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Complex Systems, Sustainability and Innovation

Edited by Ciza Thomas

COMPLEX SYSTEMS, SUSTAINABILITY AND INNOVATION

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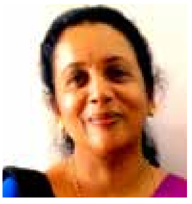
Meet the editor



Dr. Ciza Thomas is currently working as a professor in Electronics and Communication Department of College of Engineering, Trivandrum, India. Her area of expertise is network security with research interest in the fields of information security, data mining, sensor fusion, pattern recognition, information retrieval, digital signal processing, and image processing. She has publications in more than 40 International Journals and International Conference Proceedings. She has edited two books in the field of sensor fusion and published five book chapters in the field of network security and pattern recognition. She is a reviewer of more than ten reputed international journals including *IEEE Transactions on Signal Processing*, *IEEE Transactions on Neural Networks*, *International Journal of Network Security*, *International Journal of Network Management*, and *IEEE-John Wiley International Journal on Security and Communications Network*. She is a recipient of achievement award in 2010 and the e-learning IT award in 2014 from the Government of Kerala.

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Preface

This book on complex systems, sustainability, and innovation explores a broad set of ideas and presents some of the state-of-the-art research in this field. The book is triggered by ubiquitous applications of real-world complex problems. Complex systems may have many diverse and autonomous components that interact and create a functioning whole. In a complex system, it is difficult to know exactly how the individual components contribute to an observed behavior and the extent of each component's contributions. It is the interactions of the individual components that determine the emergent functionalities. This makes it difficult to understand and predict the behavior of complex systems.

In the technological front, significant progress has been made to increase the system performance and thereby the living standards. However, all innovations where their impact far exceeds the knowledge are identified as one of the quandaries of sustainability. This is because humans have through decades experimented and created ever-increasing complex systems that outperformed every system that existed at that time. However, as time passed by, the complexity has exponentially increased, and now, that complexity itself is the problem. Hence, a new age of innovations has to emerge with the main focus on user orientation and sustainability. An advanced dynamical understanding of complex systems and their dependence on the environment is essential for a long-term perspective and innovations supporting practical applications that aid in a sustainable society. Present studies need to focus on sustainability and innovation that include awareness of the consequences of complex systems. It is necessary to learn from the past, constructing causative narratives; at the same time, we need to learn for the future, which requires thinking differently and no longer linearly but in terms of alternatives.

Complex systems span the entire spectrum of science and technology including basic sciences to life sciences and medicine, to social, economic, and cognitive sciences, to engineering and computers. The book consists of six chapters. In Chapter I, the introduction to complex systems and their evolution are discussed. The knowledge of a complex system allows for sustainability when various innovations occur in the field. Chapter II to Chapter VI include the problems associated with various complex systems and the methods to address each one of them with the focus on sustainability and innovation. Chapter II includes a method to minimize the cost function of the cloud by looking at the communication possibility of service requests for multiserver in its parallel connection. Chapter III proposes a methodology for sustainable home design by applying control science. Chapter IV proposes stabilization control strategies to address the stabilization problems of periodic motions for the higher-order continuous-time chaotic systems. Chapter V discusses the quantitative methods for system-based drug discovery and design to engineer safer and more effective drugs. Chapter VI presents a platform for stochastic agent–based simulation of the role of labor in economy. The intended audience of this book will mainly consist of researchers, research students, and practitioners in the field of complex systems and sustainability.

I would like to convey my appreciation to all the contributors of this book including the authors of the accepted chapters. My special thanks to the Publishing Process Manager, Ms. Martina Usljebrka, and other staff of InTech publishing for their kind support and great efforts in bringing the book to fruition. In addition, I also thank the reviewer, Dr. T. John Tharakan, for providing very critical and constructive comments to the introductory chapter of this book. His comments helped to tremendously improve the content of the chapter.

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Chapter 1

Introduction to Complex Systems, Sustainability and Innovation

Ciza Thomas, Rendhir R. Prasad and Minu Mathew

Additional information is available at the end of the chapter

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Abstract

The technological innovations have always proved the impossible possible. Humans have all the time obliterated barriers and set records with astounding regularity. However, there are issues springing up in terms of complexity and sustainability in this context, which we were ignoring for long. Today, in every walk of life, we encounter complex systems, whether it is the Internet, communication systems, electrical power grids, or the financial markets. Due to its unpredictable behavior, any creative change in a complex system poses a threat of systemic risks. This is because an innovation is always introducing something new, introducing a change, possibly to solve an existing problem, the effect of which is nonlinear. Failure to predict the future states of the system due to the nonlinear nature makes any system unsustainable. This necessitates the need for any development to be sustainable by meeting the needs of people today without destroying the potential of future generations to meet their needs. This chapter, which studies systems that are complex due to intricateness in their connectivity, gives insights into their ways of emergence and the nonlinear cause and effects pattern the complex systems use to follow, effectively paving way for sustainable innovation.

Keywords: chaos, complex systems, complex networks, complexity theory, information systems security, sustainable networks

1. Introduction

Today, in every walk of life, we encounter complex networks, whether it is the Internet, which is a global system of interconnected computer networks; or the communication systems, which is a collection of individual communications networks, transmission systems, relay stations, tributary stations, and data terminal equipment usually capable of interconnection and interoperation to form an integrated whole; or the electrical power grids, which is an interconnected network for delivering electricity from suppliers to consumers; or the financial markets, which is any collection of traders, firms, banks, and financial exchanges; or the food web, which is a system of interlocking and interdependent food chains; or the metabolic networks, which is the complete set of metabolic and physical processes that determine the physiological and biochemical properties of a cell; or the social networks, which is a network of social interactions and personal relationships. The interacting units and intricate connections make these systems complex. Though these complex systems perform diverse functions, studies show that there are similarities in its structure.

Complexity has been defined in various ways in different fields. Moses [1] defines complex systems as "A system is complex when it is composed of many parts that interconnect in intricate ways." According to this definition, the number and types of parts of a system decide its complexity. The systems become complex when these parts are connected in a nonregular way. The information about the nature of interconnections is usually insufficient and this makes modeling difficult.

Rechtin and Maier [2] define a complex system to consist of a set of different elements so connected or related as to perform a unique function not performable by the elements alone. The complex system acts as "whole is greater than parts," which means a complete knowledge about the parts will not be sufficient to predict the working of a system as a whole. Parts show different behavior than when working together as a whole. The traditional scientific method of studying a system is to dissect a system into its parts, model them into a formal system, study individually, and then combine them to get the whole information about the system. This works on the assumption that the parts combined together will correctly give complete information about the system as a whole and the behavior of the system can be predicted completely. However, in the case of complex systems, it is not possible to get the complete information about the system just by combining parts, because information is generated, not in parts per se but in the intricate connections between them. The component parts of a complex system are more or less complex entities linked with one another and organized within an ordered structure of mutual interaction. It is not mandatory that the web of linkages is visible—instead, it may consist of cause and effect relations which originate by the way of communication. Hence, studying the behavior of complex systems, in effect, is the study of the system as a network of individual parts and the emergence of complex networks from the interconnection between individual parts.

Strogatz [3] describes the complications in studying complex systems. Complex systems show structural complexity because the nature of connection is intricate, with connections changing dynamically over time as in the case of World Wide Web, where pages and links are created and deleted all the time, making the evolution of network very dynamic and hence complex. These links are not homogenous and they show considerable diversion in terms of weights, direction, and signs. The nodes itself can be nonlinear dynamic systems since the state of nodes is varying in time. The nodes can be of diverse types as in the case of biochemical networks. Moreover, they affect each other and this interdependency result from networked risks, which means a small disturbance caused by a component, can result in a catastrophic failure of the system. Global financial meltdown of 2008 can be cited as an example of this type of cascading failure. In today's highly interconnected world, coupling of different kinds of systems makes the effects of failure uncontrollable in a global scale. Any naturally occurring complex system has a tendency to evolve automatically and those networks are quite resistant to small initial variations causing a tremendous effect on the entire system.

Helbing [4] argues that global interdependent systems produced by intricate networking are prone to cascading global-level failures even when external shocks are absent. He discusses various anecdotes of failures and calls for a new approach called Global Systems Science for the study of these phenomena and gives a detailed description of drivers and examples of systemic instabilities.

Networks have interconnected the distributed, heterogeneous systems and offer a wide variety of applications that were never dreamt of. However, there are issues springing up in terms of complexity and sustainability in this context, which we were ignoring for long. Any creative change in a complex system poses a threat of systemic risks. The exploitation of the technologies has of late led to the verge of a complexity crisis. Due to its unpredictable behavior, these networks are vulnerable to a cascade of overload failures, which can in turn cause the entire or a substantial part of the network to collapse. It is the artificial or the man-made complex systems like the Internet that gets affected by cascading failures capable of disabling the network almost entirely. Even though humans have all the time obliterated barriers and set records with astounding regularity, the irony is that an innovation is always introducing something new, introducing a change, possibly to solve an existing problem, the effect of which is nonlinear. Failure to predict the future states of the system due to the nonlinear nature makes any innovation vulnerable. Hence, there is a high possibility that an innovation can make a system unsustainable. Many examples like invention of plastics, usage of fossil fuels, etc., can be cited especially from global climate change studies. A disturbing question arises in this context: Is there a contradiction existing between innovation and sustainability? However, innovation is the only way to progress, and hence in the case of complex systems, innovation has to happen in the backdrop of sustainability. This necessitates the need for any development to be sustainable by meeting the needs of people today without destroying the potential of future generations to meet their needs. Hence, the study of complex systems, stability of complex systems, and the interdependence of the complex system components is inevitable today and is discussed in detail in this chapter. The remaining part of this chapter is to study systems that are complex due to intricateness in its connectivity and provides insights into its ways of emergence, and the nonlinear cause and effects pattern the complex systems use to follow, effectively paving way for sustainable innovation.

This chapter is organized as follows. Section 2 gives an introduction to reductionism and discusses the insufficiency of reductive approach in addressing the behavior of chaotic systems. Emergent behavior and order in chaotic system is addressed in Section 3. Section 4 discusses the relation between chaotic systems and the structure of complex systems. Section 5 looks at the Internet as a typical example of complex system with information system security as the main focus. Self-organized criticality and interdependence and its effects are also discussed in this section. Section 6 concludes the chapter.

2. Reductive approach

Nature and all its phenomena are innately mathematical. That was the confidence history accepted for a long time. All of nature's intricate and beautiful phenomena were simplified into mathematical abstractions and discussed extensively. This notion got a firmer foothold when Sir Isaac Newton discovered a common law that governed an apple falling from a tree and the splendid "planetary motion." The Newtonian theory came with all intelligibility for an acceptable explanation. There was no notion of a complex system as all observable phenomena were represented by mathematical equations, more precisely, differential equations. Newtonian physics took up the center stage and paved way to reductionism. Reductionism is the practice of simplifying or minimizing a complex issue or condition, and it deals with the theory that every complex phenomenon can be explained by analyzing the most basic and simple component that exists during the phenomenon.

Reductionism is the first footstep of modern science. The reductionist philosophy holds that a complex system is nothing but the sum of its parts and a complex phenomenon can be explained completely in terms of the interactions between more fundamental phenomena. To put it simple, analysis is done by breaking down the larger system into pieces or individual parts and determining the connections between the parts. We credit this procedure to the mathematical concept of linearity and additivity. If we add the small individual parts together, the complexity will increase in a linear manner resulting in the same original complex system.

Furthermore, reductionism infers that there exists a point-to-point connection from the starting state to the mature state of a complex system. If we know the starting state, we have 100 percent predictability of the mature state. If we know the rule that governs a system to go from state 1 to state 2, we can apply the same rule and calculate the parameter changes from state 2 to state 3. This notion is the concept of extrapolation in mathematics. The concept nullifies going stage by stage to find out the mature state of a system. Instead, it demands that applying the same rule for as many iterations as needed, we can find out the mature state just by knowing the starting state of a system and vice versa [5].

With all these rules of reductionism and definition of procedures in terms of mathematics taken seriously, the Universe becomes a clockwork machine. This type of Universe (also known as the Laplace demon), made famous by Laplace, enjoyed an established set of rules. According to Laplace, it is possible to both calculate the entire history of the Universe and to predict its entire future if there is sufficient information about the current state of the Universe in addition to all of its fundamental and unchanging laws. However, scientists have always scrambled to find a mathematical model for the natural phenomena like weather, tides, clouds, and the human body.

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Last century saw physicists investigating the dynamics of atoms and everything smaller than them, as if matter and all its wonderful properties can be explained by protons, neutrons, and going further deep into quarks and gluons [6]. Subsequent research in medical sciences devoted time in understanding and developing the tools for comprehending the workings of genes. The reductionist mindset has pervaded the field of molecular biology for half a century. Since the biological systems are composed solely of atoms and molecules, it is assumed that it should be possible to explain them using the physicochemical properties of their individual components, down to the atomic level, until and unless there is the influence of "alien" or "spiritual" forces.

For science, measurement of properties of minute particles was obviously the next step. However, physicists encountered variability, or noise as it is known in the reductive world, in those measurements of fundamental particles. Variability was stated as the discrepancy from the actual true measure. This noise represented system error and it is something that has to be avoided to get the true result. The way to reduce noise is to become more and more reductive. Reductionists argued that the closer we look at a system, the closer the obtained result will be to the actual result.

Human body is a scale-free system. Consider the tree-like bifurcating structure of the nervous system, or the circulatory system, or the pulmonary system. If the genes specify the bifurcations in a human body, there is not enough genome to code for this entire scale-free structure and all the activities that each cell is capable of. The neurons, arteries, and dendrites have a bifurcating structure which cannot be coded for and each individual part given a specific function. For a point-to-point connection to exist between the genes and the various things that a human is capable of, there is a lack of genes in our body. All the information is not coded in a single cell; it is coded in the interactions between different cells. Biological problems cannot be solved in a reductive manner [5]. We know the qualities of oxygen atoms and we know the qualities of carbon atoms. By reductive philosophy, we should be able to determine the qualities of carbon dioxide. Actually we cannot. We are familiar with the qualities of carbon dioxide only because we have observed them empirically. This does not concede with the additive philosophy. Brownian motion of molecules cannot be explained by reductionism. Reductive philosophy does not count for a role of chance. With randomness in a system, we will not be able to have absolute knowledge of its mature state from the initial state. In the reductive world, anything without an established absolute certainty becomes invalid.

3. Chaos in nature

Today, advances in both physics and biology have exploded the myths laid out by the reductionist approach. Accordingly, how inanimate and animate things work, and are made, cannot be explained simply by breaking it down into their components. Scientific developments obviously state that the specificity of a complex biological activity does not arise from the specificity of the individual molecules that are involved. Experiments have shown time and again that reality does not obey classical deterministic rules. General relativity is a good conceptual tool that describes many phenomena very accurately on fairly small scales. This being a deterministic rule, it is often argued that it serves as a limitation for reaching out to a unified theory. As opposed to Laplace's claim, mathematics begins to fall apart—as indicated by infinities and time anomalies (what they call variabilities) that pop up—when it is (mis) applied or when trying to "solve" the state of the entire Universe [7]. When some very fundamental questions on life and Universe come to the fore, the general relativity theory remained inept to answer. For as long as science inquired about the laws of nature, it has suffered ignorance about the sudden changes and the disorder in the atmosphere, the turbulence of the wind and the sea, the fluctuations in wildlife and human populations, and the variations of signals from the brain and heart. The most simple and interesting things could not be regulated in a simple reductive way. No consensus on a satisfactory answer has led to the emergence of the concept of chaos.

> "As far as the laws of mathematics refer to reality, they are not certain, and as far as they are certain, they do not refer to reality."
>
> *– Albert Einstein*

3.1. Chaos and complexity

In the scientific world, we realize chaos everywhere. A rising column of smoke breaks into wild swirls. A flag snaps back and forth in the wind. A dripping faucet goes from a steady pattern to a random one. Similar is the fluttering of leaves in the wind or the trajectory followed by a double rod pendulum or the ball in a pinball machine. Chaos appears in the behavior of weather, behavior of an airplane in flight, behavior of road traffic, behavior of oil flowing in underground pipes, population changes, or swarm formation of bees. Chaotic systems are not reductive. If a cloud does not rain, we cannot examine the cloud's component parts and come up with a solution. If we divide up a complex system into its pieces and add them up again, the resultant can be another system as the individual parts may add up differently. Knowing the initial state of a complex system will not result in a 100 percent predictability of the final state. The concept of extrapolation, linearity, and additivity does not apply to a complex system. The only way to know the mature state of a complex system is to go step by step. There are no patterns that the system follows over and over again. Chaos breaks across the lines that separate scientific disciplines. That realization has begun to change the way neurologists look at brain activity, the way business executives make decisions about insurance, the way astronomers look at the solar system, the way political theorists talk about the stresses leading to armed conflict, and the way economists look at organizational structure. Last 20 years, science saw an increase in specialization, looking for an order in all of nature. Dramatically, that hunt for specialization and order has reversed because of chaos. As Glieck [7] mentions in his book of *Chaos-Making a New Science*, "Where chaos begins, classical science stops." Chaos is a science of process rather than state, of becoming rather than being. Being a science of the global nature of systems, it has brought together thinkers from fields that had been widely separated.

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Traditionally, when physicists saw complex systems, they tried to model it by complex functions and interactions. For complex results, they looked for complex causes. When they encounter a seemingly random relationship between an input to a system and its output, they simulated it by introducing artificial noise or error. They were ignorant of the fact that variability is intrinsic to the system and that quite simple mathematical equations could model systems every bit as violent as a thunder storm. Senge [8] defines complex systems based on cause and effect in it as "A system presents dynamic complexity when cause and effect are subtle, over time." The cause and effect pattern is not static over the time, but it changes along with the emergence of the system. A local effect may not give a clue about the global effect, so the interventions produce complex unpredictable effects. Tiny differences in input could quickly escalate and become overwhelming differences in output. This phenomenon of chaotic systems being highly sensitive to initial conditions is termed as the "butterfly effect"—a notion that a butterfly flapping its wings in Perkin would result in a thunder storm in New York a month later [7].

3.2. The butterfly effect

The butterfly effect was first observed by Edward Lorenz, a research meteorologist at the Massachusetts Institute of Technology. In 1960, Lorenz created a weather model on his computer [9]. It consisted of an extensive array of complex formulas, but the computer system had neither the speed nor the memory to manage a realistic simulation of the earth's atmosphere and oceans. Yet the program behaved quite like the real weather; it never seemed to repeat a sequence. One day Lorentz had let the program run on certain parameters to generate a certain weather pattern, and he wanted to take a better look at the outcome. Instead of starting the whole run over, he started midway through. To give the machine its initial conditions, he typed the numbers that had come up in the earlier run. This new run should have exactly duplicated the old as he inputted the exact results from the preceding run. The program had not changed. Yet the weather result diverged so rapidly from the previous run such that all resemblance to the old one was gone. It was not a malfunctioning of the system, but an infinitesimal difference in the input that scaled exponentially to cause an overwhelming difference in the output. In the computer's memory, six decimal places were stored: 0.506127. On the printout of the result, to save space, just three appeared: 0.506. Lorenz had entered the shorter, rounded-off numbers. And that puny little inaccuracy appeared to amplify and cause the entire system to swing out of whack. Lorenz weather toy was implementing the classical program. It used a purely deterministic system of equations and the small errors proved catastrophic. Given a particular starting point, the weather would unfold exactly the same way each time. Given a slightly different starting point, the weather at the next moment would unfold in a slightly different way. This is the new initial condition which results in totally different mature state values compared to the previous run. This variability continues in a scale-free manner to result in a weather pattern with no similarities. Now the question arises: what if we give Lorenz weather machine results accurate to six decimal places? Remember, the Heisenberg's uncertainty principle prohibits accuracy of measurement. An infinitesimal change in the input values can result in a totally different outcome. Therefore, the initial situation of a complex system cannot be accurately determined, and the evolution of a complex system can therefore not be accurately predicted. This shattered the classical theory that one can calculate the approximate behavior of the system given an approximate knowledge of a system's initial conditions and an understanding of the natural law [7]. As chaos theory progressed, the research community saw journals which compared strange dynamics of a ball bouncing on a table side by side with articles on quantum physics. The simplest systems now seemed to be unpredictable.

