random values 1 or 2, and m_g is the (mature male) global answer at the present iteration. At last, *Crand* is the location of an MG that is randomly chosen from the total MGs.

3.4.3 Bachelor male flocks

When the male MGs become mature, they wanted to construct zone and occupy female MGs. Then, the young male MGs struggled with the male

Iran. J. Numer. Anal. Optim., Vol. ??, No. ??, ??, pp ??

MGs over the area and possession of the female MGs, so there is a lot of violence. Relation below ([32\)](#page-18-0) is implemented to model this action of MGs:

$$
BMF = (C(t) - D) + ei_5 \times m_g - ei_6 \times BF) \times Cof_e.
$$
 (32)

In relation (32) (32) , $C(t)$ is the MG location in the present repetition, and *D* is computed based on relation (33) (33) . Also, ei_5 and ei_6 are numbers 1 or 2, and m_g is the location of the male MG (the best answer). As well, BF is the affect coefficient of the young male flock, which is computed based on the relation (27) (27) . Moreover, Cof_e is a randomly chosen factor, computed depending on the relation [\(29](#page-17-0)) below:

$$
D = (|C(t)| + |m_g|) \times (2 \times e_6 - 1).
$$
 (33)

In relation [\(33](#page-18-1)), $C(t)$ and m_g are the locations of the MGs in the present repetition, correspondingly, and the location is the best answer (mature male). Also, e_6 is a random value from the interval $[0, 1]$.

3.4.4 Movement to seek for food

MGs continually search and move far away distances to gain food. Meanwhile, MGs have favorable velocity and great jump strength. Relation below ([34\)](#page-18-2) had been applied to model this action of MGs:

$$
MSF = (ub - lb) \times e_7 + lb.
$$
\n(34)

In relation (34) (34) , *ub* and *lb* are the NLP's upper and lower bounds, correspondingly. At last, r_7 is an integer and random number 0 and 1 .

The four TAM, MF, BMF, and MSF strategies are executed to the whole MGs to generate new MGs. A new generation joins the entire MGs, and each generation is a solution. Also, all MGs are in ascending order at the end of each generation. The best MGs that had acceptable quality and favorable answers and objective less, are maintained in the whole MGs. Then, old or weak MGs are deleted from the total MGs. The best MG is considered as the mature male MG that possessed the zone.

Iran. J. Numer. Anal. Optim., Vol. ??, No. ??, ??, pp ??

The pseudo-code of the MGA is indicated in Algorithm [1](#page-19-0). The flowchart of MGA is shown in Figure [2.](#page-20-0)

3.4.5 Computational complexity of the MGA

The complexity of MGA depends on the following factors:

Iran. J. Numer. Anal. Optim., Vol. ??, No. ??, ??, pp ??

Figure 2: The flowchart of MGA for solving the presented NLP

Ebrahimzadeh, Khanduzi, Mirabbasi and Hashemizadeh 22

- 1) Initialization
- 2) Fitness assessment
- 3) Gazelle update

The computational cost of the initialization procedure is *O* concerning the presence of *N* Gazelles (*N*). Also, the computational complexity of the operation for generating and updating new answers that is executed on all search agents in the NLP space, is $O(T \times N \times D \times 4)$, where *D* is the NLP dimension, and *T* is the maximum number of repetitions. So, the complexity of MGA is considered as $O(T \times N \times 4) \times O(J(W, S, I, \mathcal{U}))$, where the objective function is appraised.

3.4.6 Convergence of MGA

The MGA is designed to ensure convergence through a structured approach that integrates four distinct mechanisms aimed at enhancing its search capabilities. These mechanisms facilitate diverse movement patterns for search agents, allowing for effective exploration and exploitation of the solution space. By employing varying coefficient vectors, the MGA prevents stagnation in local optima and promotes parallel exploration, ensuring that agents can navigate towards promising solutions. The algorithm continuously updates its population, prioritizing agents with higher-quality solutions, which further drives convergence towards a single optimal solution. Through iterative improvements and the application of its mechanisms, the MGA systematically refines its search process. This structured design balances exploration and exploitation, enabling the algorithm to effectively traverse the problem space. As a result, search agents are consistently directed towards the most promising areas for solution discovery, leading to robust convergence towards optimal solutions. The MGA's ability to maintain this balance is crucial for its performance, allowing it to efficiently identify and converge on global optima in various optimization scenarios.