3.3. Patterns in chaos

The second law of thermodynamics can be stated as follows, "In an isolated system, entropy never decreases." The second law of thermodynamics is just another way of saying that all physical systems tend to move toward their most probable states, which shows up as increased entropy. Viewed in that context, entropy can be thought of as measuring disorder or randomness. The Universe is governed by entropy and constant changes and growing toward greater and greater disorder. Yet, chaos is not simply disorder. Chaos explores the transitions between order and disorder, which often occur in surprising ways. An order arises from the ever-growing disorder of the Universe—chaos and order together. Let us take a close look at nature in **Figure 1**.

Figure 1. Pattern of river networks, lightning bolts, trees, snowflakes, metal crystals, and pinecones.

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River networks, lightning bolts, and trees have a self-similar pattern. Snowflakes, metal crystals, and pinecones have similar structural pattern. In all these structures, the same pattern gets repeated. They are said to have fractal-like features. Fractal, by definition, is a curve or geometrical figure, each part of which has the same statistical character as the whole. Fractal-like patterns are found throughout the nature. It can be seen in the formation of ice crystals and veins in the human body, in leaves, in water drops, in air bubbles, etc. It is often been said that nature is an excellent designer and fractals can be thought of as the design principle nature follows when putting things together. Fractals are the best existing mathematical descriptions of many natural forms, such as coastlines, mountains, or parts of living organisms. Fractals are infinitely complex patterns that are self-similar across different scales and infinitely detailed.

Most physical systems of nature and many human artifacts are not regular geometric shapes of the standard geometry derived from Euclid. Fractal geometry offers almost unlimited ways of describing and measuring these natural phenomena. Scientists discovered that the basic architecture of a chromosome is tree-like; every chromosome consists of many "mini-chromosomes" and therefore can be treated as fractal. This self-similarity has also been found in DNA sequences. Even the rhythm of our heart is a fractal pattern as a function of time. Many image compression schemes use fractal algorithms to compress computer graphic files to less than a quarter of their original size. Recent study shows that the Universe and our brain cell follow a very similar pattern as shown in **Figure 2**.

Figure 2(a) is an image, which is only micrometers wide and shows three neuron cells and their connections in the brain of a mouse, whereas **Figure 2(b)** is an image, which is billions of light-years across and is a computer-simulated image, which shows how the Universe grew and evolved. Together, they suggest the surprisingly similar patterns found in vastly different natural phenomena.

Fractals are related to chaos because they are complex systems that have definite properties. Chaotic systems and fractals are both iterated functions. Each iteration takes the state of the previous iteration as an input to produce the next state. Although fractals can show

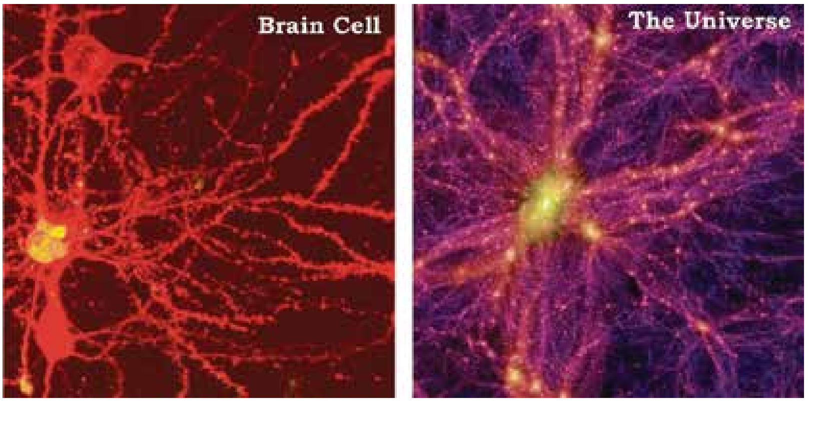

Figure 2. (a) Pattern of the brain cell. (b) Pattern of the Universe.

beautiful patterns, we cannot actually predict what their value is going to be of a specific iteration other than by calculating all the preceding iterations. So in a sense, fractals are just beautiful chaos.

The process of making a fractal is a type of self-ordering process. These self-organizing processes are very local in nature but lead to highly organized structures on very large scales. An order arises from the ever-growing disorder of the Universe. We cannot see the order in chaos if we are looking moment to moment. We cannot see order if we are managing individual behaviors. However, if we stand back far enough, if we wait over time, scale, or distance, we will observe the order that is in chaos, a pattern emerges from the otherwise disordered system.

3.3.1. The strange attractor

In a deterministic linear system, variability is not significant. There is a definite answer, a mathematical proof and solution for its characteristics and problems. A perfectly periodic system has the concept of a regular attractor. The damped pendulum has two invariant points; one is the point of minimum height and the other of maximum height. Due to the dissipation of energy, point of minimum height behaves as a regular attractor. The system tends to evolve toward the attractor. Into a structured linear system, if the amount of input force is increased, the system undergoes a transition to a chaotic system. The periodically repeating pattern previously present in the linear system breaks apart and gives rise to a pattern that never repeats. The system loses its predictability. A system in chaos is totally unpredictable from moment to moment. When converted into multidimensional space on high-speed computers, one could track many variables at once and could plot the movement of a system in chaos. The system is in total disorder when it is observed from moment to moment. Prediction of the next state is impossible. However, over a period of time, we come to realize that the system conforms to a boundary. There is an inherent shape that it never violates and never will it move out of a defined boundary. The plots that are based on nonlinear equations may appear to be random or chaotic but over many iterations will evolve to be simple and tend to produce patterns called strange attractors that confine to a boundary. These strange attractors need not be symmetrical always.

The behavior strange attractor can be seen from the first chaotic system discovered by Edward Lorenz, the Lorenzian (or chaotic) waterwheel. A chaotic waterwheel is just like a normal waterwheel except for the fact that the buckets leak. The entire waterwheel system is mounted under a water sprout. In the working of the waterwheel, water pours in from the top at a steady state and gives the system energy while water leaks out from each bucket at a steady state and removes energy from the system. Water trickles into the top bucket and immediately trickles out through the hole in the bottom at low speeds. With an increase in the inflow of water, the waterwheel will begin to revolve as the buckets fill up faster than they can empty. The heavier buckets containing more water on descending will let the water out, and when empty, it ascends on the other side to be refilled. The system is in a steady state; the wheel will continue to spin at a fairly constant rate. On increasing the input flow of water, increasing the system's entropy, the system transitions into a chaotic behavior. Rather than spinning in one direction at a constant speed, the wheel will speed up, slow down, change directions, and

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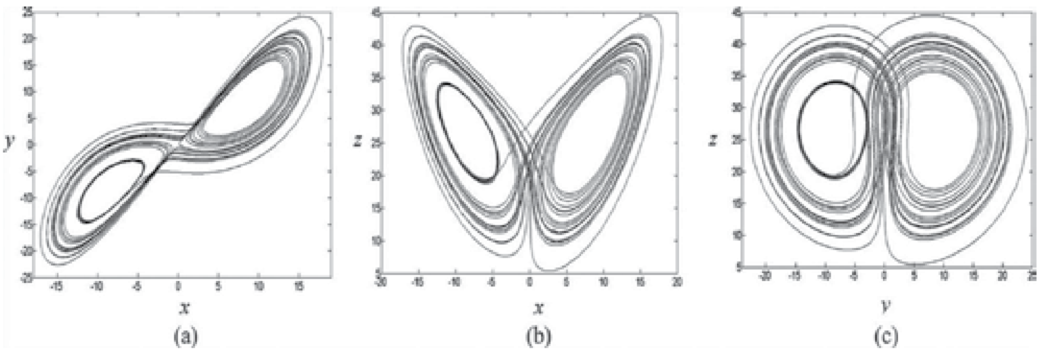

Figure 3. Chaotic patterns followed by the center of mass of the bucket in Lorenzian waterwheel with x, y, and z being the coordinates of the center of mass in (a) x-y plane, (b) x-z plane and (c) y-z plane [10].

oscillate back and forth, between the combinations of behaviors in an unpredictable manner. However, the entire system is within some bounds. Because the system never exactly repeats itself, the trajectory of a particular bucket never intersects itself. Instead it loops around and around forever in a strange pattern. It seems to be attracted toward a point in space. The system does not reach the ideal attraction point but is constantly pulled to it. There emerges an order in the chaotic system as shown in **Figure 3**. Hence, simply put, a chaotic system is a deterministic and unpredictable system.

4. Complex systems

Complex systems exhibit chaotic behavior that is characterized by extreme sensitivity to initial conditions, fractal geometry, and self-organized criticality [11]. The concept of sensitive dependence on initial conditions has been popularized in the "butterfly effect": minute differences in the initial conditions for such a system result in extremely different outcomes.

Fractal geometry refers to self-similarity, which implies that an object looks the same at any scale. Mathematically, self-similarity requires a power law distribution of representative objects. In other words, as the size of an object decreases, there is a corresponding power law increase in the number of objects of that size [12].

Self-organized criticality (SOC) is the concept that a dynamic system will move toward a critical, an emergent, or a metastable state, by natural processes [13]. A metastable system is in a delicate state of equilibrium where even a small change in conditions may precipitate a major change in the system. The chaotic nature of complex systems and its sensitivity to initial conditions make it prone to be in a metastable state and not in an equilibrium state.

The knowledge about the emergent properties of chaotic system and similarities across various natural systems opens up new possibilities. First, it boosts the effort to explore the secrets of the nature in the sense that these conspicuous similarities encourage to think about the common mechanisms connecting all these systems. Second, it gives a tool to study the chaotic system. Chaotic systems are highly complex systems due to the randomness and nonlinearity existing in these systems. Chaotic systems are usually defined as deterministic systems whose trajectories diverge exponentially over time. It involves few parameters and the dynamics of their values. Complex systems are essentially chaotic systems, and hence, all these properties are relevant to complex systems too. However, as complex systems comprise of many interacting parts, they are ever-growing dynamic systems. It always interacts with the environment. So, the scientific study of chaos is the root of the modern study of complex systems [14]. The big question is how we can study the complex systems based on the insights obtained from the study of chaotic systems.

Complex systems manifest themselves as complex networks because complexity stems from intricacies that exist in the interconnections. Hence, the study of complex systems is the statistical study of network matrices as graphs representing complex networks. Networks can be represented as regular or nonregular graphs. Regular graphs are those having regular topologies, and algorithms in graph theory are used to analyze their properties. However, many complex systems, for example, World Wide Web or social networks, do not follow a regular graph structure. There is randomness associated with the existence of a connection between two nodes in a complex network. The random graph as proposed by Erdös and Rényi [15] tries to capture this randomness. It is observed by Strogatz [3] that the small-world effect is exhibited in complex networks. When a rewiring is done in a regular lattice with some random connections, short paths are produced between any pair of nodes and the network is highly clustered than random graphs. Many complex systems like social networks show this property of high significance in the way people are connected with each other.

The quest for finding the underlying laws in the emergence of complex systems is a very important one. With the knowledge that a small change during the emergence plays a big role in forming the final form, the question arises as to whether there exists any simple law that resulted in the systems that exist now. This enquiry starts with the analysis of complex networks and tries to find the similarities in them. Barabási and Albert [16] have observed that the degrees of distribution among the nodes are dissimilar. Some nodes are highly connected than others. This means, if p_k denote the fraction of nodes that have k links where k is the degree and p_k is the degree distribution, the random graph model predicts a bell-shaped Poisson distribution for *pk*. However, in the case of real networks, p_k is highly skewed and decays much more slowly than Poisson's distribution. For instance, the distribution decays as a power law $p_k \sim k$ for the Internet backbone, metabolic reaction networks, the telephone call graph, and the World Wide Web. These networks are called "scale-free" networks by analogy with fractals, phase transitions, and other situations where power laws arise and no single characteristic scale can be defined. Though power law distribution is not universal, it is quite common among real networks. Hence, this result is quite significant when the laws for emergence of these networks are concerned. Turcotte [11] has shown that this emerges due to the existence of two simple rules during the emergence: the growth of network and its preferential attachment. This means that if the network expands continuously by the addition of new vertices and the new vertices attach preferentially to the sites that are already well connected, a power law distribution in degree distribution will occur. In complex systems improbable events are orders of magnitude more likely than events that

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follow the Gaussian distribution. Complex systems exhibit non-Gaussian outputs since the estimates and predictions of system's future behavior, particularly Gaussian estimates, formed by observations collected over short time periods provide an incorrect picture of large-scale fluctuations [17].

5. Internet as a complex system

After the Internet became widely available in the early nineties, it has enabled new services and transformed access to information, improved economic efficiency, and facilitated greater collaboration among individuals, businesses, and government. The Internet and the internetworking infrastructures underpin every aspect of our lives. More than 50% of the world's population now uses the Internet, a proportion that is growing every year. The Internet provides the supporting platform for an emerging digital economy, which depends on broadband networks and services like social media and cloud computing.

The computers and network which form the information system is an important and natural application domain for complex systems. Those systems are dynamic in nature, with continuously changing patterns of behavior, programs getting modified or removed or new programs included, users being removed or added, and configurations getting changed over time. The information system security problems are quite challenging due to the growing complexity and interconnected nature of these systems. It happens to be additionally complex with its multidimensionality as problems at different layers of the system are to be addressed. These problems include the physical layer security problems, network layer routing problems, application layer privacy, authentication and encryption problems, information security management problems, etc.

The Internet is identified as a critical enabler for sustainable development since it aids in unlocking human capabilities and enables communication and integration of the large information society. Forecasting the development of innovative and new technologies in this field is very difficult. The developments of the Internet were not anticipated by anyone. Most forecasts turn out to be too optimistic about the short-term introduction and too conservative about the societal consequences in the long term. Sustainability necessitates the reliability and resilience of the Internet if governments and businesses are to use the Internet to deliver services and for economic prosperity. Participation in the digital economy, including cloud computing, requires uninterrupted and safe access to high-speed networks.

5.1. Information systems security

The Internet evolves at a rapid rate in terms of the number and variety of the individual components and the possible applications that were never expected at all. The main reason for instability of the Internet is that many of the engineering innovative applications for ease of use are not being matched by engineering for ease of security. Now, large number of people, even with little technical knowledge or skill, all over the world are using the power of application software and new hardware to work with greater effectiveness and efficiency. However, it is difficult to securely configure and operate many of these services or products. This mismatch between the knowledge needed to operate a system and that needed to keep it secure results in increasing the number of system exploits. Additionally, the Internet has evolved so rapidly that any service provider or application developer will be concentrating on reducing the time taken to bring a new innovation to market. Hence, security is given the least priority in a competitive market for new products. This results in a high chance of exploits and attacks on the Internet that involve direct participation of many components including people and systems (software and hardware including networks). Hence, there is a fundamental relationship between the networking components and network security problems.

Additionally, the complexity of the Internet adds to the risk in the system usage as it allows attackers to find novel ways to gain improper access to the information on computer systems or intrude into network systems. The security analysis in such a complex context has to be investigated rather than depending only on heuristics. This paradigm shift leads to employ complexity theory to model the interactions of networking components in security problems. In these decision-making security models, the decision makers play the role of either the attacker or the defender. They have conflicting goals, with attacker attempting to breach security of the system so as to interrupt the services offered or damage the information available on systems, whereas a defender takes either preventive or corrective measures to enhance the system performance.

There are situations of uncertainty in predicting the behavior, interaction, and intention of both the malicious attackers and the defenders. It is necessary to understand the interaction between the attackers and defenders. Also, there is an increasing interaction and collaboration between various organizations that are interconnected as there are security interdependencies among them. This is because the vulnerability of one organization may result in compromises for others and in cascading failures affecting many nodes. The equilibrium analysis of the entire system provides insights on the decisions like security investment and patch management. Complexity theory aids in analyzing and investigating the decision process by the proper prediction of the behavior of networking components.

It is therefore necessary to give a top priority to analyze, model, and better understand the interconnected large-scale complex systems due to the increasing vulnerability of these network infrastructures. The Leontief-based input-output infrastructure model [18] can be made use of to represent the added and ever-increasing interdependence, intraconnectedness, and interconnectedness among the networking infrastructures. Additionally, the entire system becomes complex due to its architecture involving decision-making at multiple levels. The Leontief-based model can be used in managing the vulnerabilities of these complex network systems and the threats on these infrastructures in a more cost-effective manner. This will ensure the continued performance of these complex infrastructures. This will enable the total protection of the information stored in the systems or the information that gets communicated over the network.

Sustainable development has been a focus of international public policy since the Earth Summit in 1992. It identifies that economic growth, social inclusion, and environmental sustainability are essential to achieve human development that meets the needs of the present without compromising the ability of future generations to meet their own needs. Any innovation happening in a field becomes sustainable if it can meet the needs of people without adversely affecting the future generations to meet their needs. Thus, sustainable innovation has a close linkage with value choices. Any naturally occurring complex system has a tendency to evolve automatically, and those networks are quite resistant to small initial variations causing a tremendous effect on the entire system. It is only the artificial or the man-made complex networks like the Internet that get affected by cascading failures capable of disabling the network almost entirely.

5.2. Self-organized criticality

As many vital systems for the existence of human beings follow chaotic pattern, the quest for finding out the measure of the stability and predictability of a complex system is a very active research field. The stability of the Internet system is getting affected both from the internal and external threats. Internal threats stem from the growing instability inherent in the system. Self-organized criticality introduced by Bak et al. [13] addresses this issue. SOC is a property of dynamic systems to organize its microscopic behavior to be spatial (and/or temporal) scale independent. SOC is typically observed in slowly driven nonequilibrium systems with extended degrees of freedom and a high level of nonlinearity. Phenomena of strikingly different backgrounds were claimed to exhibit SOC behavior: sand piles, earthquakes, forest fires, rivers, mountains, cities, literary texts, electric breakdown, motion of magnetic flux lines in superconductors, water droplets on surfaces, dynamics of magnetic domains, growing surfaces, human brains, etc. [19]. SOC models are useful in analyzing systemic instabilities inherently present in the system. Growth, i.e., addition of the new components to the system, is a ubiquitous feature of the complex system. SOC models study whether this growth will reach critical state and in which further addition of a component leads to failure of the system. This scenario may be in direct relation to the issue of sustainability of the Internet system. Many concerns of the Internet usage in modern life are the unprecedented growth that raises the concerns of sustainability. The studies are conducted using SOC model to analyze the growth dynamics of these systems and effect of human interventions in the system. For example, the effect of introducing a new species into an ecosystem [20], external threats to the system, attack from outside targeting a random member or targeting a special member of the system, etc.

Peculiar structure existing in the Internet influences the effectiveness of these attacks. In many complex systems like social networks or the Internet, very few nodes are rich in their connections, whereas most of the nodes are poor. This gives rise to the formation of hubs in these kinds of networks. These hubs are important and the significance of their security is integral to the stability of the whole system. Albert et al. [21] have studied about the attack tolerance of scale-free network and have shown that scale-free networks are more tolerant to random attacks. Change in diameter (longest geodesic) is analyzed for both random attacks and targeted attacks, and their study shows that scale-free network is less resilient against targeted attack. This shows that the nature of possible attack and the resultant failure that can happen are highly important in systems like the Internet. A similar result is shown by Xiao et al. [22] when they examine the robustness of communication networks under intentional attacks from a complex network point of view. They have found that incomplete information may significantly degrade the efficiency of intentional attack, especially if a big hub is missed. After analyzing local information–based distributed attacks such as greedy sequential attack, coordinated attack, and lower-bounded parallel attack, it is shown that distributed attacks can be highly effective, sometimes almost as efficient as an accurate global information–based attack. This observation shows that attack is possible even when complete information about a hub is not available.

The question of how effectively information can be spread in a complex network or conversely how fatal a malicious node or the information it spreads is very significant. In this regard, Kitsak et al. [23] investigated on the question of which nodes can be the most influential spreaders in a complex network. The most efficient spreaders were identified by the k-shell decomposition analysis to be those located within the core of the network. When multiple spreaders are considered simultaneously, the distance between them becomes the crucial parameter that determines the extent of the spreading. Basaras et al. [24] explore the possibility of blocking virus propagation in complex networks. They found that removing edges is more practical than removing nodes to prevent the spread of a malware infection. Identification of edges that have to be removed is discussed and they propose an algorithm that detects critical connections based on their diffusion capabilities, namely, critical edge detector (CED).

Due to the nonlinear nature of complex networks, a failure starting at some point can cause unpredictable damage to the whole system. An attack can cascade through the nodes too. Lai et al. [25] review two problems in the security of complex networks: *cascades of overload failures on nodes and range-based attacks on links*. They argue that many scale-free networks are more sensitive to attacks on short-range than on long-range links because short-range links tend to link together highly connected nodes, while long-range links tend to connect nodes with very few links. Another finding is that the small-world phenomenon in these scale-free networks is caused by short-range links. The removal of a node with a tremendously large load is likely to significantly affect the loads at other nodes. There is hence a chance to trigger a sequence of overload failures. Thus, in networks with some degree of randomness, the distribution of loads and the distribution of links are highly correlated.

Buldyrev et al. [26] developed a framework for understanding the robustness of interacting networks that are subject to cascading failures. They have presented the analytical solutions for finding the critical fraction of nodes that, on removal, will lead to a cascading failure and to a complete fragmentation of two interdependent networks. It is also found that a broader distribution with the same average degree implies that there are more low-degree nodes. The advantage of a broad distribution for a single network becomes a disadvantage for interdependent networks as the low-degree nodes are more easily disconnected.

5.3. Interdependence and its effects

Complexity is multiplied when one complex network intricately depends on other complex networks. The nonlinearity in the effect discussed so far makes most of the systems vulnerable to even the smallest perturbation. In a highly networked world, interdependence causes many uncertainties. The effects of climate system on financial system, social network on political system, power grid on the Internet, etc., are some of the examples. Buldyrev et al. [26] discuss about the problem of interdependence failure. Vespignani [27] analyzes the number of nodes that must fail before network is totally fragmented. Using percolation theory it is shown that the number of nodes is very less for interdependent networks compared to isolated networks. Chen et al. [28] investigate the emergence of extreme events in interdependent networks and found that when the number of network layers and/or the overlap among the layers is increased, extreme events can emerge in a cascading manner on a global scale. Thorough analysis has been carried out to understand the emergence of global-scale extreme events based on the concept of effective betweenness. A cost-effective control scheme to suppress the cascading process of extreme events so as to protect the entire multilayer infrastructure against global-scale breakdown is undertaken in his work by increasing the capacity of very few hubs. Buldyrev et al. [26] developed a framework to understand the robustness of interacting networks that are subject to cascading failures.

6. Conclusion

The possibility of studying systems that are complex gives insights into the ways of emergence and the nonlinear cause and effects pattern that are followed. Most natural systems follow a complex structure. The interdependence of seemingly disparate systems is getting more evident with a tiny change in one parameter producing disastrous effect in many interconnected systems. A system becomes unsustainable when it causes those effects, which are never expected out of it. This is exactly because of the inability to predict the effect of a system on other systems.

Sustainability is crucial in organizational and technological innovations that yield both bottom-line and top-line returns. Sustainability in a sense is being environment friendly with a reduced consumption of resources or, in simple terms, by reducing the inputs used by a system, in terms lowering the cost of production or innovation. Additionally, the entire process generates extra revenues from better products or enables to create new businesses. In fact, it is smart to treat sustainability as innovation's new frontier. Hence, complex systems are to be taken as a whole for a long-term analysis. Complexity theory, which studies about the emergence of systems with a "whole is greater than part" approach, is the very suitable tool to attack the effects.

Research challenges in the field of complex systems are about creating models and finding metrics that can capture the true nature of any real-world complex system. Representing complex systems as a network provides a powerful tool to decipher the secrets of their complexities. This inquiry is yet another epoch of comprehending the difficult riddles nature poses before humans, the most intelligent life form of the Universe. Maybe, victory in this through a proper understanding of the system gives the ability to innovate and sustain.

Finally poised between chaos and order, sustainability, and innovation, chaos theory has an edge that promises to clarify the simple and yet mysteriously complex nature of this Universe and all its beings and phenomena. Its ramifications are the information available, strong claims made, more lucid answers sought and driven by the sustainability of nature, and the innovative and problem-solving capacity of humans. Driven by the need for better problem solving, we continue to structure knowledge, recognize new problems, and create new knowledge with innovation at the center to sustain the flow.

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Chapter 2

Measurement of the Communication Possibility of Service Requests for Multiservers in Parallel Connection in Cloud Computing Systems

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Additional information is available at the end of the chapter

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Abstract

Newly, growing amount of data-demanding applications arrangement with continuous fluctuating data substances, have been investigated by many researchers recently. In these applications, the underlying data management system must support new types of the space-time changing that indicates to the paths of the cloud computing system (CCS). The time-space changing causes change in the dimension of data and, consequently, in the CCS. One of the solutions regarding this case is suggesting an integrated cloud computing system (ICCS). In this effort, we introduce a new ICCS, based on fractional formal operators, taking into account the symmetrical delay in it. This model is useful for higher dimensional data, moving data, and chaos data. Moreover, we employ a fractional differential method to discover the paths (outcomes) of the system by minimizing the cost function. The proposed system delivers a sequence of paths that converge to the optimal path. The theoretical technique is supported by the applications.

Keywords: fractional calculus, fractional formal, fractional dynamical system, cloud computing

1. Introduction

Cloud computing system (CCS) is the technique industries and organizations use to do their trades. In that dynamically accessible and visualized resources are delivered as a service over the Internet. This system constructs a new type of chance for organizations. CCS is developing as one of the most important factors for the business industry: it can convert the traditional industrial business prototypical, aid it to support product improvement with business approach, and construct able manufacturing networks that reassure effective cooperation. Various categories of CCS adoptions in the industrial area have been studied with direct adoption utilizing technologies and manufacturing. CCS has been in some of the important parts of developed Information Technology (IT). In CCS, entirety is preserved as a service such as platform, infrastructure, and software. These services express a layered system assembly for CCS. There are different kinds of CCS: private (single-tenant setting), public (idea of sharing), hybrid (mixed internal and external clouds), and community (multitenant setting shared by numerous organizations) clouds. The integrated CCS may refer to one of them. These cloud services are permeating as a particular plug of access. Various types of placement simulations outfit various states. The main study in CCS is to minimize the cost of the cloud, keeping the good and stable quality with less time [1–5].

The cost assistance of accepting clouds in a characteristic developed prize can be manifold. The savings acquired from the exclusion of selected functions that were necessary in customary Information Technology (IT) can be important. With cloud paths (solutions), some applications may be distributed with the company's Information Technology (IT) region along CCS technologies. Thus, the Information Technology (IT) control can create the modification that occurs seamlessly to reduce the cost. scheming is significant for creating schedules and controlling decisions. Cost itemization analysis, finding the developed movement, adaptive cost scheming, clearness of feeding, and billings are imperative concerns. Virtualization states to the idea of rational resources from their fundamental physical features in order to progress and enhance flexibility and decrease cost. Integrated cloud computing system (ICCS) platform paths show a significant character in converting prize systems, funding to cost reduction [1, 6–9].

A diversity of smart phones and handheld computers prepared with a GPS and further sensory devices previously exists for clients. A collective sensor that can discover and report separate motivations plots a sequence of data arguments in a higher dimensional data (HDD) time-space (one time dimension and n data dimensions). Consequently, to improve a practical database application, one requires to examine the following categories: the nature, the presentation, the store, the management, the environment, and the support of data. The challenging phase of HDD organization is considerably more obvious in training, particularly when inadequate recognition, such as intervals, reduces the frequency of accelerators and GPS interval. The HDD is adopted to deal with partial capacity, highly dynamic clients, and partial scalability to larger data sets. Recently, numerous application path simulations have been presented. These models suggested the point-time and location of data in the information space. If the item transfers farther, it reports its new position and changes the inform threshold for the next apprise [10–14].

Fractional calculus is a field of various studies with applications not only in mathematics but also in other sciences, engineering, economics, and social presentations. It agrees with differential and integral operators, including random powers: real and complex [15, 16]. The essential benefit of the constructing technique of fractional differential equations (ordinary and partial) in methodical forming is their nonlocal property. It is standard that the normal derivative is a local, linear operator, while the derivative of arbitrary order is nonlocal and

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nonlinear. This proceeds that the successive recognized by a system is not only susceptible upon its present proper but also reliable upon all of its ancient formals. This additionally defined why fractional calculus has industrialized more and more extensively in mechanical, engineering, information theory, and industrial areas. Fractional calculus is received in information theory [17].

In this study, we impose a new ICCS, based on fractional formal operators, taking into account the symmetrical delay in it. This model is useful for higher dimensional data, moving data, and chaos data. Moreover, we employ a fractional differential method to discover the paths (outcomes) of the system by minimizing the cost function. The proposed system delivers a sequence of paths that converge to the optimal path. The theoretical technique is supported by applications.

2. Seeking

In this section, we illustrate the algorithm that we use to minimize the cost of the Information Technology (IT) in the cloud. Here, we suppose that the agents have nonhomogeneous options and pay the cost in order to translate from a position to another one in the state space $X \in [0, 1]$, where X is the level of utilizing Information Technology (IT) of the CCS. All agents have the common cost function Φ to have the request χ. Every user applies his optimal decision on the utility of the CCS by minimizing the cost function. Thus, the issue for each user is the minimized control function $U(t,X)$.

The method is based on a new fractional differential transform (FDT). It is well known that this method has solved many problems not only in mathematics but also in physics and engineering (see [18–20]). We need the following fractional formal: the Riemann-Liouville operators are defined by the formal

$$D_s^{\nu}\wp(t) = \frac{d}{ds}\int_0^t \frac{(t-\varsigma)^{-\nu}}{\Gamma(1-\nu)}\wp(\varsigma)d\varsigma, \tag{1}$$

which coincides with the fractional integral operator

$$I_a^{\nu}\wp(t) = \int_a^t \frac{(t-\varsigma)^{\nu-1}}{\Gamma(\nu)}\wp(\varsigma)d\varsigma, \tag{2}$$

such that $\nu \in (0, 1)$ and $\wp$ is a continuous function on $J = [0, T], T < \infty$. We use the notation $I_0^{\nu}\wp(t) = I^{\nu}\wp(t)$.

In this effort, we deal with the FCCS of the form minimize:

$$\frac{\partial}{\partial t}U(t,\chi) = \Phi(t,\chi(\tau_0 t), D^{\nu}\chi(\tau_1 t), D^{2\nu}\chi(\tau_2 t),\dots,D^{n\nu}\chi(\tau_n t), I^{\nu}\phi(t)),$$
$$\text{Initial condition}: \quad (\chi_i(\tilde{t}) = y_i(\tilde{t})), \forall i = 1,\dots,n, \tilde{t} < t \in J, \tag{3}$$

where

$$\phi(t) := \phi(t,\varsigma,\chi(\rho_0\varsigma), D^{\nu}\chi(\rho_1\varsigma), D^{2\nu}\chi(\rho_2\varsigma),\dots,D^{n\nu}\chi(\rho_n\varsigma)), \quad t \geq 0, \varsigma \leq t, \tag{4}$$

is the objective function (we suggested integrable function in order to make the minimization of the cost function), $\chi = (\chi_1,\dots,\chi_n)^T$ is the request function for $n-$ agent in the cloud, and Φ is the cost function of the cloud system. We aim for a given company a degree of CCS in its present operation, $X(\tilde{t}) = \chi(\tilde{t}) = y(\tilde{t}) \in [0,1]$. Therefore, $\chi = 0$ is represented to a company that is not yet translated to advanced position. Therefore, the dynamic of the company's position develops depending on Eq. (3). We proposed the system (3) in terms of the fractional formal operator to include the delay in the CCS. The objective function deals with optimal state of the usage of the Information Technology (IT) in the cloud system depending on the cost.

CCS influences notions from utility computing to deliver elements the services used. Such elements are at the fundamental of the public cloud paid-per-use representations. Moreover, measured services are a critical part of the reactive loop in autonomic computing, agreeing services to scale on-demand and to achieve automatic disappointment recovery. Also, CCS delivers the tools and technologies to measure data/compute demanding parallel applications with much more reasonable prices compared to traditional computing system techniques. Our aim is to minimize (3). Therefore, we proceed to introduce a solution for the system (3). In this section, we introduce a numerical solution for Eq. (3) by using a new technique based on the fractional formal concept. The CCS (3) is equivalent to the problem

$$\Phi(t,\chi(\tau_0 t), D^{\nu}\chi(\tau_1 t), D^{2\nu}\chi(\tau_2 t),\dots,D^{n\nu}\chi(\tau_n t), I^{\nu}\phi(t)) = 0. \tag{5}$$

An arbitrary function $\chi(t)$ can be formulated in terms of fractional Taylor series (see [21]) about the point t_0

$$\begin{aligned}\chi(t) &= \sum_{\kappa=0}^{\infty}\frac{(t-t_0)^{\kappa\nu}}{(\nu\kappa)!}[D^{\kappa\nu}\chi(t)]_{t=t_0}\\ &:= \sum_{\kappa=0}^{\infty}(t-t_0)^{\kappa\nu}\Lambda_{\nu}(\kappa),\end{aligned} \tag{6}$$

where $(\nu\kappa)! = \Gamma(\nu\kappa + 1)$, $D^{\kappa\nu}\chi(t) = (D^{\nu}...D^{\nu})_{\kappa - times}\chi(t)$ and

$$\Lambda_{\nu}(\kappa) = \frac{[D^{\nu\kappa}\chi(t)]_{t=t_0}}{(\nu\kappa)!}, \nu \in (0,1], \tag{7}$$

is FDT of $\chi(t)$.

Equation (3) represents various types of fractional and integer control systems such as the Hamilton Jacobi Bellman equation, Euler equation, Fokker-Planck equation, and Hybrid systems. The major important advantage of FCCS is their nonlocal property. The CCS (integer case) is a local, linear system, while the FCCS is a nonlocal, nonlinear system. Therefore, the subsequent formal of a system is simulated by its current and previous positions (this asset is beneficial in CC). Thus, fractional formal has developed progressively into practical and manufacturing areas. A virtuous consequence is attained in FCCS by minimizing the time of utility function ($\chi(t)$) and the cost function (Φ) of the cloud. The change in the quality of the cloud may calculate the difference in the promised quality (Q_p) and the recent quality (Q_r)

$$\Delta Q = Q_p - Q_r. \tag{8}$$

We accept that cost, request, profit, and income functions are continuous and different with respect to time. The request is dwindling in the cost for the service and growing in quality delivered. The CCS is expected to determine its request for Information Technology (IT) services for any assumed value and quality. The base flat of quality essential to function the system is zero, and the base flat of request is at zero quality and cost. The request of the internal customer is such that at a satisfactorily high cost, there will be no feeding the services. Therefore, the quantity of the CCS can be expended as a function of the amount and quality.

We have the following properties:

Proposition 2.1. Suppose that $\Theta(\kappa)$ and $\Lambda(\kappa)$ are FDTs of $\theta(t)$ and $\chi(t)$, respectively, then

1. If $\theta(t) = \chi(\rho t)$, then $\Theta_{\nu}(\kappa) = \rho^{\kappa}\Lambda_{\nu}(\kappa)$.

2. If $\theta(t) = D^{m\nu}\chi(\rho t)$, then $\Theta_{\nu}(\kappa) = \frac{(\nu(m+\kappa))!}{(\nu\kappa)!}\rho^{m+\kappa}\Lambda_{\nu}(m+\kappa), m \in \mathbb{N}$.

3. If $\theta(t) = I^{\nu}\chi(\rho t)$, then $\Theta_{\nu}(\kappa) = \frac{(\nu(\kappa-1))!}{(\nu\kappa)!}\rho^{\kappa-1}\Lambda_{\nu}(\kappa-1)$.

for $\rho \in (0,1)$

Proof: From Eq. (7), we have

$$D^{\nu\kappa}\theta(t) = D^{\nu\kappa}\chi(\rho t) = \rho^{\kappa}D^{\nu\kappa}\chi(\rho t); \tag{9}$$

therefore, we get

$$D^{\nu\kappa}\theta(t)|_{t=t_0} = \rho^{\kappa} D^{\nu\kappa}\chi(\rho t)|_{t=t_0} = \rho^{\kappa}(\nu\kappa)!\Lambda_{\nu}(\kappa); \tag{10}$$

thus, we obtain

$$\Theta_{\nu}(\kappa) = \frac{[D^{\nu\kappa}\theta(t)]_{t=t_0}}{(\nu\kappa)!} = \rho^{\kappa}\Lambda_{\nu}(\kappa). \tag{11}$$

This proves the first part. By using the first part, we conclude that

$$D^{\nu\kappa}\theta(t)|_{t=t_0} = D^{\nu\kappa}(D^{m\nu}\chi(\rho t))|_{t=t_0} = D^{\nu(m+\kappa)}\chi(\rho t))|_{t=t_0}, \text{ and} \tag{12}$$

consequently, we receive

$$D^{\nu\kappa}\theta(t)|_{t=t_0} = (\nu(m+\kappa))!\rho^{m+\kappa}\Lambda_{\nu}(m+\kappa). \tag{13}$$

Hence, we arrive at the part two,

$$\Theta_{\nu}(\kappa) = \frac{(\nu(m+\kappa))!}{(\nu\kappa)!}\rho^{m+\kappa}\Lambda_{\nu}(m+\kappa). \tag{14}$$

Finally, to prove the last part,

$$\begin{aligned} D^{\nu\kappa}\theta(t)|_{t=t_0} &= D^{\nu\kappa}(I^{\nu}\chi(\rho t))|_{t=t_0} = D^{\nu(\kappa-1)}\chi(\rho t))|_{t=t_0} \\ &= \frac{(\nu(\kappa-1))!}{(\nu\kappa)!}\rho^{\kappa-1}\Lambda_{\nu}(\kappa-1) \\ &= \Theta_{\nu}(\kappa). \end{aligned} \tag{15}$$

This completes the proof.