Iran. J. Numer. Anal. Optim., Vol. ??, No. ??, ??, pp ??

4 Convergence analysis

At first, we rewrite the OCP in Section [2](#page-6-0) in a vectorial form to gain a deeper understanding of its mathematical structure and enable more effective convergence analysis. Let $x(t) = \begin{bmatrix} W(t), S(t), I(t), \mathcal{T}(t) \end{bmatrix}$ be the state vector, where $W(t)$, $S(t)$, $I(t)$, and $\mathcal{T}(t)$ are the state variables defined in Section [2.](#page-6-0) Similarly, let $\mathcal{U}(t) = C_5^T \phi(t)$ be the control vector. We define

$$
x'(t) = F(x(t), \mathcal{U}(t)),\tag{35}
$$

where $x'(t) = (W'(t), S'(t), I'(t), T'(t))$ and

$$
F(x(t),\mathcal{U}(t)) = \begin{bmatrix} \Lambda - \alpha_1 WS - \alpha_2 WI + \rho \alpha_2 I - \mu W \\ \alpha_1 WS + (\delta + \mathcal{U}(t))I - (\theta_1 + \mu)S \\ \alpha_2 WI - \rho \alpha_2 I - (\delta + \mathcal{U}(t) + \theta_2 + \mu)I \\ \theta_1 S + \theta_2 I - \mu \mathcal{T} \end{bmatrix}.
$$

Let us define the *N*th order approximation as follows:

$$
x_N(t) = [C_1^T \phi(t), C_2^T \phi(t), C_3^T \phi(t), C_4^T \phi(t)].
$$

This represents the *N*th order approximation x_N^* . Additionally, let $\mathcal{U}_N(t)$ = $C_5^T \phi(t)$ denote any approximation of the optimal control $\mathcal{U}_N^*(t)$, where $\phi(t)$ is the vector of SJPs defined in (8) (8) . It is important to note that $\phi(t)$ can be replaced with any set of orthogonal polynomials.

Next, we consider a sequence of problems denoted as \mathcal{P}_N , where N increases from N_1 to infinity. Consequently, we obtain a sequence of discrete optimal solutions represented as

$$
\{(x_i^*, \mathcal{U}_i^*): i = 0, \ldots, N\}_{N=N_1}^{\infty},
$$

where *i* indicates the number of basis functions. This also leads to a corresponding sequence of approximation functions given by

$$
\{(x_N,\mathcal{U}_N)\}_{N=N_1}^{\infty}.
$$

Theorem [1](#page-23-0) establishes that if the problem *P* has feasible solutions, then the problem P_N will also have feasible solutions. By introducing these vector

Iran. J. Numer. Anal. Optim., Vol. ??, No. ??, ??, pp ??

notations, we can compactly represent the state and control variables, as well as their optimal trajectories. This vector-based formulation allows for a more concise and generalized analysis of the OCP, which can be particularly useful when dealing with complex systems with multiple state and control variables. Now, we consider a sequence of problem \mathcal{P}_N , with *N* which increases from N_1 to infinity. Correspondingly, we get a sequence of discrete optimal solutions $\{(x_i^*, \mathcal{U}_i^*) : i = 0, \ldots, N\}_{N=N_1}^{\infty}$, where *i* is the number of basis, and their approximation function sequence $\{(x_N, \mathcal{U}_N)\}_{N=N_1}^{\infty}$ $\{(x_N, \mathcal{U}_N)\}_{N=N_1}^{\infty}$ $\{(x_N, \mathcal{U}_N)\}_{N=N_1}^{\infty}$. Theorem 1 demonstrates that if the problem P has feasible solutions, then the problem P_N also has feasible solutions. First, we need the following definition.

Definition 2. A Sobolev space $W^{m,\infty}(\Omega)$ is defined as the space of functions $g: \Omega \to \mathbb{R}$ such that

- 1 : *g* is essentially bounded, that is, $u \in L^{\infty}(\Omega)$;
- 2 : all weak derivatives of *g* up to order *m* exist and are also essentially bounded, that is, for each multi-index α with $|\alpha| \leq m$, the weak derivative $D^{\alpha}g$ satisfies $D^{\alpha}g \in L^{\infty}(\Omega)$.