Proposition 2.2. Consider that $\Theta_{\nu}(\kappa)$, $\Lambda_{\nu}(\kappa)$ and $\Omega_{\nu}(\kappa)$ are the FDT of the functions $\theta(t)$, $\chi(t)$ and $\omega(t)$, respectively, then

1. If $\theta(t) = \chi(t) \pm \omega(t)$, then $\Theta_{\nu}(\kappa) = \Lambda_{\nu}(\kappa) \pm \Omega_{\nu}(\kappa)$.

2. If $\theta(t) = \delta\chi(t)$, then $\Theta_{\nu}(\kappa) = \delta\Lambda_{\nu}(\kappa)$.

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Proof: By applying Eq. (7) in the first part, we obtain

$$\begin{aligned}\Theta_{\nu}(\kappa) &= \frac{[D^{\nu\kappa}\theta(t)]_{t=t_0}}{(\nu\kappa)!} = \frac{[D^{\nu\kappa}(\chi(t)\pm\omega(t))]_{t=t_0}}{(\nu\kappa)!} \\ &= \frac{[D^{\nu\kappa}\chi(t)]_{t=t_0}}{(\nu\kappa)!} \pm \frac{[D^{\nu\kappa}\omega(t)]_{t=t_0}}{(\nu\kappa)!} \\ &= \Lambda_{\nu}(\kappa)\pm\Omega_{\nu}(\kappa).\end{aligned} \tag{16}$$

Similarly, for the second part, we have

$$\Theta_{\nu}(\kappa) = \frac{[D^{\nu\kappa}\theta(t)]_{t=t_0}}{(\nu\kappa)!} = \frac{[D^{\nu\kappa}\delta\chi(t)]_{t=t_0}}{(\nu\kappa)!} = \delta\Lambda_{\nu}(\kappa). \tag{17}$$

The procedure of CCS as a contribution to the Information Technology (IT) section can be observed as a resource chain. The Information Technology (IT) section improves the cost of the external part of CCS and deliveries such improved services to the inner consuming parts. Therefore, there are correspondences and there are parts of differences between the traditional resource chain techniques [22] and the suggested one that introduced in this effort (see **Figure 1**). The proposed CCS model shows dual relegation under the incomes because the Information Technology (IT) section scripts the cost of the incoming cloud system. Nevertheless, the cost reports double relegation by posing Information Technology (IT) services at no control. Moreover, apart from the differing reasons of the numerous objects, information irregularity is an additional problem in resource chain coordination, which causes the bullwhip result.

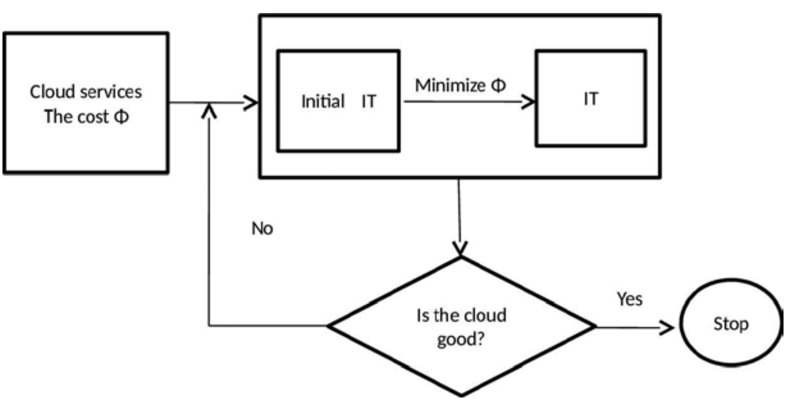

Figure 1. The proposed method of FCCS.

The proposed FCCS model theoretically looks like a resource chain construction. However, there are significant parts of the changes. We contain the stability and convergence of the system to the optimal solution by using the FDT, which implies the authority to inflict the operating organizational arrangement. The optimizing owns benefit discretely, or the models optimize the cost. The ICCS model, in the recent studies in Information Technology (IT) services, does not meet the resource problems for physical properties such as stock-outs or excess record. Moreover, we take into account the quality of Information Technology (IT) services under the ICCS model. Value development under CCS is expected to formulate a stationary price component and a quality-related minimal cost component. This is the new ICCS model that fixed the cost organization and increased the variable labor cost. Under this seeking, higher internal Information Technology (IT) value stages need a suitably high level of value from the ICCS because the price of a considerable value development is gross.

3. Applications

In this section, we illustrate some prototype applications to explain the accuracy of the FCCS.

3.1. System 1

Assume the following cost function:

$$\begin{aligned}\Phi(t,\chi) &= D^{\nu}\chi(t)-\chi(t)\\ &= 0\\ &\text{Initial condition}: \chi(0)=1, \chi'(0)=1.\end{aligned} \tag{18}$$

In view of Proposition 2.1, we obtain the fractional differential transform type of Eq. (18) as follows:

$$\begin{aligned}&\frac{(\nu(1+\kappa))!}{(\nu\kappa)!}\Lambda_{\nu}(1+\kappa)-\Lambda_{\nu}(\kappa)=0\\ &\text{Initial condition}: \Lambda_{\nu}(0)=\Lambda_{\nu}(1)=1,\end{aligned} \tag{19}$$

where Λ_{ν} is the fractional differential transform of $\chi(t)$, which is read in Eq. (7). By utilizing Eq. (19), we obtain the following system:

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$$\begin{aligned}
&\frac{(2\nu)!}{\nu!}\Lambda_\nu(2)-1=0,\\
&\frac{(3\nu)!}{(2\nu)!}\Lambda_\nu(3)-\Lambda_\nu(2)=0,\\
&\frac{(4\nu)!}{(3\nu)!}\Lambda_\nu(4)-\Lambda_\nu(3)=0,\\
&\frac{(5\nu)!}{(4\nu)!}\Lambda_\nu(5)-\Lambda_\nu(4)=0.
\end{aligned} \tag{20}$$

Solving the above system, we obtain the following outcome:

$$\Lambda_\nu(t)\approx 1+t+\frac{1}{\Gamma(2\nu+1)}t^2+\frac{1}{\Gamma(3\nu+1)}t^3+\frac{1}{\Gamma(4\nu+1)}t^4+\frac{1}{\Gamma(5\nu+1)}t^5. \tag{21}$$

In general, we attain to the solution

$$\Lambda_\nu(t)\approx E_{\nu,1}(t), \tag{22}$$

where $E_{\nu,1}$ is the Mittag-Leffler function defined by the series:

$$E_{\nu,\mu}(t)=\sum_{\kappa=0}^{\infty}\frac{t^\kappa}{\Gamma(\nu\kappa+\mu)}. \tag{23}$$

3.2. System 2

Assume the following cost function:

$$\begin{aligned}
&\frac{(\nu(1+\kappa))!}{(\nu\kappa)!}\Lambda_\nu(1+\kappa)-\frac{1}{2}\Lambda_\nu(\kappa)-\frac{1}{2}\frac{(\nu(\kappa-1))!}{(\nu\kappa)!}\Lambda_\nu(\kappa-1)=0\\
&\text{Initial condition}:\Lambda_\nu(0)=\Lambda_\nu(1)=\frac{1}{2},
\end{aligned} \tag{24}$$

In view of Proposition 2.1, we get the fractional differential transform of Eq. (24) as follows:

$$\begin{aligned}&\frac{(\nu(1+\kappa))!}{(\nu\kappa)!}\Lambda_{\nu}(1+\kappa)-\frac{1}{2}\Lambda_{\nu}(\kappa)-\frac{1}{2}\frac{(\nu(\kappa-1))!}{(\nu\kappa)!}\Lambda_{\nu}(\kappa-1)=0\\&\text{Initial condition}:\Lambda_{\nu}(0)=\Lambda_{\nu}(1)=\frac{1}{2},\end{aligned}\tag{25}$$

where Λ_ν is the fractional differential transform of $\chi(t)$, which is given in Eq. (7). By utilizing Eq. (25), we obtain the following system:

$$\begin{aligned}&\frac{(2\nu)!}{\nu!}\Lambda_{\nu}(2)-\frac{1}{2}\Lambda_{\nu}(1)-\frac{1}{2}\frac{1}{\nu!}\Lambda_{\nu}(0)=0,\\&\frac{(3\nu)!}{(2\nu)!}\Lambda_{\nu}(3)-\frac{1}{2}\Lambda_{\nu}(2)-\frac{1}{2}\frac{\nu!}{(2\nu)!}\Lambda_{\nu}(1)=0,\\&\frac{(4\nu)!}{(3\nu)!}\Lambda_{\nu}(4)-\frac{1}{2}\Lambda_{\nu}(3)-\frac{1}{2}\frac{(2\nu)!}{(3\nu)!}\Lambda_{\nu}(2)=0,\\&\frac{(5\nu)!}{(4\nu)!}\Lambda_{\nu}(5)-\frac{1}{2}\Lambda_{\nu}(4)-\frac{1}{2}\frac{(3\nu)!}{(4\nu)!}\Lambda_{\nu}(3)=0.\end{aligned}\tag{26}$$

Solving the above system, we obtain the following outcome for $\nu \in (0,1]$:

$$\Lambda_{\nu}(t)\approx\frac{1}{2}\left[1+t+\frac{1}{\Gamma(2\nu+1)}t^{2}+\frac{1}{\Gamma(3\nu+1)}t^{3}+\frac{1}{\Gamma(4\nu+1)}t^{4}+\frac{1}{\Gamma(5\nu+1)}t^{5}\right].\tag{27}$$

In general, we attain the solution

$$\Lambda_{\nu}(t)\approx\frac{1}{2}E_{\nu,1}(t).\tag{28}$$

3.3. System 3

Suppose the following cost function:

$$\begin{aligned}\Phi(t,\chi)&=D^{2\nu}\chi(t)+D^{\nu}\chi(t)-\chi(t)+I^{\nu}\chi(t)\\&=0\\&\text{Initial condition}:\chi(0)=1,\chi'(0)=-1.\end{aligned}\tag{29}$$

In view of Proposition 2.1, we have the fractional differential transform of Eq. (29) as follows:

$$\frac{(\nu(2+\kappa))!}{(\nu\kappa)!}\Lambda_\nu(2+\kappa)+\frac{(\nu(1+\kappa))!}{(\nu\kappa)!}\Lambda_\nu(1+\kappa)-\Lambda_\nu(\kappa)+\frac{(\nu(\kappa-1))!}{(\nu\kappa)!}\Lambda_\nu(\kappa-1)=0$$
$$\text{Initial condition}: \Lambda_\nu(0)=1, \Lambda_\nu(1)=-1, \tag{30}$$

where Λ_ν is the fractional differential transform of $\chi(t)$, which is given in Eq. (7). By utilizing Eq. (25), we obtain the following system:

$$\begin{aligned}
&\frac{(3\nu)!}{\nu!}\Lambda_\nu(3)+\frac{(2\nu)!}{\nu!}\Lambda_\nu(2)-\Lambda_\nu(1)+\frac{1}{\nu!}\Lambda_\nu(0)=0,\\
&\frac{(4\nu)!}{(2\nu)!}\Lambda_\nu(4)+\frac{(3\nu)!}{(2\nu)!}\Lambda_\nu(3)-\Lambda_\nu(2)+\frac{\nu!}{(2\nu)!}\Lambda_\nu(1)=0,\\
&\frac{(5\nu)!}{(3\nu)!}\Lambda_\nu(5)+\frac{(4\nu)!}{(3\nu)!}\Lambda_\nu(4)-\Lambda_\nu(3)+\frac{(2\nu)!}{(3\nu)!}\Lambda_\nu(2)=0,\\
&\frac{(6\nu)!}{(4\nu)!}\Lambda_\nu(6)+\frac{(5\nu)!}{(4\nu)!}\Lambda_\nu(5)-\Lambda_\nu(4)+\frac{(3\nu)!}{(4\nu)!}\Lambda_\nu(3)=0.
\end{aligned} \tag{31}$$

Solving the above system, we get the following outcome for $\nu \in (0,1)$:

$$\Lambda_\nu(t)\approx\left[1-t+\frac{1}{\Gamma(2\nu+1)}t^2-\frac{1}{\Gamma(3\nu+1)}t^3+\frac{1}{\Gamma(4\nu+1)}t^4-\frac{1}{\Gamma(5\nu+1)}t^5\right]. \tag{32}$$

In general, we attain the solution

$$\Lambda_\nu(t)\approx E_{\nu,1}(-t). \tag{33}$$

From above examples, we conclude that the solution of a fractional system, taking the formal (3), has the following general formula:

$$\chi(t)=(\chi(0))E_\nu(\lambda t^\nu). \tag{34}$$

4. Results and discussion

For the extra model improvement, it is essential to form some model considerations that come across the demand of applicability and to study major information and price styles.

- Every worker has a computer linked to the internet. Therefore, the price of acquiring and the price of the network (switches, routers, and network security) are not recognized to the CCS.
- The effort of the analysis deceits in the price evaluation of different CCS and service structures. As a consequence, the price for servers is reflected in the mathematical model.
- The price (cost) construction and empathy of cost styles have been initially formed in the source of the CCS.

The cost function is suggested and studied by many researchers in various methods [23–25]. For example, the authors used the form

$$\text{Total Cost} = \text{Expenditure of time} = \text{Total time* The cost per hour.} \tag{35}$$

Most of these methods do not request the quality of the CCS. Our technique requested the quality and integrated it. **Table 1** shows the experimental results, the proposed method, and comparison with the usual method for calculating the cost of CCS. It is well known that E_ν satisfies the following asymptotic behavior (see [26]; Theorem 1):

$$E_\nu(t) \sim \frac{1}{\nu} e^{t^{1/\nu}}, \quad \nu \neq 0. \tag{36}$$

Hence, we have the solution

$$\chi(t) \approx \frac{\lambda}{\nu} e^{t(\Delta Q)^{1/\nu}}, \tag{37}$$

where ΔQ is the difference in the quality of the CCS, which is suggested in $[0, 1]$ and $\lambda = \chi(0)$ is the initial cost of the cloud. In this effort, based on the above discussion, we impose the following formal of the total cost

$$\text{Total Cost} = \text{Total time* The cost per hour * } \chi(t), \tag{38}$$

where $\chi(t)$ is given in Eq. (37).

Obviously, the quality of the cloud plays an important role in the cost. Increasing the quality leads to higher cost. At the level $\Delta Q = \nu = 0.1$ (high quality, low fractional value), we see that the cost is minimized to the quarter, while the level $\Delta Q = \nu = 0.5$ (the quality is less and higher fractional power), we obtain no much minimization for the cost. Moreover, in the case $\Delta Q = 0.1, \ = \nu = 0.75$, we have a minimum up to the half. Hence, we conclude that the fractional

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power of the cloud system also plays an important role to minimize the cost. The fractional power of the system may be realized as the rate of the gain of the FCCS.

Time	**[23–25]**	**FCCS**	**[Eq. (38)]**			
		$\Delta Q = \nu = 0.1$	$\Delta Q = \nu = 0.25$	$\Delta Q = \nu = 0.4$	$\Delta Q = \nu = 0.5$	$\Delta Q = 0.1, \nu = 0.75$
10	$112.0	$246.6	$560	$896	$1131.1	$896
12	$134.4	$295.68	$672	$1075.2	$1357.44	$1075.2
14	$156.8	$344.96	$784	$1254.4	$1583.66	$1254.4
16	$179.2	$394.24	$896	$1433.6	$1809.92	$1433.6
18	$201.6	$433.5	$1008	$1612.8	$2036.16	$1612.8
20	$224.0	$492.8	$1120	$1792	$2262.4	$1792

Table 1. The cost of FCCS with initial cost = $112.

5. Conclusion

The cloud computing system moves the manner activities (business, economy, and industries) and deals with their plans. The cloud computing system uses a new method to improve the economy, industries, and businesses, that is, everything is supposed as a service, be a service you demand or a service you deliver. We employed the concept of fractional formal calculus to impose a mathematical model of the cloud computing system. This system is obligated to various factors such as the controller, the utility of the cloud, structure for the Information Technology (IT) unit, and the cost taking into account the gain of the producers. Although the model has created simplifying conditions, it yielded a selection of outcomes that enhance the literature and have management suggestions. Obviously, any concept that is essential for a dynamic system is restricted in its ability to internment the complexity of Information Technology (IT) control. The proposed system may be viewed as a hybrid system, integrated system, as well as a perturbed system. It included various types of well-known systems (see [22, 27]). Also, the suggested system is addressed with huge number of data (time and space). Our goal was to introduce a method to minimize the cost function of the cloud. The anticipated framework is comprehensive in that the coverage contains the conceptual model, quantitative computation, logical representation, straddling both the theory and the applications of the problem. The results in **Table 1** show the performance of the method, by using fractional formal calculus. The obtainable method raises the quality of the system as well as minimizes the cost in the cloud computing system.

6. Competing interests

The author declares that there are no competing interests.

7. Author's contributions

There is no conflict of interests regarding the publication of this article.

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Chapter 3

System Control for Sustainability: Application to Building Design

Kazutoshi Fujihira

Additional information is available at the end of the chapter

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Abstract

In order to meet environmental, social and economic sustainability objectives, an immediate transformation needs to occur in housing design. We have been investigating a methodology for sustainable home design by applying control science because it can be applied to all of goal-oriented tasks. Our first study has shown the basic control system for sustainability. After that, regarding home as the complex of material and spatial elements, we have identified each element's variables and their desired values that lead to sustainability. Utilizing these schemes, we have composed the "control system for promoting sustainable home design" in which the "sustainable design guidelines" and "sustainability checklist" are incorporated. Following this control system, we have actually designed a home and constructed it. The results of this study indicate that if system users closely follow the methodology, they can design comprehensively sustainable and sufficiently energy-saving homes. Furthermore, the studies imply that this methodology is superior in user-friendliness as well as adaptable to regional differences and changes over time.

Keywords: control system, sustainable housing, climate change, adaptation, ageing population, material elements, spatial elements

1. Introduction

Buildings including homes have been causing various environmental problems such as climate change, environmental destruction, pollution, and depletion of natural resources. According to the IPCC, in 2010, buildings accounted for 32% of total global final energy use (24% for residential and 8% for commercial) and 19% of all global greenhouse gas emissions [1]. In the twenty-first century, continued emission of greenhouse gases will cause further warming, increasing the likelihood of severe, pervasive, and irreversible impacts on people and ecosystems [2].

Reducing climate change risks would require both "mitigation" and "adaptation" measures [2, 3], typically shown in **Table 1**. The chapter of "Climate-Resilient Pathways: Adaptation, Mitigation and Sustainable Development" in *Climate Change 2014* explains, "It takes sustainable development as the ultimate goal, and considers mitigation as a way to keep climate change moderate rather than extreme. Adaptation is considered a response strategy to anticipate and cope with impacts that cannot be (or are not) avoided under different scenarios of climate change" [4].

Mitigation measures	Adaptation measures
• Energy conservation	• Measures against inland and coastal floods
• Harnessing renewable energy	• Measures for dealing with water shortages
• Conserving timber resources	• Heatstroke warning systems
• Carbon dioxide capture and storage	• Building resilient infrastructure

Table 1. Typical examples of mitigation and adaptation measures.

While growing human activities are aggravating climate change and seriously harming environmental sustainability, "ageing population" is becoming a fierce challenge to social and economic sustainability. According to the book titled *Agequake*, in the twenty-first century there will be more people older than younger ones. The "agequake" will turn the age pyramids upside down, first in Japan and Europe, but ultimately throughout the world [5]. Demographic pressures will continue to mount and add to concerns about fiscal sustainability [6, 7]. Ed Harding – International Longevity Centre UK clearly states, "Suitable housing is central to the challenge of population ageing. Appropriate housing offers the potential to reduce expenditure on public services and promote older people's independence and wellbeing" [8].

It is obvious that an immediate transformation needs to occur in housing design, in order to meet sustainability objectives. Achieving sustainable development or sustainability is the ultimate goal-oriented task of humankind. It is a rational and reliable approach to apply control science to this challenge. Control science can be applied to all of goal-oriented tasks; it has already produced remarkable results in various fields, including engineering [9].

Based on the above recognition, we have been investigating a methodology for sustainable housing design by applying control science. Our first study has demonstrated the basic control system for sustainability. After that, we have systematically determined the relationships between the elements of home and sustainability. Utilizing these schemes, we have shown the control system for promoting sustainable home design and started putting it into practice. This paper reviews these studies and discusses the characteristics of the methodology and future prospects of our research.

2. Basic control system for sustainability

In the basic control system for sustainability (**Figure 1**), "controlled objects" are human activities which need to be controlled [10, 11]. "Disturbances" are harmful influences on controlled objects, which are caused by environmental, social, or economic problems. Examples of the disturbances are damaging influences caused by environmental pollution, floods or landslides resulting from environmental destruction, and various impacts caused by climate change. Moreover, "adaptation" has been added as the route from "disturbances" to "sustainability," based on the recent IPCC's recognition. "Controlled variables" are the variables that are related to the human activities and need to be controlled for basically solving or preventing the problems or adapting to disturbances.

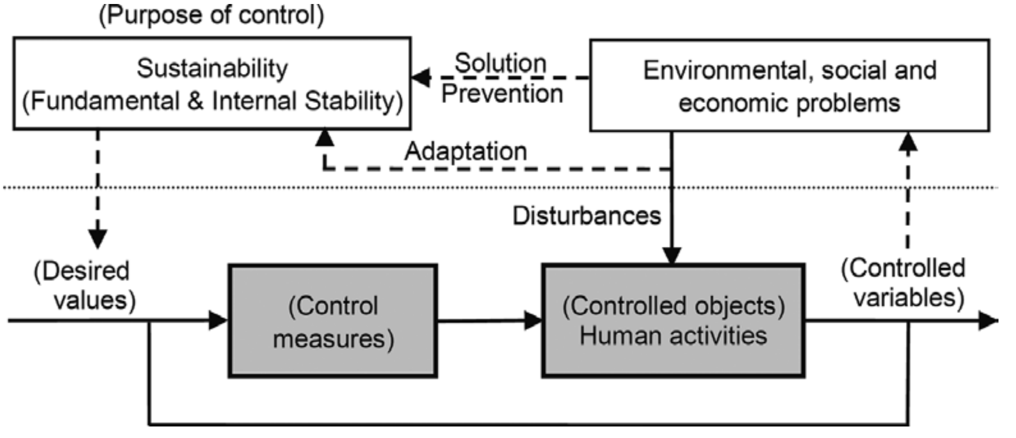

Figure 1. Basic control system for sustainability.

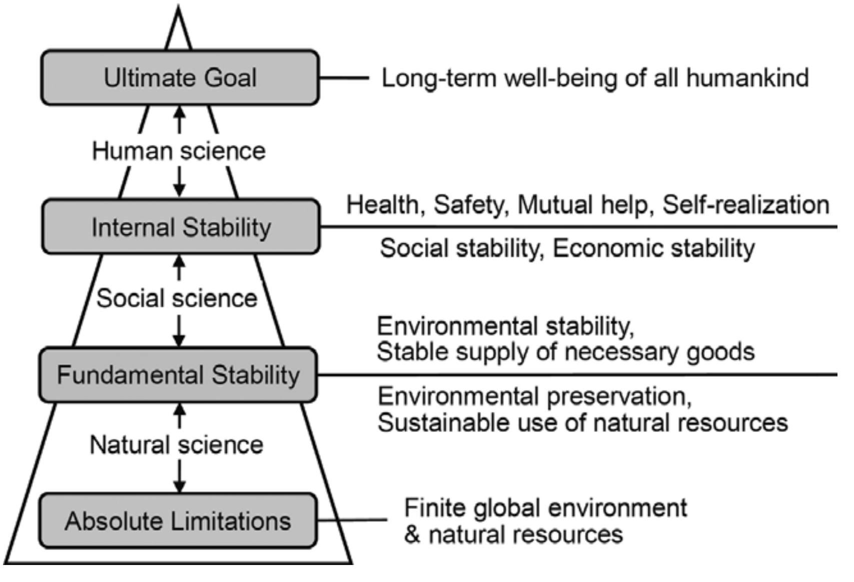

Figure 2. Model of sustainability.

"Desired values" are derived from the purpose of control, that is to say, sustainability. The model of sustainability (**Figure 2**) demonstrates that sustainability requires both "fundamental stability" and "internal stability," in order to accomplish the long-term well-being of humankind or ultimate goal, within the finite global environment and natural resources, or absolute limitations [10, 11]. Fundamental stability means environmental stability and a stable supply of necessary goods; the conditions for fundamental stability are environmental preservation and the sustainable use of natural resources. On the other hand, internal stability means social and economic stability; the conditions for internal stability are health, safety, mutual help, and self-realization, which are essential for well-being of humans.

The control objective is to adjust the controlled variables to their desired values. Furthermore, the control system requires designing and implementing "control measures," or measures for achieving the control objective.

3. Methodology for sustainable housing design

3.1. Two-step preparatory work

Our previous study has provided the two-step preparatory work for sustainable home design. The two steps are (1) "determining the relationships between the standard home and sustainability" and (2) "sustainability checkup on a home as an object" [12, 13]. The following sections show the essence of these two steps.

3.1.1. Determining the relationships between the standard home and sustainability

In the first step, system designers select important elements of the standard home and determine the relationships between such elements and sustainability.

When selecting important elements, we have analyzed two main factors: "material" and "space" [12]. "Material" regards the home as the aggregate of material elements such as framework, exterior, interior, and piping; "space" considers it as the aggregate of spatial elements, such as rooms and areas. Based on these two factors, we have selected important elements, from which extracts are shown in the central column of **Table 2**. "Material elements" are from "framework" to "equipment for harnessing natural energy;" "spatial elements" are from "specified bedroom" to "garden area."

After that, we have determined the relationships between these elements and sustainability. The left side of **Table 2** shows the relationships between the elements and fundamental stability; the right side demonstrates the relationships between the elements and internal stability. Considering the relationships between each element and the stability conditions, we have identified variables that indicate the degree of stability. Moreover, we have set the desired values of these variables that can meet relevant stability conditions.

Choosing only one element from **Table 2**, that is, "framework," I concretely describe the relationships. Considering the relationship between "framework" and "sustainable use of natural resources," a condition for fundamental stability, we have identified "durability" and "materials" as variables. The desired value of "durability" is set at "Grade 3" in the deterioration resistance grades (building frames, etc.) of JHPIS, that is, the Japan housing performance

Relationships with fundamental stability			Element	Relationships with internal stability		
Condition	**Desired value**	**Variable**		**Variable**	**Desired value**	**Condition**
Sustainable use of resources	JHPIS 3.1: Grade 3	Durability	**Framework**	Resistance to earthquakes	JHPIS 1.1: Grade 2 or over	Safety
Sustainable use of resources	CASBEE LR$_{H}$2 1.1: Level 4 or over	Materials				
Sustainable use of resources	CASBEE LR$_{H}$2 1.3: Level 4 or over	Durability	**Exterior** (outer wall, roof, etc.)	Fire resistance (outer wall)	JHPIS 2.6: Grade 3 or over	Safety
Sustainable use of resources	CASBEE Q$_{H}$2 1.2 & 3: Level 4 or over	Materials		Shape & color	Consideration for the landscape	Health
Enviro-preserve Sustainable use of resources	JHPIS 5.1: Grade 4	Thermal insulation performance	**Windows & doors**	Sound insulation performance	JHPIS 8.4: Grade 2 or over	Health
Enviro-preserve Sustainable use of resources	CASBEE Q$_{H}$1 1.1.2: Level 4 or over	Sunlight adjustment capability		Protection of glass against impacts	With shutters	Safety
Sustainable use of resources	CASBEE LR$_{H}$2 1.4: Level 4 or over	Materials	**Interior**	Measures against formaldehyde	JHPIS 6.1: Grade 3	Health
Enviro-preserve Sustainable use of resources	LED	Type of light	**Lighting fixtures**			
Enviro-preserve Sustainable use of resources	CASBEE LR$_{H}$1 3.2: Level 4 or over	Rainwater equipment	**Equipment for rainwater use**	Rainwater equipment	CASBEE LR$_{H}$1 3.2: Level 4 or over	Health Safety (in crisis)
Enviro-preserve Sustainable use of resources	100% or more of the total energy usage	Harnessed natural energy	**Equipment for harnessing natural energy**	Harnessed natural energy	100% or more of the total energy usage	Health Safety (in crisis)
			Specified bedroom	Routes to toilet & bath area, dining room, kitchen, and entrance	Accessible without steps	Health safety
Enviro-preserve Sustainable use of resources	Placing them closer	Areas in the home	**Areas relating to water use & hot water supply**			
			Doorways	Differences in level	No differences	Health safety
				Width	75 cm or more	
Enviro-preserve	40% or more	Ratio to the exterior area	**Garden area**			

Note: (1) JHPIS means the Japan housing performance indication standards (for new homes).
(2) CASBEE means CASBEE for detached houses (for new construction)—technical manual 2010 edition.

Table 2. Relationships between the standard home and sustainability [Essence].

Relationships with fundamental stability				Element	Relationships with internal stability			
Desired value	**Assess.**	**Measured or estimated value**	**Variable**		**Variable**	**Measured or estimated value**	**Assess.**	**Desired value**
JHPIS 3.1: Grade 3	No	JHPIS 3.1: Grade 1	Durability	**Framework**	Resistance to earthquakes	JHPIS 1.1 & 1.2: Grade 1	No	JHPIS 1.1: Grade 2 or over
CASBEE LR_H2 1.1: Level 4 or over	OK	CASBEE LR_H2 1.1: Level 4	Materials					
CASBEE Q_H2 1.2 & 3: Level 4 or over	No	CASBEE Q_H2 1.2 & 3: Level 2	Durability	**Exterior** (Outer wall, roof, etc.)	Fire resistance (Outer wall)	JHPIS 2.6: Grade 3	OK	JHPIS 2.6: Grade 3 or over
CASBEE LR_H2 1.3: Level 4 or over	No	CASBEE LR_H2 1.3: Level 3	Materials		Shape & color	Consideration for the landscape	OK	Consideration for the landscape
JHPIS 5.1: Grade 4	No	JHPIS 5.1: Grade 1	Thermal insulation performance	**Windows & doors**	Sound insulation performance	JHPIS 8.4: Grade 1	No	JHPIS 8.4: Grade 2 or over
CASBEE Q_H1 1.1.2: Level 4 or over	No	CASBEE Q_H1 1.1.2: Level 3	Sunlight adjustment capability		Protection of glass against impacts	With shutters	OK	With shutters
CASBEE LR_H2 1.4: Level 4 or over	OK	CASBEE LR_H2 1.4: Level 4	Materials	**Interior**	Measures against formaldehyde	JHPIS 6.1: Grade 3	OK	JHPIS 6.1: Grade 3
LED	No	Fluorescent	Type of light	**Lighting fixtures**				
CASBEE LR_H1 3.2: Level 4 or over	No	No equipment	Rainwater equipment	**Equipment for rainwater use**	Rainwater equipment	No equipment	No	CASBEE LR_H1 3.2: Level 4 or over
100% or more of the total energy	No	0 (zero)	Harnessed natural energy	**Equipment harnessing natural energy**	Harnessed natural energy	0 (zero)	No	100% or more of the total energy
				Specified bedroom	Routes to toilet & bath area, dining, kitchen, and entrance	With steps	No	Accessible without steps
Placing them closer	OK	Placing them closer	Areas in the home	**Areas water use & hot-water supply**				
				Doorways	Differences in level	With differences	No	No differences
					Width	60-70 cm	No	75 cm or more
40% or more	OK	45%	Ratio to the exterior area	**Garden area**				

Note: (1) JHPIS means the Japan housing performance indication standards (for new homes).
(2) CASBEE means CASBEE for detached houses (for new construction)—technical manual 2010 edition.
(3) When this checklist is used for the inspection or evaluation of existing homes, JHPIS (for existing homes) and CASBEE for detached houses (for existing building)—technical manual 2011 edition need to be referred to, instead of the "for new homes" version and "for new construction" version, respectively.

Table 3. An example of sustainability checkup on a home as an object [Essence].

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indication standards (for new homes) [14]. Meanwhile, the desired value of "materials" is set at "Level 4 or over" in the assessment levels of the "use of materials effective for resource saving and waste prevention" of CASBEE, that is, CASBEE for detached houses (for new construction)—technical manual 2010 edition [15].

On the other hand, considering the relationship with "safety," a condition for internal stability, we have selected "resistance to earthquakes" as a variable and set its desired value at "Grade 2 or over" in the "seismic resistance grades (prevention of collapse of building structures)" of JHPIS [14].

In addition, **Table 2** is the first updated version, which has been revised due to several reasons. First, we have revised the table so that following it leads to obtain long-life quality housing (*Choki Yuryo Jutaku*) certification. The long-life quality housing certification started in 2009 and has rapidly spread in Japan because of various incentives, such as tax reduction [16]. The second reason is the addition of adaptation measures against impacts caused by climate change. Other reasons are rapid spread of new technology, namely LED light, and minor changes in expressions and desired values.

3.1.2. Sustainability checkup on a home as an object

In the second step, "sustainability checkup on a home as an object" is conducted. To be concrete, first, the variables of a home as an object are measured or estimated. Next, the measured or estimated values are compared with the desired values and the comparison results are assessed. **Table 3** demonstrates the essence of "sustainability checkup," which includes an example of the results.

In this case, the comparison results have simply been assessed, whether the variable reaches the desired value or not, that is, "OK" or "No." The variables that have been assessed as "No" need to be identified as "controlled variables."

3.2. Control system for promoting sustainable home design

Based on the basic control system and the two-step preparatory work, we have composed the control system for promoting sustainable home design.

First, as shown in **Figure 3**, we have derived two functions from the two-step preparatory work, that is, the "sustainable design guidelines" from step 1 and the "sustainability checklist" from step 2, respectively.

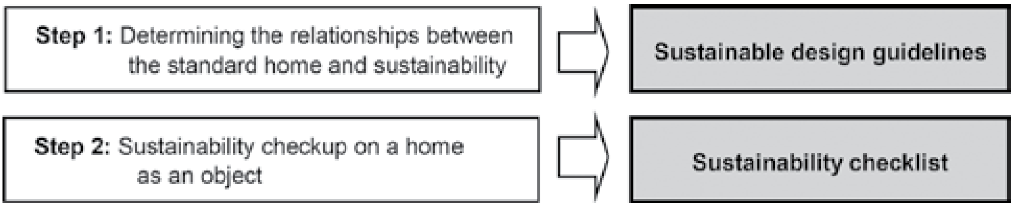

Figure 3. Two functions derived from the two-step preparatory work.

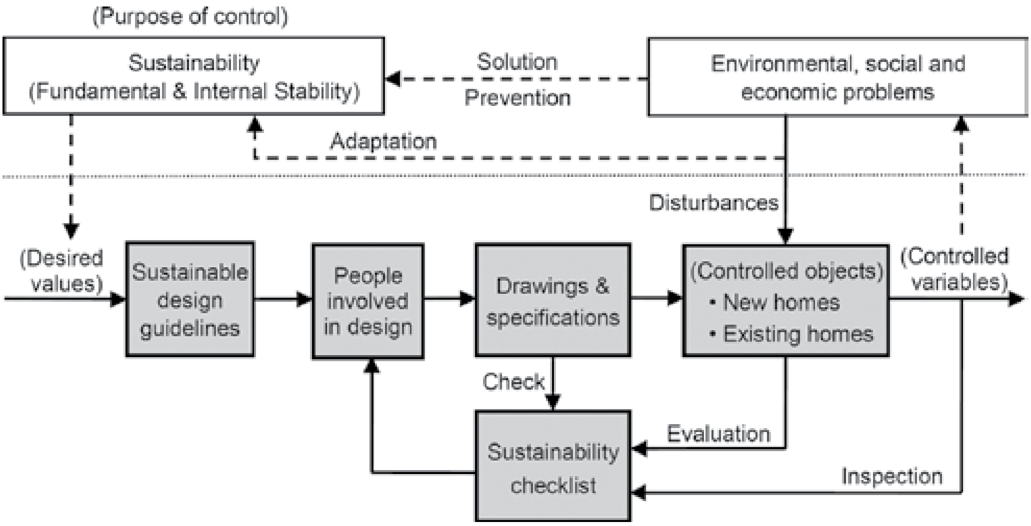

Figure 4. Control system for promoting sustainable home design.

Next, we have composed the control system for promoting sustainable home design in which these two functions are incorporated. **Figure 4** demonstrates the block diagram of the control system. In this control system, "controlled objects" include both "new homes" and "existing homes." The following describes how to use the two functions in the process of sustainable home design, on the order of "new homes" and "existing homes."

3.2.1. New homes

In the case of new homes, first, information on the desired values reaches "people involved in design" through the "sustainable design guidelines" [17]. "People involved in design" include homeowners, architects, designers, and homebuilders. Such people make a design so that the variables of home's elements can attain their desired values as close as possible. At important steps in the design process, they check the drawings and specifications by referring to the "sustainability checklist." After the construction is finished, the new home can be also evaluated against the "sustainability checklist."

3.2.2. Existing homes

When existing homes are the objects, the design process starts with "inspection" on the home as an object. The "people involved in design" measure or estimate each element's variables of that home by using the "sustainability checklist." Next, they compare the measured or estimated variables with their desired values and assess the comparison results.

Table 3 in the last section is equivalent to an example of such inspection results. In addition, when inspecting an existing home and measuring or estimating variables by referring to the JHPIS or CASBEE for detached houses, "people involved" use the "for existing homes" version or "for existing building" version, instead of the "for new homes" version or "new construction" version, respectively. The "JHPIS (for existing homes)" and "CASBEE for detached houses (for existing building)" are almost the same as their new home versions; however, these existing home versions include suitable assessment criteria for existing homes [14, 18].

After the inspection, the "people involved" usually make a design for improvement so that controlled variables meet their desired values as close as possible. When improvement is assumed to be technically difficult or costly, reconstruction can be chosen. Similar to the cases of new homes, they check the drawings and specifications for improvement or reconstruction against the "sustainability checklist." Moreover, sustainability of actually improved or reconstructed homes can be evaluated against the "checklist."

4. Case study

Following the above methodology, we designed a new home and constructed it. After this home began to be used, we objectively assessed its environmental performances.

4.1. Design process

In this case, the homeowner, who is the author of this paper, made the basic design by himself. After that, he made a contract with a housing manufacturer whose skills seemed sufficient to achieve the desired values as shown in **Table 2**.