The norm on this space is given by

$$
\|g\|_{W^{m,\infty}(\Omega)} = \sup_{|\alpha| \le m} \|D^{\alpha}g\|_{L^{\infty}(\Omega)},
$$

where $||D^{\alpha}u||_{L^{\infty}(\Omega)}$ denotes the essential supremum of the weak derivative $D^{\alpha}g$ over the domain Ω .

Theorem 1. Let (x, \mathcal{U}) be feasible solutions to the problem \mathcal{P} , and assume that the state function $x(t)$ belongs to the Sobolev space $W^{m,\infty}$ with $m \geq 2$. For sufficiently large *N*, the problem \mathcal{P}_N has a feasible solution (\bar{x}_i, \bar{u}_i) , such that $\bar{u}_i = u(s_i)$ and

$$
||x(s_i) - \bar{x}_i||_{\infty} \le M(N-1)^{1-m}, \quad 0 \le i \le N,
$$
\n(36)

where s_i are the Legendre–Gauss–Lobatto nodes and M is a positive constant independent of *N* [[9\]](#page-30-6).

Iran. J. Numer. Anal. Optim., Vol. ??, No. ??, ??, pp ??

Theorem [2](#page-24-0) demonstrates that a sequence of optimal solutions for the problem P converges to the optimal solution of the problem P_N . The following lemma and definition are employed in the proof of Theorem [2](#page-24-0).

Lemma 2. Let τ_j for $j = 0, 1, ..., N$ be the GL nodes, and let w_j be the GL weights. If $f(t)$ is Riemann integrable, then it holds that

$$
\int_{-1}^{1} f(t) dt = \lim_{N \to \infty} \sum_{j=0}^{N} f(\tau_j) w_j.
$$

Definition 3. A continuous function $\zeta(t)$ is called uniform accumulation point of a function sequence $\{\zeta_N(t)\}_{N=0}^{\infty}$, $t \in [-1, 1]$, if there is a subsequence of $\{\zeta_N(t)\}_{N=0}^{\infty}$ that uniformly converges to $\zeta(t)$.

Theorem [1](#page-23-0) guarantees the existence of high-quality feasible solutions for Problem P_N when N is sufficiently large. In this case, the control variables closely approximate the true control function, and the state variables are near the true state trajectory. The subsequent theorem is significant as it provides a theoretical assurance that the pseudospectral method, which discretizes the OCP, can be effectively utilized to approximate the solution of the original continuous problem.

Theorem 2. Let $\{(x_i^*, \mathcal{U}_i^*)\}_{i=N_1}^{\infty}$ be a sequence of optimal solutions for the problem \mathcal{P}_N , and let $\{(x_N(t), \mathcal{U}_N(t))\}_{N=N_1}^{\infty}$ denote their corresponding interpolating functions. Suppose that $(q(t), u(t))$ is any uniform accumulation point of the sequence $\{(x'_N(t), \mathcal{U}_N(t))\}_{N=N_1}^{\infty}$. Then, $q(t)$ is an optimal control for the original continuous problem P , and $\bar{x}(t) = \int_0^t q(\tau) d\tau + x(0)$ represents the corresponding optimal trajectory [[9\]](#page-30-6).

Thus, under relatively mild conditions, Theorems [1](#page-23-0) and [2](#page-24-0) guarantee the existence and convergence of the discrete-time optimal solution to the continuous-time solution of the original problem.

5 Applicable example

This section presents the results of numerical simulations conducted in Mathworks Matlab R2023a on a 64-bit computer Intel Core i7, 3.3GHz processor,

Iran. J. Numer. Anal. Optim., Vol. ??, No. ??, ??, pp ??

and 4GB of RAM to investigate the OCP of transmission rate of water pollutants. References [\[10](#page-31-1)] and [\[25](#page-32-1)] are used as the basis for the parameter values and initial conditions in this study as follows: $\Lambda = 0.8$, $\rho = 0.25$, $\alpha_1 =$ 0.18, $\alpha_2 = 0.02$, $\delta = 0.3$; $\mu = 0.4$, $\theta_1 = 0.2$, $\theta_2 = 0.5$, $W_0 = 500$, $I_0 =$ 100*,* $S_0 = 400$ *,* and $T_0 = 0$. The values of the constants are $a_1 = 0.1$, $a_2 = 0.1, a_3 = 0.1,$ and $a_4 = 1$. The numerical results were obtained using $n = 5$, $\alpha = 0$, and $\beta = 0$. The behavior of water pollutant variables in OCP described in section [3](#page-10-1) is illustrated in Figures [3,](#page-25-0) [4,](#page-26-0) [5,](#page-27-0) and [6](#page-27-1).