In the basic design stage, the homeowner used the "sustainable design guidelines" and "sustainability checklist," in addition to following related laws and regulations. First, when making the site plan and floor plans, he considered spatial elements, such as "specified bedroom," "areas relating to water use and hot water supply," and "garden area." In addition, considering natural ventilation and day lighting, he planned "position and area of windows," which is omitted from the tables due to space limitations. Moreover, he examined how to install "equipment for harnessing natural energy" and "equipment for rainwater use" so as to satisfy the desired values of these material elements' variables.

At the beginning of the detailed design stage, the homeowner requested the architects of the housing manufacturer to refer to the "guidelines" and "checklist." They readily accepted them because the material and spatial elements are equivalent to real parts of the home. Next, we determined the site plan, floor plans, elevation, and fundamental specifications. After that, the architects designed the home's elements such as framework, exterior, windows and doors, interior, and lighting fixtures, so that as much as possible, the elements' variables meet their desired values.

After the design stage, we obtained long-life quality housing certification as well as building confirmation. Subsequently, the home, a wooden structure with two stories, was constructed in a residential area of suburban Tokyo.

4.2. Results

This section shows the results of the design and construction, focusing on main elements' variables.

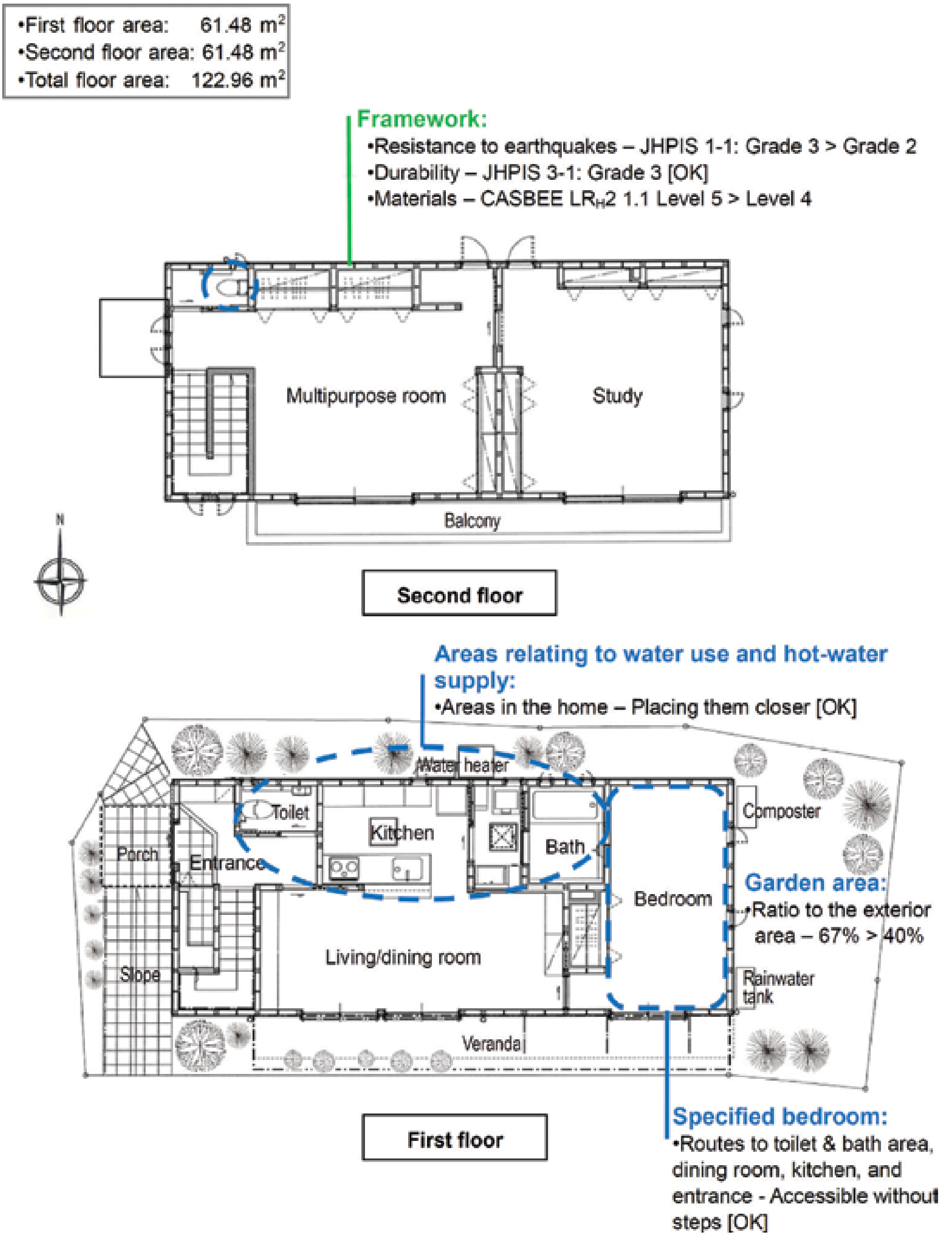

Figure 5. Site and floor plans.

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First, **Figure 5** demonstrates the site plan and floor plans in which three spatial elements and one material element are referred to:

• Specified bedroom

A "specified bedroom" is a bedroom which is used or expected to be used by elderly or wheelchair users. The owner couple was in their late fifties and not handicapped when they moved in. However, in order to prepare for their future, both their bedroom and other essential areas for their daily living, all have been placed on the same first floor. This arrangement enables them to have access to such areas without any steps.

• Areas relating to water use and hot water supply

"Areas relating to water use and hot water supply," that is, kitchen, bath, washing room, toilet, and a place to put the water heater, have been placed closer. This planning reduces the total length of water piping and drainage piping. Moreover, this consideration helps to reduce heat loss from hot water piping.

• Garden area

A "garden area" is an area with plants such as trees, shrubs, herbs, grasses and vegetables. The ratio of this home's garden area to the total exterior area is 67%, which surpasses its desired value, 40%. A larger garden area is favorable for environmental preservation, including mitigation of heat island phenomenon, and a higher level of biodiversity.

• Framework

This home has been designed so that the "resistance to earthquakes" of the framework meets "Grade 3" in the seismic resistance grades of JHPIS, which surpasses the required level, Grade 2.

The "durability" of the framework satisfies the desired value, or "Grade 3" in the deterioration resistance grades of JHPIS. Grade 3, the highest grade, requires measures to extend the period up to when large-scale renovation becomes necessary after three generations, or about 75–90 years, under normally assumed conditions and maintenance [14].

As for "materials," more than half of the wood is domestically produced timber, legality and sustainability of which are authorized. This consideration has sufficiently satisfied the desired value.

Figure 6 shows external appearance, including a panoramic view, with the descriptions of four material elements: exterior, windows and doors, equipment for harnessing natural energy, and equipment for rainwater use.

• Exterior

The "fire resistance" capacity of the outer walls fulfills the desired value, namely "Grade 3" in the fire resistance grades of JHPIS [14]. Meanwhile, the "shape" is simple but accented by

Figure 6. External appearance.

the balcony; the "color" of the outer walls, light beige, is coordinated with the colors of other parts, such as the windows and doors, entrance porch, and rainwater pipes. We are expecting that these considerations bring harmony and stability to the landscape.

• Windows and doors

Higher "thermal insulation performance" and "sunlight adjustment capability" of the openings contribute to reducing energy for heating and air conditioning as well as the occupants' health and comfort [15, 19, 20]. However, both of these variables appear on only the left side of **Tables 2** and **3** as the space is limited. The "thermal insulation performance" of this house's openings meets the desired value, or the highest grade of the relevant item of JHPIS. Meanwhile, the "sunlight adjustment capability" reaches "Level 5" in the assessment levels of the CASBEE's relevant item. "Level 5" means that the sunlight penetration ratio of the subject windows can be reduced to 0.3 or less in the summer and 0.6 or over in the winter [15].

We have installed "shutters" on the large windows facing south, in order to "protect the glass against impacts" such as fire, hurricane, and flying objects. This installment is also expected to decrease the risk of being damaged by tornados or huge typhoons, which can be caused by serious climate change.

• Equipment for harnessing natural energy

The surface of the single-pitch roof is almost entirely covered with solar panels. The total generating capacity of the 49 solar panels amounts to 11.4 kW. In the first year, after moving-in, this solar system produced the electricity of 15,911 kWh. In the same period, the energy used in this home has been 3085 kWh. Accordingly, the energy self-sufficiency reached an amazing 516%. This value substantially exceeded the desired value, 100%.

In addition, equipment for harnessing natural energy secures alternative energy sources and increases resilience or passive survivability in crisis. Therefore, it is recognized as an "adaptation" measure as well as "mitigation" [3, 21].

• Equipment for rainwater use

"Equipment for rainwater use," in this case, a 200-l rainwater tank, meets the desired value. The rainwater in this tank is used for watering the garden, which can reduce the quantity of

Figure 7. Interior, lighting fixtures and doorways.

water supply. At the same time, storing rainwater is also considered one of "adaptation" measures because it leads to securing emergency water supply [3, 21].

Figure 7 illustrates two material elements, namely "interior" and "lighting fixtures," and one spatial element, namely "doorways."

• Interior

Interior, which includes floors, walls and ceilings, requires "measures against formaldehyde" as an important variable. Formaldehyde is a harmful pollutant; therefore, its desired value is set at the highest level of the countermeasures against formaldehyde in JHPIS. All of the interior finish and base materials used in this house are certified materials that meet the desired value.

• Lighting fixtures

All of the "lighting fixtures" of this house use '"LED" lights, which meets the desired value.

• Doorways

We have taken barrier-free and universal design into maximum consideration. All of the "doorways" in this home have no "difference in level," and "width" of the doorways on the first floor except for the bath is 75 cm.

4.3. Performance evaluation

4.3.1. Sustainability performance

After the home started to be used, we had its sustainability evaluated by the "CASBEE for detached houses (for new construction, 2010 edition)." The evaluation results show that the "environmental quality (Q)" and "environmental load (L)" have been "88" and "13" respectively. Consequently, as demonstrated in **Figure 8(A)**, the score of Building Environmental

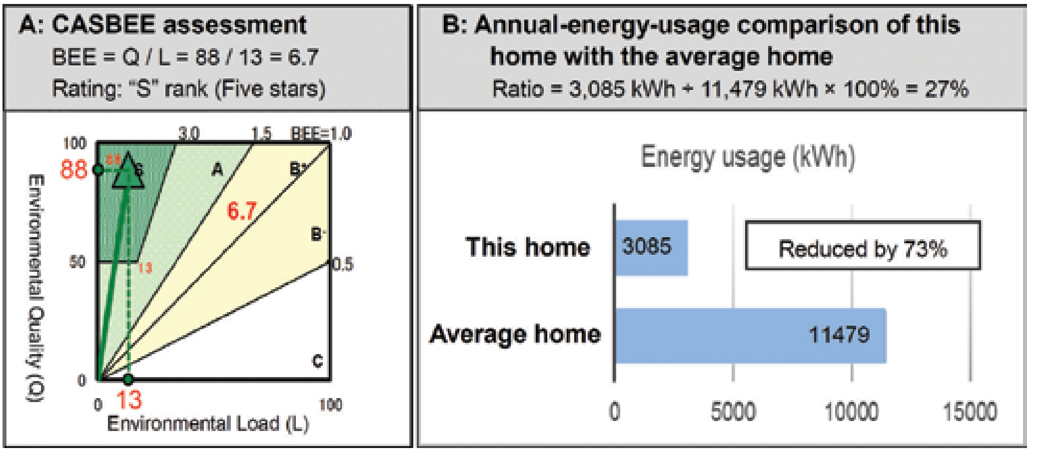

Figure 8. Sustainability performance and energy-saving performance of this home.

Efficiency (BEE) has reached 6.7, which has rated and certified the home with the highest "S," or "five stars" [22].

4.3.2. Energy-saving performance.

We have analyzed the energy-saving performance of this home, by comparing its annual energy usage with that of the average home. The actual total energy usage in this home in a year was 3085 kWh. On the other hand, the average annual energy usage of the same two-person-household detached houses amounts to 41,325 MJ [23], which is equivalent to 11,479 kWh. The usage of 3085 kWh is equal to 27% of 11,479 kWh. Therefore, as shown in **Figure 8(B)**, this house has reduced energy consumption by over 70%, as compared to the average house under the same conditions.

5. Discussion

This chapter discusses the results of this study from the following perspectives: (1) effects of the methodology on achieving sustainable homes, (2) characteristics of the methodology, (3) future work, and (4) applicability of the methodology.

5.1. Effects of the methodology on achieving sustainable homes

As shown in the case study, we have designed a home, following the methodology. To be concrete, we have designed the home's parts, or elements, so that as much as possible the elements' variables meet their desired values. After the home started to be used, we have objectively assessed its environmental performances. First, CASBEE for detached houses, a comprehensive assessment system, has readily ranked the home in the highest "S," with an extremely high score of BEE. Meanwhile, the energy-saving performance assessment has shown that the total energy usage of this home is equal to about 27% of the average home under the same conditions. These assessment results indicate that if system users closely follow the methodology, they can achieve comprehensively sustainable and sufficiently energy-saving homes.

5.2. Characteristics of the methodology

The characteristics of the methodology includes (1) visualization of the processes for promoting sustainable home design, (2) user-friendliness, (3) adaptability to regional differences and changes over time. In addition, the third point is beneficial for the system designers, whereas the second point is convenient for the system users.

5.2.1. Visualization of the processes

Figure 4 has demonstrated the control system in which the "sustainable design guidelines" and "sustainability checklist" are incorporated. It concisely shows processes for promoting sustainable design on both new and existing homes. Moreover, this schematic diagram contains "disturbances" caused by problems, such as climate change. Accordingly, we consider that this diagram itself explains the whole picture of the sustainable design processes with the guidelines and checklist and helps people concerned to recognize them.

5.2.2. User-friendliness

The "sustainable design guidelines" and "sustainability checklist" are simple tables. The material and spatial elements in these functions are equivalent to real parts of homes. Therefore, the system users smoothly design, check, evaluate, and inspect the home, by easily comparing the drawings or real home with the guidelines or checklist. In fact, the design process in the case study has supported the user-friendliness of the functions; the designers of the home easily accepted them and efficiently made drawings.

5.2.3. Adaptability to regional differences and changes over time

This methodology originally has a mechanism of easily adapting to regional differences. As shown in Section 3.1., system designers determine the elements' variables and their desired values, considering the relationships between the elements and sustainability conditions. This determination process has a mechanism of reflecting various regional features, such as natural, geographical, social, and cultural features. For example, a variable of the framework, "resistance to earthquakes," reflects a geological feature of earthquake-prone Japan. This mechanism also enables the system designers to easily vary the guidelines according to the characteristics of the region. For instance, if the region is in a snowy area or strong wind area, they can adjust the guidelines to the region, by adding "resistance to snowfall" or "resistance to wind" as a variable of the framework.

This characteristic also leads to the flexibility of the functions toward changes over time. In fact, in order to adjust to ageing population, we could smoothly take basic barrier-free design in the guidelines and checklist. To be concrete, we have added necessary spatial elements, such as "specified bedroom" and "doorways." Similarly, in order to adapt housing to climate change, we have taken adaptation measures in the functions. That is to say, we have added relevant variables including "protection of glass against impacts."

5.3. Future work

5.3.1. Further case studies

The case study has successfully demonstrated the effects of the methodology on achieving sustainable homes. However, in order to confirm the effects, we need to conduct more case studies, applying it to both new and existing homes. We expect that an increase in the number of case studies will also strengthen the credibility of the methodology and help it to be widely used.

5.3.2. Update of the guidelines and checklist

It is necessary to update the "guidelines" and "checklist," as the occasion arises. Probably, such revision will have to be made due to several reasons, for example, in response to the results of case studies, changes in the natural and social environment, developments in related sciences, and innovations in related technologies. Furthermore, through such processes, we are planning to examine how to revise them efficiently.

5.4. Applicability of the methodology

This section discusses the applicability of the methodology from two viewpoints: (1) application to other regions, (2) application possibility to other kinds of objects.

5.4.1. Application to other regions

As shown in Section 2, this methodology, specifically the "guidelines" and "checklist," has a characteristic of being adaptable to regional differences. Therefore, it will probably be easy for system designers in another region to adapt the functions for that region. To be concrete, the system designers can compile its regional version, by examining the elements and adapting the elements' variables and their desired values to the region's features.

5.4.2. Application possibility to other kinds of objects

Theoretically, the methodology can be applied to various kinds of objects, or human activities. That is to say, in the control system of **Figure 4**, "homes" in the block of "controlled objects" can be replaced with other kinds of objects. Possibility of such replacement depends on if the table of relationships, or the "guidelines," can be compiled or not.

It will not be difficult to apply it to other types of buildings besides the home, since the structure is similar to one another. It is also possible in theory to apply it to other sorts of infrastructure, such as roads and parks. Furthermore, we consider it possible to apply the methodology to more complex and large-scale objects, such as the city and town, for they are also regarded as the complex of material and spatial elements.

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Chapter 4

Stabilization Control for the Giant Swing Motion of the Horizontal Bar Gymnastic Robot Using Delayed Feedback Control

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Additional information is available at the end of the chapter

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Abstract

Open-loop dynamic characteristics of an underactuated system with nonholonomic constraints, such as a horizontal bar gymnastic robot, show the chaotic nature due to its nonlinearity. This chapter deals with the stabilization problems of periodic motions for the giant swing motion of gymnastic robot using chaos control methods. In order to make an extension of the chaos control method and apply it to a new practical use, some stabilization control strategies were proposed, which were, based on the idea of delayed feedback control (DFC), devised to stabilize the periodic motions embedded in the movements of the gymnastic robot. Moreover, its validity has been investigated by numerical simulations. First, a method named as prediction-based DFC was proposed for a two-link gymnastic robot using a Poincaré section. Meanwhile, a way to calculate analytically the error transfer matrix and the input matrix that are necessary for discretization was investigated. Second, an improved DFC method, multiprediction delayed feedback control, using a periodic gain, was extended to a four-link gymnastic robot. A set of plural Poincare maps were defined with regard to the original continuous-time system as a T-periodic discrete-time system. Finally, some simulation results showed the effectiveness of the proposed methods.

Keywords: gymnastic robot, nonholonomic system, giant swing motion, delayed feedback control, chaos control, stabilization

1. Introduction

In the past decades, scientists have found that unusual and unexpected evolution patterns arise frequently in numerous natural and model nonlinear systems in physics, chemistry, biology, engineering, medicine, economics, and so forth, since Lorenz [1] in 1963, May [2] in 1976, and others reported chaotic behavior in very simple dynamical models. The most peculiar aspect of these patterns is their random-like behavior, although the systems are deterministic, in other words, the deterministic nature of these systems does not make them predictable [3]. This behavior is known as deterministic chaos, or simply chaos. It is considered that chaos is due to sensitive dependence on the initial conditions. This property implies that two trajectories emerging from two different close-by initial conditions separate exponentially in the course of time. Due to this property, and due to the fact that, in general, experimental initial conditions are never known perfectly, chaotic systems cannot be predicted by their long-term behaviors.

This feature of their critical sensitivity to initial conditions, often regarded as a troublesome property, made chaos undesirable in engineering control practice, and most experimentalists considered such characteristics as something to be strongly avoided since it restricts the operating range of many electronic and mechanic devices. Besides that, chaotic systems exhibit two other important properties. One is that there is an infinite number of unstable periodic orbits embedded in the underlying chaotic set. The other is that the dynamics in the chaotic attractor is ergodic; that is to say, the system visits ergodically small neighborhood of every unstable fixed point during its temporal evolution [4].