Figure 3: Transmission of the concentration of water pollutant

Figure [3](#page-25-0) demonstrates that the concentration of water pollutants does not change significantly with an increase in the number of days and also shows the impact of managing treatment for water pollutants to rid our planet of toxins. As time progresses, we observe that the concentration of pollutants does not exhibit a significant increase or decrease. This plateau could be due to the implementation of effective treatment strategies that maintain the pollutant levels at a manageable state. Additionally, this figure highlights the effectiveness of continuous pollution control measures in maintaining water quality over an extended period. The lack of significant fluctuation emphasizes the importance of consistent monitoring and treatment to prevent sudden spikes in pollutant levels that could harm the environment and public health.

Iran. J. Numer. Anal. Optim., Vol. ??, No. ??, ??, pp ??

Figure 4: Transmission of the concentration of soluble Water Pollutant

Figure [4](#page-26-0) shows the transmission of soluble water pollutants, which are typically more responsive to environmental changes than insoluble pollutants. Initially, the concentration of soluble pollutants increases rapidly, likely due to the breakdown of insoluble pollutants into soluble forms or an influx of new soluble pollutants into the water system. However, after reaching a peak, the concentration starts to decline. This decrease could be attributed to several factors: the natural settling of pollutants, the implementation of treatment processes that specifically target soluble pollutants, or the dilution effect in larger bodies of water. The decline over time suggests that the treatment efforts are effectively reducing the concentration of soluble pollutants, thereby decreasing the overall pollutant load in the water. This figure emphasizes the dynamic nature of soluble pollutant concentrations and the critical need for timely intervention to mitigate their impact.

Figure [5](#page-27-0) depicts the concentration changes of insoluble water pollutants over time. Insoluble pollutants tend to settle more slowly compared to their soluble counterparts, as indicated by the gradual decrease observed in the graph. The downward trend may result from ongoing water treatment efforts that transform insoluble pollutants into less harmful or more easily removable forms, such as precipitates. The steady decline suggests that the treatment methods employed are effective in continuously reducing the levels of insoluble pollutants. Moreover, the figure underlines the importance of

Iran. J. Numer. Anal. Optim., Vol. ??, No. ??, ??, pp ??

Figure 5: Transmission of the concentration of insoluble Water Pollutant

Figure 6: Transmission of the concentration of treated water Pollutant

addressing insoluble pollutants to prevent long-term contamination of water bodies, which can result in sediment pollution and negatively impact aquatic life. The continuous treatment helps mitigate the risks associated with insoluble pollutants, contributing to improved water quality and ecosystem health.

Figure [6](#page-27-1) illustrates the changes in the concentration of treated water pollutants over time. Initially, there is a high concentration of both soluble and insoluble pollutants, necessitating a robust treatment response. The graph

Iran. J. Numer. Anal. Optim., Vol. ??, No. ??, ??, pp ??

Figure 7: Optimal control function

shows that the concentration of treated pollutants increases during the early stages, likely due to the intensified treatment efforts to manage the high initial pollutant load. As treatment progresses, the concentration of treated pollutants begins to decrease, indicating a reduction in the overall pollution levels due to effective treatment strategies. This decrease could also reflect the diminishing returns of treatment as the pollutant concentration approaches lower levels, making further reductions more challenging. The figure highlights the effectiveness of early and aggressive treatment interventions in managing water pollution and the importance of sustained efforts to maintain low pollutant levels over time. The graph of the optimal control function is demonstrated in Figure [7](#page-28-0).