Although the existence of steady states and an infinity of different unstable periodic orbits embedded in chaotic motion is not usually obvious in free-running chaotic evolution, these orbits offer a great potential advantage if one wants to control a chaotic system. The presence of chaos may be a great advantage for control in a variety of situations. In a nonchaotic system, small controls typically can only change the system dynamics slightly. However, in a chaotic system, one can choose between a rich variety of dynamical behaviors. It is then not surprising that the matter of controlling chaotic systems has come under detailed investigation by several different scientific communities. Chaotic dynamics consists of a motion where the system moves in the neighborhood of one of the unstable periodic orbits (UPO) for a while, then falls close to a different UPO and remains for a limited time. Thus, it allows to exploit a single dynamical system for the production of a large number of different periodic behaviors so that the single system can carry out different performances with different yields [5]. The result is to render an otherwise chaotic motion more stable and predictable, which is often an advantage. The perturbation must be tiny, to avoid significant modification of the system's natural dynamics.

Since Ott, Grebogi, and Yorke [6], in 1990, pointed out the existence of many unstable periodic orbits (UPOs) embedded in chaotic attractors that raise the possibility of using very small external forces to obtain various types of regular behavior, Pyragas [7] in 1992, proposed a so-called "Delayed Feedback Control (DFC)" idea that an appropriate continuous controlling signal formed from the difference between the current state and the delayed state is injected into the system, whose intensity is practically zero as the system evolves close to the desired periodic orbit but increases when it drifts away from the desired orbit, several techniques were devised for controlling chaos [8–21] during the past years and applied to various systems [22–31]. It is worth noting that in spite of the enormous number of applications among the chaos control, very few rigorous results are so far available. Most results are justified by computer simulations rather than by analytical tools. Therefore, many problems remain unsolved.

On the other hand, recently in the field of mechanical and control engineering, the open-loop link mechanism, in terms of diversity and ease of movement, has been used in industrial robots, although a large control input is needed due to speeding up, and the opposing force to the joint and the base increases. Therefore, the actuator with a large driving performance is needed, and the mass of the entire mechanism is increased. It is thought that the control method using the opposing force and gravity is important to achieve the desired movement with high speed and high efficiency by the limited driving performance. The joint type movement robot is actively researched in recent years, and the achievement of dynamic walking and running with high speed and efficiency becomes a problem. Although living creatures, such as humans or animals, have achieved the high-speed movement by using the open-loop link mechanism, it is thought that this is because that a good movement possessing the energy efficiency and small joint drive power and small impact power, and so forth in the gravitational filed had been acquired adaptively during the process of evolution. For example, the human biped locomotion is performed by dynamic link mechanism coupled to the pendulum motion [32, 33], and brachiation (movement across branches) used by the monkeys is a specialized form of arboreal locomotion that can be seen as a continuous pendulum motion [34, 35]. In addition, humans have competed for the manipulation of their own multi-degree of freedom link mechanism through sports or physical exercise, and so forth, and the achievement of a complex movement meeting a specific initial terminal requirement as a technique.

The systems, such as humans and robots, which control the internal force to achieve motions by using reaction force from the outside world, can be modeled as an underactuated link mechanism. These systems usually have nonholonomic second-order constraints due to the presence of passive joints, which makes development of control methods a difficult task. In recent years, studies on underactuated mechanical systems that possess fewer actuators than degrees of freedom have received increased interest [36–40].

Open-loop dynamic characteristics of an underactuated system with nonholonomic constraints show the chaotic nature that even though there are small differences in the initial conditions, the amplitude grows to be a completely different movement for its nonlinearity due to centrifugal force, Coriolis force, and gravity. Motions control of underactuated systems known also as nonholonomic control, such as wheeled robot positioning control [41], aerial posture control of space robots [42], and positioning control of underactuated link mechanism robot [43, 44], have been studied. However, a generalized control method has not yet been established to this kind of system due to the difficulties in analysis, and the fact that for an underactuated system, it cannot be directly controlled because of the generalized coordinates of its passive parts. Control methods, which utilize empirical skills catching the motion characteristics and proper motion of the system, are desirable. From the above-mentioned viewpoint, in order to achieve a robot with a high-speed, highly effective optimal motion, and the skill in movement seen in living creatures, fundamental researches on the control method and the trajectory planning method using periodic free movement for the linkage with a passive joint have been done [45–51].

The remaining parts of this chapter are organized as follows: Section 2 discusses a kind of DFC method, PDFC, for a two-link gymnastic robot by using of a Poincaré section. In the Section 3, an improved DFC method, Multiprediction Delayed Feedback Control, is extended to a four-link gymnastic robot. Section 4 gives some numerical simulations to show the effectiveness of the proposed method. Section 5 summarizes the chapter.

2. Delayed feedback control for a two-link horizontal bar gymnastic robot

The two-link horizontal bar gymnastic robot is a highly simplified model of a human gymnast on a high bar, where the underactuated first joint models the gymnast's hands on the bar and the actuated second joint models the gymnast's waist [52]. Studies on such underactuated mechanical systems that possess fewer actuators than degrees of freedom, as gymnastic robot with the underactuated first joint, have received considerable interest in recent years. Open-loop dynamic characteristics of such a linkage as this kind of system, which is classified as an underactuated systems with nonholonomic constraints, show the chaotic nature that even though there are small differences in initial conditions, the amplitude grows to be a completely different movement for its nonlinearity due to centrifugal force, Coriolis force, and gravity. Since a generalized control method has not yet been established to this kind of system for the difficulties in analysis, their control problems are challenging.

While applying the original DFC to the continuous system, such as gymnastic robot, stability analysis of the closed-loop system becomes a very difficult task because of the time-delay dynamics described by a difference-differential equation. A modified delayed feedback control method, called Prediction-based DFC (PDFC), is proposed to stabilize the giant swing motion of two-link horizontal bar gymnastic robot.

2.1. Two-link gymnastic robot model

The two-link horizontal bar gymnastic robot is a simplified model of a human gymnast on a high bar, where the first joint being passive models the gymnast's hands on the bar and the second joint comprising of an actuator models the gymnast's hips. The formula m_i, l_i, a_i, $I_i (i = 1, 2)$ in **Figure 1** denotes the ith link's mass, length, distance from joint to its center of mass, inertia moment around its center of mass, respectively.

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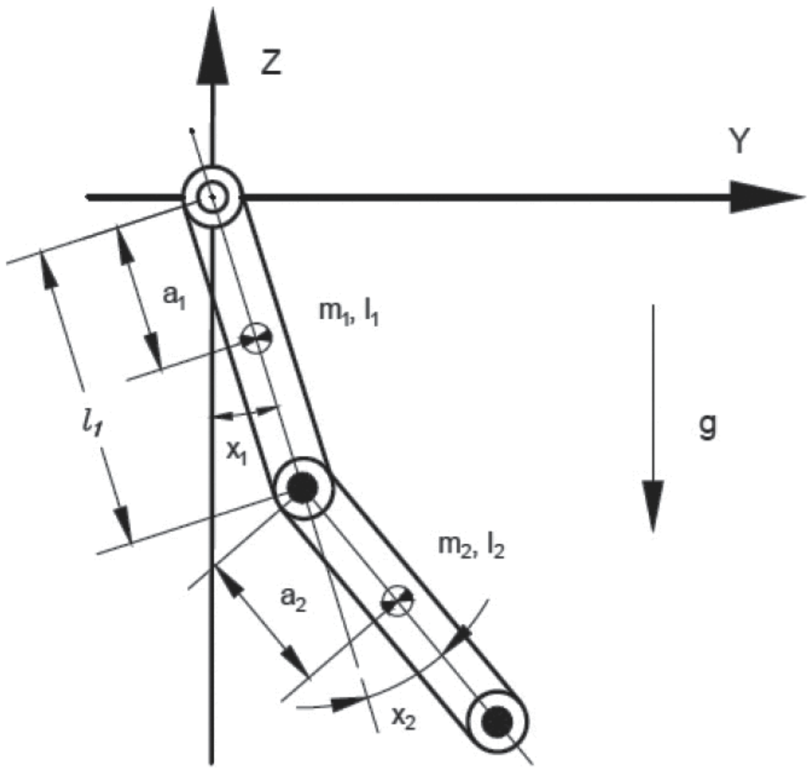

Figure 1. Two-link gymnastic robot model.

The equation of motion of the gymnastic robot is as follows:

$$\begin{bmatrix} u_1 \\ u_2 \end{bmatrix} = \underbrace{\begin{bmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{bmatrix}}_{M} \begin{bmatrix} \ddot{x}_1 \\ \ddot{x}_2 \end{bmatrix} + \underbrace{\begin{bmatrix} C_1 \\ C_2 \end{bmatrix}}_{C} + \underbrace{\begin{bmatrix} G_1 \\ G_2 \end{bmatrix}}_{G}, \tag{1}$$

where $\mathbf{x} = (x_1, x_2)^T \in \mathrm{R}^2$ is the generalized coordinate vector, $\mathbf{u} = (u_1, u_2)^T \in \mathrm{R}^2$ is the joint torque vector, and $M \in \mathrm{R}^{2 \times 2}$, $C \in \mathrm{R}^{2 \times 1}$, $G \in \mathrm{R}^{2 \times 1}$ denote the inertia matrix, Coriolis matrix, and gravitational matrix, respectively.

$$M_{11} = I_1 + I_2 + m_1 a_1^2 + m_2 \left(l_1^2 + a_2^2 + 2 l_1 a_2 \cos x_2 \right)$$

$$M_{12} = I_2 + m_2 \left(a_2^2 + l_1 a_2 \cos x_2 \right)$$

$$M_{21} = I_2 + m_2 \left(a_2^2 + l_1 a_2 \cos x_2 \right)$$

$$M_{22} = I_2 + m_2 a_2^2$$

$$C_1 = -\left(\dot{x}_2^2 + 2 \dot{x}_1 \dot{x}_2 \right) m_2 l_1 a_2 \sin x_2$$

$$C_2 = \dot{x}_1^2 m_2 l_1 a_2 \sin x_2$$

$$G_1 = g\{(m_1a_1 + m_2l_1)\sin x_1 + m_2a_2\sin(x_1 + x_2)\}$$

$$G_2 = gm_2a_2\sin(x_1 + x_2)$$

In addition, since the first joint cannot generate active torque, the following constraint must be satisfied.

$$u_1 \equiv h(\ddot{\mathbf{x}}, \dot{\mathbf{x}}, \mathbf{x}) = 0 \tag{2}$$

In order to facilitate the analysis, we rewrite the motion Eq. (1) into the following equation of state:

$$\dot{x} = \begin{bmatrix} \dot{\mathbf{x}} \\ M^{-1}(\mathbf{x})(-C(\mathbf{x}, \dot{\mathbf{x}}) - G(\mathbf{x})) \end{bmatrix} + \begin{bmatrix} 0 \\ M^{-1}(\mathbf{x})E \end{bmatrix} u \equiv f(x, u), \tag{3}$$

where

$$\begin{aligned} M(\mathbf{x}) &= \begin{bmatrix} c_1 + c_2 + 2d\cos x_2 & c_2 + d\cos x_2 \\ c_2 + d\cos x_2 & c_2 \end{bmatrix}, \\ C(\mathbf{x}, \dot{\mathbf{x}}) &= \begin{bmatrix} -(\dot{x}_2^2 + 2\dot{x}_1\dot{x}_2)d\sin x_2 \\ \dot{x}_1^2 d\sin x_2 \end{bmatrix}, \\ G(\mathbf{x}) &= \begin{bmatrix} g_1\sin x_1 + g_2\sin(x_1 + x_2) \\ g_2\sin(x_1 + x_2) \end{bmatrix}, \\ E &= \begin{bmatrix} 0 \\ 1 \end{bmatrix}. \end{aligned} \tag{4}$$

Here, $x = [\mathbf{x}, \dot{\mathbf{x}}]^T \in \mathrm{R}^4$ denotes the state vector, and $u \in \mathrm{R}^1$ represents the control input. Meanwhile, the variables among the above equations are defined as follows:

$$c_1 = I_1 + m_1a_1^2 + m_2l_1^2C$$

$$c_2 = I_2 + m_2a_2^2C$$

$$d = m_2l_1a_2C$$

$$g_1 = g(m_1a_1 + m_2l_1)C$$

$$g_2 = gm_2a_2.$$

2.2. Prediction-based delayed feedback control

As is known, the stability of a periodic orbit of the original continuous-time system is closely related to the stability of the fixed point of the corresponding Poincaré map. Since the stability of the periodic orbit means that the sequence of points converges to a fixed point in the phase plane, the objective system can be expressed as the following difference equation for the discrete-time systems.

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$$\tilde{x}(k+1) = A\tilde{x}(k) + Bu(k) \equiv f(\tilde{x}(k), u(k)) \tag{5}$$

where k, $\tilde{x} \in R^4$, $u \in R^1$ denote the discrete time, the state error, and the control input, respectively. And $A \in R^{4\times 4}$ is named as the error transfer matrix (ETM), $B \in R^{4\times 1}$ is called the Input Matrix.

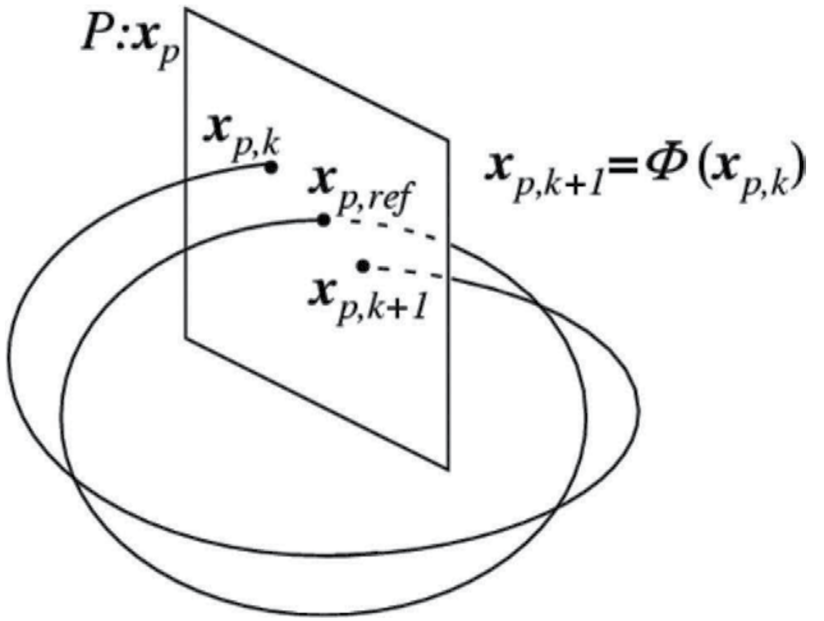

Figure 2. Poincaré map of a closed periodic trajectory.

2.2.1. *Solution for obtaining the error transfer matrix* **A**

Here, let $y_1 = \dot{x}_1$, $y_2 = \dot{x}_2$. Then the state vector of two-link gymnastic robot can be written in the following form:

$$x = (x_1, x_2, y_1, y_2) \tag{6}$$

As shown in **Figure 2**, the $(k+1)$th state vector $x_{p,k+1}$ can be calculated by one-cycle integration in accordance with the control law by defining the kth state vector passing through the section P as $x_{p,k}$.

This relationship representing this state transfer map is defined as ϕ as follows:

$$x_{p,k+1} = \phi(x_{p,k}) \tag{7}$$

If given an initial condition from which a periodic orbit can be formed, it will return to the same point after one period. Hence, the following equation holds:

$$x_{p,ref} = \phi(x_{p,ref}) \tag{8}$$

While a difference occurs in the initial state, the motion will stray away from the periodic orbit. Suppose that there was an error corresponding to $e_{p,k}$ in kth state vector, the $(k+1)$th state $x_{p,k+1}$ can be described as

$$x_{p,k+1} = \phi(x_{p,ref} + e_{p,k}). \tag{9}$$

Using the above equation's Taylor series at $e_{p,k}$ and neglecting the higher-order terms can yield

$$e_{p,k+1} = \frac{\partial \phi(x_{p,ref})}{\partial x_p} e_{p,k} \equiv A e_{p,k}. \tag{10}$$

It is obvious that $\partial \phi(x_{p,ref})/\partial x_p$ is equivalent to the ETM A defined in Eq. (5). It can be judged from this equation that if the absolute value of the ETM's eigenvalue >1, then the error increases with each cycle, and if <1, the motion will approach asymptotically the periodic orbit. However, because the state transfer mapping cannot be stated explicitly as a function, in previous studies, this ETM had been computed based on numerical differentiation. In this work, we obtained ETM with an analytical method by using variational equation.

Now consider the objective system given by the equation of motion in Eq. (3). First, given the case of $u = 0$, the objective system becomes

$$\dot{x} = f(x(t)) \equiv [f_1, f_2, f_3, f_4]^T \tag{11}$$

Assume the state x to be the following vector function

$$x(t) = \varphi(t, x) \equiv [\varphi_1, \varphi_2, \varphi_3, \varphi_4]^T, \tag{12}$$

where f_i, φ_i ($i = 1 \sim 4$) are the functions of x. The solution of equation passing through $x(0)$ at $t = 0$ is defined as follows:

$$x(0) = x_0. \tag{13}$$

Moreover, the periodic solution satisfies the following equation.

$$x(T) = x(0) = \varphi(T, x_0) \tag{14}$$

Here, a Poincaré map is defined as follows:

$$P: \begin{array}{l} \mathbf{R}^n \to \mathbf{R}^n \quad (n = 4) \\ x_0 \mapsto x_1 = P(x_0) = \varphi(T, x_0) \end{array}$$

Then, the T-period sequence of points obtained by sampling the trajectory from the initial value x_0 is

$$\{x_0, x_1, ., x_k, \dots\} = \{x_0, P(x_0), P^2(x_0), ., P^k(x_0), \dots\}. \tag{15}$$

Thus, it is obvious that the periodic solution is shown as a point passing through the same position. Substituting $x = \varphi(t, x_0)$ into Eq. (11), we obtain an equation for the variable $\varphi(t, x_0)$, which can be written as

$$\frac{d\varphi(t, x_0)}{dt} = f(\varphi(t, x_0)). \tag{16}$$

Next, taking differentiation for Eq. (16) at x_0, we can obtain

$$\frac{\partial}{\partial x_0}\left(\frac{d\varphi}{dt}(t, x_0)\right) = \frac{\partial}{\partial x_0}(f(\varphi(t, x_0))). \tag{17}$$

The differential order of the left-hand side in the above equation can be modified as

$$\frac{d}{dt}\left(\frac{\partial\varphi}{\partial x_0}(t, x_0)\right) = \frac{\partial f}{\partial x}(\varphi(t, x_0))\frac{\partial\varphi}{\partial x_0}(t, x_0) \equiv \tilde{A}(t)\frac{\partial\varphi}{\partial x_0}(t, x_0). \tag{18}$$

Thus, it becomes a time-varying linear matrix differential equation with the form of

$$\frac{dX(t, x_0)}{dt} = \tilde{A}(t)X(t, x_0), \tag{19}$$

which is called the Variational Equation if defining $X(t, x_0) = \frac{\partial\varphi}{\partial x_0}(t, x_0)$. From Eqs. (11) and (12), the above equation is equivalent to

$$\frac{d}{dt}\begin{bmatrix}\partial\varphi_1/\partial x_{i,0}\\ \partial\varphi_2/\partial x_{i,0}\\ \partial\varphi_3/\partial x_{i,0}\\ \partial\varphi_4/\partial x_{i,0}\end{bmatrix} = \begin{bmatrix}\partial f_1/\partial x_1 & \partial f_1/\partial x_2 & \partial f_1/\partial y_1 & \partial f_1/\partial y_2\\ \partial f_2/\partial x_1 & \partial f_2/\partial x_2 & \partial f_2/\partial y_1 & \partial f_2/\partial y_2\\ \partial f_3/\partial x_1 & \partial f_3/\partial x_2 & \partial f_3/\partial y_1 & \partial f_3/\partial y_2\\ \partial f_4/\partial x_1 & \partial f_4/\partial x_2 & \partial f_4/\partial y_1 & \partial f_4/\partial y_2\end{bmatrix}\begin{bmatrix}\partial\varphi_1/\partial x_{i,0}\\ \partial\varphi_2/\partial x_{i,0}\\ \partial\varphi_3/\partial x_{i,0}\\ \partial\varphi_4/\partial x_{i,0}\end{bmatrix}, \tag{20}$$

where $x_{i,0}$ refers to the solution at $t = 0$ of the ith state corresponding to the state vector x defined in Eq. (12).