6 Conclusion

The survival of humanity depends on water as a main resource. Water pollution is a significant problem that can have a harm impact on the environment and human health. Micro-pollutants have significant potential impacts on water ecosystems and human health [\[5](#page-30-7)]. Treatment can be used to remove pollutants from water. The study presents a numerical approach for an OCP governed by a mathematical model of the transmission of water pol-

Iran. J. Numer. Anal. Optim., Vol. ??, No. ??, ??, pp ??

lutants formulated in a system of ordinary differential equations. This OCP is transformed into an NLP using a collocation approach based on SJPs and its derivative operational matrix. Then, the resulted NLP is solved by the MGA to derive the solutions of the optimal control and state. The presented method can be implemented quickly and efficiently for solving mathematical models of water pollutant transmission. The conclusion of water contamination treatment shows that the risk of pollutants spreading into surface water has decreased. In order to minimize pollution, it is essential to treat water pollutants before being released into water bodies. This can be achieved through a variety of methods [[28\]](#page-32-9), including physical, chemical, and biological treatments. Physical treatments involve removing pollutants from the water through processes such as sedimentation and filtration. Chemical treatments include using chemicals to remove contaminants from the water. Biological treatments use microorganisms to break down pollutants. By implementing a water treatment strategy, we can quickly purify water and insure it does not include pollutants. Proper management of our water supplies is also a need to ensure that they remain pollutant-free. This includes monitoring water quality, reducing the consumption of harmful chemicals, and properly disposing of waste.

Acknowledgment

The corresponding author is thankful to the Water Research Center of Shahrekord University for the executive and technical support during the sabbatical visit to that center.

Conflict of interest On behalf of all authors, the corresponding author states that there is no conflict of interest.

References

[1] Abdollahzadeh, B., Gharehchopogh, F.S., Khodadadi, N., and Mirjalili, S. *Mountain gazelle optimizer: a new nature-inspired metaheuristic al-*

Iran. J. Numer. Anal. Optim., Vol. ??, No. ??, ??, pp ??

31 Optimal control of water pollutant transmission by utilizing a combined ... *gorithm for global optimization problems,* Adv. Eng. Softw. 174 (2022), 103282.

- [2] Aribowo, W., Abualigah, L., Oliva, D., and Prapanca, A. *A novel modified mountain gazelle optimizer for tuning parameter proportional integral derivative of DC motor,* Bull. Electr. Eng. Inform. 13(2) (2024) 745–752.
- [3] Bonyaha, E., Agbekpornub, P., and Unlud, C. *Mathematical modeling of transmission of water pollution,* J. Prime Res. Math., 17(2) (2021), 20–38.
- [4] Canuto, C., Hussaini, M.Y., Quarteroni, A., and Zang, T.A., *Spectral methods: fundamentals in single domains,* Springer Science and Business Media, 2007.
- [5] Cizmas, L., Sharma, V.K., Gray, C.M., and McDonald, T.J., *Pharmaceuticals and personal care products in waters: occurrence, toxicity, and risk,* Environ. Chem. Lett. 13 (2015) 381–394.
- [6] Doha, E.H., Bhrawy, A.H., and Ezz-Eldien, S.S., *A new Jacobi operational matrix: an application for solving fractional differential equations,* Appl. Math. Model. 36(10) (2012) 4931–4943.
- [7] Doha, E.H., *On the construction of recurrence relations for the expansion and connection coefficients in series of Jacobi polynomials,* J. Phys. A: Math. Gen. 37(3) (2004) 657.
- [8] Drag, P., Styczeń, K., Kwiatkowska, M., and Szczurek, A., *A review on the direct and indirect methods for solving optimal control problems with differential-algebraic constraints.* In Recent Advances in Computational Optimization: Results of the Workshop on Computational Optimization WCO 2014 (pp. 91–105). Springer International Publishing, 2016.
- [9] Gong, Q., Ross, I.M., Kang, W., and Fahroo, F., *On the pseudospectral covector mapping theorem for nonlinear optimal control,* In Proceedings of the 45th IEEE Conference on Decision and Control (pp. 2679–2686) (2006) IEEE.
- [10] Ebrahimzadeh, A., Hashemizadeh, E., Mirabbasi, R., *A numerical solution of the mathematical models for water pollution by shifted Jacobi polynomials,* TWMS J. Appl. Eng. Math. 14 (2023) 1–15.
- [11] Gael, P.K. *Water pollution: Causes, effects and control,* New Age International, 2006.
- [12] Guo, G., and Cheng, G. *Mathematical modelling and application for simulation of water pollution accidents,* Process Saf. Environ. Prot. 127 (2019), 189–196.
- [13] Khodadadi, N., El-Kenawy, E.S.M., De Caso, F., Alharbi, A.H., Khafaga, D.S., and Nanni, A. *The mountain Gazelle optimizer for truss structures optimization,* Appl. Comput. Inform. 3(2) (2023), 116–144.
- [14] Hashemizadeh, E., and Ebadi, M.A. *A numerical solution by alternative Legendre polynomials on a model for novel coronavirus (COVID-19),* Adv. Differ. Equ. 2020(1) (2020), 223.
- [15] Hussaini, M.Y., and Zang, T.A. S*pectral methods in fluid dynamics,* Annu. Rev. Fluid Mech. , 19(1) (1987), 339–367.
- [16] Kroeze, C., Gabbert, S., Hofstra, N., Koelmans, A.A., Li, A., Löhr, A., Ludwig, F., Strokal, M., Verburg, C., Vermeulen, L. and van Vliet, M.T. G*lobal modelling of surface water quality: a multi-pollutant approach,* Curr. Opim. Environ. Sustain. 23 (2016), 35–45.
- [17] Luke, Y. *The special functions and their approximations,* vol. 2, Academic Press, New York, 1969.
- [18] Maleknejad, K., and Ebrahimzadeh, A. *An efficient hybrid pseudospectral method for solving optimal control of Volterra integral systems,* Math. Commun., 19(2) (2014) 417–435.
- [19] Magdy, F. E. Z., Hasanien, H. M., Sabry, W., Ullah, Z., Alkuhayli, A., and Yakout, A. H. Mountain gazelle algorithm-based optimal control strategy for improving LVRT capability of grid-tied wind power stations. IEEE Access, 11 (2023) 129479-129492.

Iran. J. Numer. Anal. Optim., Vol. ??, No. ??, ??, pp ??

- [20] Maashi, M., Alabdulkreem, E., Maray, M., Shankar, K., Darem, A.A., Alzahrani, A., and Yaseen, I. *Elevating survivability in next-gen IoT-Fog-Cloud networks: Scheduling optimization with the metaheuristic mountain gazelle algorithm,* IEEE Transactions on Consumer Electronics, 2024.
- [21] Parsaie, A., and Haghiabi, A.H. *Computational modeling of pollution transmission in rivers,* Appl. Water Sci. 7 (2017), 1213-1222.
- [22] Rao, A. V. *A survey of numerical methods for optimal control,* Adv. Astronaut. Sci. 135(1) (2009) 497–528.
- [23] Ren, H., Lin, F., Tao, Y., Wei, T., Kang, B., Li, Y., and Li, X. *Research on the Optimal Regulation of Sudden Water Pollution,* Toxics, 11(2) (2023), 149.
- [24] Sadjadi, S.J., and Ponnambalam, K. *Advances in trust region algorithms for constrained optimization,* Appl. Numer. Math. 29(3) (1999), 423–443.
- [25] Shah, N.H., Patel, S.N., Satia, M.H., and Thakkar, F.A. *Optimal control for transmission of water pollutants,* Int. J.Math. Eng. Manag. Sci. 3(4) (2018), 381–391.
- [26] Tang, W., Pei, Y., Zheng, H., Zhao, Y., Shu, L., and Zhang, H. *Twenty years of China's water pollution control: Experiences and challenges,* Chemosphere, 295 (2022) 133875.
- [27] Utama, D.M., Sanjaya, B.D., and Nugraha, A. *A modified mountain gazelle optimizer for minimizing energy consumption on no-wait permutation flow shop scheduling problem,* Int. J. Intell. Eng. Syst. 17(2) (2024) 609–620.
- [28] Weng, C.H. *Water environment and recent advances in pollution control technologies,* Environ. Sci. Pollut. Res. 29(9) (2022), 12462–12464.
- [29] Yuan, Y.X. *A review of trust region algorithms for optimization,* In Iciam, 99(1) (2000), 271–282.

Iran. J. Numer. Anal. Optim., Vol. ??, No. ??, ??, pp ??

[30] Zellagui, M., Belbachir, N., and El-Sehiemy, R.A. *Solving the optimal power flow problem in power systems using the mountain gazelle algorithm,* Eng. Proc. 56(1) (2023), 176.

Iran. J. Numer. Anal. Optim., Vol. ??, No. ??, ??, pp ??