Note that $X(0, x_0) = I$. Carrying out integrals in numerical integration to the above variational equations over the interval $t \in [0, T]$, one column of the matrix $X(T, x_0)$ can be obtained. Hence, repeating it four times, all of its values can be calculated. It should be emphasized here that to solve these equations since the value of $\tilde{A}(t)$ is required, however, $\tilde{A}(t)$ contains $x(t)$ in terms of the relevant time, they have to be solved together with Eq. (11) simultaneously. From Eqs. (10) and (15), it is not difficult to be verified that $X(T, x_0)$ can be regarded as ETM.

2.2.2. *Solution for obtaining the input matrix* B

Note that Eq. (3) can be rewritten into

$$\dot{x} = \tilde{f}(x,u) = f(x) + g(x)u, \tag{21}$$

where

$$g(x) = \begin{bmatrix} 0 \\ M^{-1}(x)E \end{bmatrix} \equiv \begin{bmatrix} 0 \\ 0 \\ g_3 \\ g_4 \end{bmatrix}. \tag{22}$$

The input torque u can be described as

$$u = \mathrm{rect}(t)u_0, \tag{23}$$

where

$$\mathrm{rect}(t) = \begin{cases} 1 & \text{if} \quad kT < t \le kT + \tau \quad (k = 0, 1, 2, \dots) \\ 0 & \text{otherwise} \end{cases}, \tag{24}$$

Here, u_0 is the control input during (t_0, τ), while $x = x_0$ and τ are control parameters.

Since the solution of equation at $x = x(0)$ can be stated as

$$x(t) = \varphi(t, x_0, u_0). \tag{25}$$

Define a Poincaré map as follows:

$$\tilde{P} : \begin{array}{l} \mathrm{R}^n \to \mathrm{R}^n \quad (n = 4) \\ x_0 \mapsto x_1 = P(x_0, u_0) = \varphi(T, x_0, u_0) \end{array}$$

The continuous system described by Eq. (21) will change to be a discrete system by mapping of $\tilde{P}$. Substituting $x = \varphi(t, x_0, u_0)$ into Eq. (21), the following equation for the variable $\varphi(t, x_0)$ can be obtained.

$$\frac{d\varphi(t, x_0, u_0)}{dt} = f(\varphi(t, x_0, u_0)) + g(x)\mathrm{rect}(t)u_0 \tag{26}$$

It is obvious here that by taking differentiation at x_0, its result will be equivalent to Eq. (18). Consider here the case of differentiation at u_0, which can yield

$$\frac{\partial}{\partial u_0}\left(\frac{d\varphi}{dt}(t, x_0, u_0)\right) = \frac{\partial}{\partial u_0}(f(\varphi(t, x_0, u_0))) + g(x)\mathrm{rect}(t). \tag{27}$$

The differential order of left-hand side in the above equation can also be changed.

$$\frac{d}{dt}\left(\frac{\partial\varphi}{\partial u_0}(t, x_0, u_0)\right) = \frac{\partial f}{\partial x}(\varphi(t, x_0, u_0))\frac{\partial\varphi}{\partial u_0}(t, x_0, u_0) + g(x)\mathrm{rect}(t) \tag{28}$$

Let $X(t, x_0, u_0) = \partial\varphi/\partial x_0(t, x_0, u_0)$. Similar to previous subsection, the above equation is equivalent to the following equation.

$$\frac{d}{dt}\begin{bmatrix}\partial\varphi_1/\partial u_0\\ \partial\varphi_2/\partial u_0\\ \partial\varphi_3/\partial u_0\\ \partial\varphi_4/\partial u_0\end{bmatrix} = \begin{bmatrix}\partial f_1/\partial x_1 & \partial f_1/\partial x_2 & \partial f_1/\partial y_1 & \partial f_1/\partial y_2\\ \partial f_2/\partial x_1 & \partial f_2/\partial x_2 & \partial f_2/\partial y_1 & \partial f_2/\partial y_2\\ \partial f_3/\partial x_1 & \partial f_3/\partial x_2 & \partial f_3/\partial y_1 & \partial f_3/\partial y_2\\ \partial f_4/\partial x_1 & \partial f_4/\partial x_2 & \partial f_4/\partial y_1 & \partial f_4/\partial y_2\end{bmatrix}\begin{bmatrix}\partial\varphi_1/\partial u_0\\ \partial\varphi_2/\partial u_0\\ \partial\varphi_3/\partial u_0\\ \partial\varphi_4/\partial u_0\end{bmatrix} + \text{rect}(t)\begin{bmatrix}0 & 0 & g_3 & g_4\end{bmatrix}^T \tag{29}$$

Note that $X(0, x_0, u_0) = 0$. Carrying out integrals in numerical integration to Eq. (29) over the interval $t \in [0, T]$, it is not difficult to obtain the value of the matrix $X(T, x_0, u_0)$ which can be regarded as the input matrix B defined in Eq. (5).

2.2.3. Stability of periodic orbits

Since the value of both the matrices A and B can be calculated analytically, i.e., the continuous system of two-link gymnastic robot can be expressed in a discrete model described in Eq. (5). In order to study the stabilization of gymnastic robot's continuous system by delayed feedback control, it is sufficient to consider the discrete model.

Consider the following Prediction-based feedback control:

$$u(k) = K\{x(k) - x_P(k)\}, \tag{30}$$

where $K \in R^{1\times 4}$ is a feedback gain, $x(k)$ is the state vector at k-step, $x_P(k)$ denotes one period future states of uncontrolled system which can be obtained from Eq. (3). Moreover, notice that the following almost equality holds.

$$x(k) - x_P(k) \approx \tilde{x}(k) - f(\tilde{x}(k), 0) \tag{31}$$

Here $f(\tilde{x}(k), 0)$ stands for the state error at $(k + 1)$th step. From Eq. (5), it is obvious that $f(\tilde{x}(k), 0) = A\tilde{x}(k)$ holds.

Therefore, the closed-loop system can be described by

$$\begin{aligned}\tilde{x}(k+1) &= A\tilde{x}(k) + BK(I-A)\tilde{x}(k)\\ &= \{A + BK(I-A)\}\tilde{x}(k).\end{aligned} \tag{32}$$

Let

$$\widehat{K} = K(I-A), \tag{33}$$

then the stabilization problem is reduced as follows:

Given a system Eq. (5), find a feedback gain $\widehat{K}$ that places the closed-loop poles of the system in the set

$$\Lambda = \{z \in C : |z| < 1\}. \tag{34}$$

By using the pole placement technique, it is not difficult to obtain the value of $\widehat{K}$, and if *det* $(I - A) \neq 0$, then the feedback gain K is given by

$$K = \widehat{K}(I - A)^{-1}. \tag{35}$$

Thus, the above design procedure can be applied to analyze the stability of two-link gymnastic robot system.

3. Delayed feedback control for a four-link horizontal bar gymnastic robot

As is known, the simplified two-link robot shown in the previous section is not an ideal physical model of a human gymnast on a high bar. In order to mimic gymnastic routine more realistically, the complicated robot model with higher degrees of freedom (DOF) needs to be considered. An improved method based on PDFC which control a three-link gymnastic robot via a periodic gain has been proposed [51]. In this section, the Multiprediction Delayed Feedback Control (MDFC), is extended to a more complicated gymnastic robot with four DOF.

3.1. Four-link gymnastic robot model

Figure 3 shows a four-link horizontal bar gymnastic robot model, which consists of four links and four joints. Shoulder, hips, and knees are active, while the pivot connecting the hand and bar is a passive joint. Assume m_i, l_i, a_i, $I_i (i = 1, 2, 3, 4)$ to be the link mass, length, distance from joint to its center of mass, and inertia moment around its center of mass, respectively.

The motion equation of the robot is

$$\begin{bmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \end{bmatrix} = \begin{bmatrix} M_{11} & M_{12} & M_{13} & M_{14} \\ M_{21} & M_{22} & M_{23} & M_{24} \\ M_{31} & M_{32} & M_{33} & M_{34} \\ M_{41} & M_{42} & M_{43} & M_{44} \end{bmatrix} \begin{bmatrix} \ddot{x}_1 \\ \ddot{x}_2 \\ \ddot{x}_3 \\ \ddot{x}_4 \end{bmatrix} + \begin{bmatrix} C_1 \\ C_2 \\ C_3 \\ C_4 \end{bmatrix} + \begin{bmatrix} G_1 \\ G_2 \\ G_3 \\ G_4 \end{bmatrix}, \tag{36}$$

where $\mathbf{x} = (x_1, x_2, x_3, x_4)^T \in \mathrm{R}^4$ is the generalized coordinate vector, $(u_1, u_2, u_3, u_4)^T \in \mathrm{R}^4$ is the joint torque vector, and M_{ij}, C_i, G_i $(i, j = 1, 2, 3, 4)$ are, respectively, the terms of inertia matrix, Coriolis matrix, and gravitational matrix. Each item of M_{ij}, C_i, G_i is as follows. Note that $M_{ij} = M_{ji}$, $(i \neq j)$.

$$\begin{gathered} \mathrm{M11} = m_2\left(2a_2l_1\cos(x_2) + a_2^2 + l_1^2\right) + m_3\{2a_3l_1\cos(x_2 + x_3) + 2a_3l_2\cos(x_3) \\ + a_3^2 + 2l_1l_2\cos(x_2) + l_1^2 + l_2^2\} + m_4\{2a_4l_1\cos(x_2 + x_3 + x_4) + 2a_4l_2\cos(x_3 + x_4) \\ + 2a_4l_3\cos(x_4) + a_4^2 + 2l_1l_2\cos(x_2) + 2l_1l_3\cos(x_2 + x_3) + 2l_2l_3\cos(x_3) + l_1^2 + l_2^2 + l_3^2\} \\ + a_1^2m_1 + I_1 + I_2 + I_3 + I_4; \end{gathered}$$

$$\begin{gathered} \mathrm{M12} = m_2\left(a_2l_1\cos(x_2) + a_2^2\right) + m_3\left\{a_3l_1\cos(x_2 + x_3) + 2a_3l_2\cos(x_3) + a_3^2 + l_1l_2\cos(x_2) + l_2^2\right\} \\ + m_4\left\{a_4l_1\cos(x_2 + x_3 + x_4) + 2a_4l_2\cos(x_3 + x_4) + 2a_4l_3\cos(x_4) + a_4^2 + l_1l_2\cos(x_2)\right. \\ \left. + l_1l_3\cos(x_2 + x_3) + 2l_2l_3\cos(x_3) + l_2^2 + l_3^2\right\} + I_2 + I_3 + I_4; \end{gathered}$$

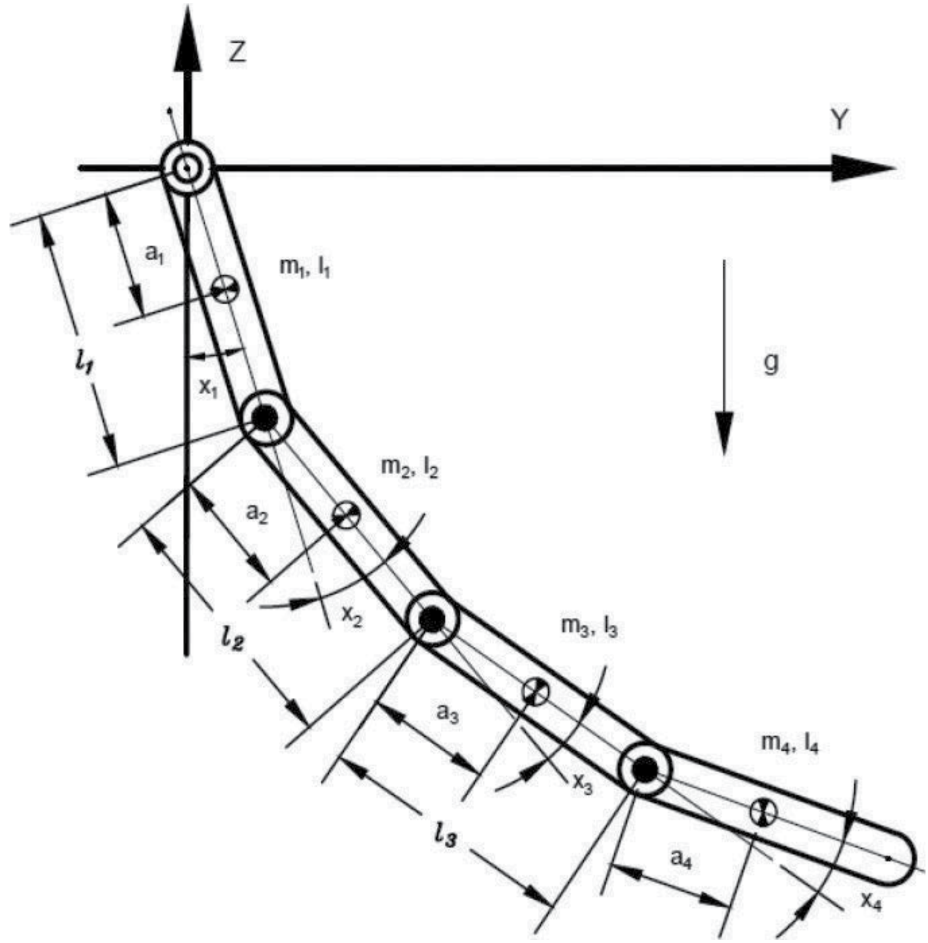

Figure 3. Four-link gymnastic robot model.

$$M13 = m_3\left(a_3l_1\cos(x_2+x_3) + a_3l_2\cos(x_3) + a_3^2\right) + m_4\{a_4l_1\cos(x_2+x_3+x_4) + a_4l_2\cos(x_3+x_4)$$
$$+2a_4l_3\cos(x_4) + a_4^2 + l_1l_3\cos(x_2+x_3) + l_3(l_2\cos(x_3) + l_3)\} + I_3 + I_4;$$

$$M14 = m_4\left(a_4l_1\cos(x_2+x_3+x_4) + a_4l_2\cos(x_3+x_4) + a_4l_3\cos(x_4) + a_4^2\right) + I_4;$$

$$M22 = m_3\left(2a_3l_2\cos(x_3) + a_3^2 + l_2^2\right) + m_4\{2a_4l_2\cos(x_3+x_4) + 2a_4l_3\cos(x_4) + a_4^2$$
$$+2l_2l_3\cos(x_3) + l_2^2 + l_3^2\} + a_2^2m_2 + I_2 + I_3 + I_4;$$

$$M23 = m_3\left(a_3l_2\cos(x_3) + a_3^2\right) + m_4\{a_4l_2\cos(x_3+x_4) + 2a_4l_3\cos(x_4) + a_4^2$$
$$+l_2l_3\cos(x_3) + l_3^2\} + I_3 + I_4;$$

$$M24 = m_4\left(a_4l_2\cos(x_3+x_4) + a_4l_3\cos(x_4) + a_4^2\right) + I_4;$$

$$M33 = m_4\left(2a_4 l_3 \cos(x_4) + a_4^2 + l_3^2\right) + a_3^2 m_3 + I_3 + I_4;$$

$$M34 = m_4\left(a_4 l_3 \cos(x_4) + a_4^2\right) + I_4;$$

$$M44 = a_4^2 m_4 + I_4;$$

$$C1 = m_3\{-a_3 l_2 \dot{q}_3\left(2\left(\dot{q}_1 + \dot{q}_2\right) + \dot{q}_3\right)\sin(x_3) - a_3 l_1\left(\dot{q}_2 + \dot{q}_3\right)\left(2\dot{q}_1 + \dot{q}_2 + \dot{q}_3\right)$$
$$\sin(x_2 + x_3) - l_1 l_2 \dot{q}_2\left(2\dot{q}_1 + \dot{q}_2\right)\sin(x_2)\} - a_2 l_1 m_2 \dot{q}_2\left(2\dot{q}_1 + \dot{q}_2\right)\sin(x_2)$$
$$+m_4\{-a_4 l_3 \dot{q}_4\left(2\left(\dot{q}_1 + \dot{q}_2 + \dot{q}_3\right) + \dot{q}_4\right)\sin(x_4) - a_4 l_2\left(\dot{q}_3 + \dot{q}_4\right)\left(2\dot{q}_1 + 2\dot{q}_2 + \dot{q}_3 + \dot{q}_4\right)$$
$$\sin(x_3 + x_4) - a_4 l_1\left(\dot{q}_2 + \dot{q}_3 + \dot{q}_4\right)\left(2\dot{q}_1 + \dot{q}_2 + \dot{q}_3 + \dot{q}_4\right)\sin(x_2 + x_3 + x_4)$$
$$+l_2 l_3 \dot{q}_3^2(-\sin(x_3)) - 2l_2 l_3\left(\dot{q}_1 + \dot{q}_2\right)\dot{q}_3 \sin(x_3) + l_2 l_3 \dot{q}_3^2(-\sin(x_3)) - 2l_2 l_3\left(\dot{q}_1 + \dot{q}_2\right)\dot{q}_3 \sin(x_3)$$

$$C2 = a_2 l_1 m_2 \dot{q}_1^2 \sin(x_2) + m_3\{a_3 l_1 \dot{q}_1^2 \sin(x_2 + x_3) - 2a_3 l_2 \dot{q}_3 \dot{q}_1 \sin(x_3) - a_3 l_2 \dot{q}_3^2 \sin(x_3)$$
$$-2a_3 l_2 \dot{q}_2 \dot{q}_3 \sin(x_3) + l_1 l_2 \dot{q}_1^2 \sin(x_2)\Big\} + m_4\{a_4 l_1 \dot{q}_1^2 \sin(x_2 + x_3 + x_4)$$
$$-2a_4 l_3 \dot{q}_4 \dot{q}_1 \sin(x_4) - 2a_4 l_2 \dot{q}_3 \dot{q}_1 \sin(x_3 + x_4) - 2a_4 l_2 \dot{q}_4 \dot{q}_1 \sin(x_3 + x_4) - a_4 l_3 \dot{q}_4^2 \sin(x_4)$$
$$-2a_4 l_3 \dot{q}_2 \dot{q}_4 \sin(x_4) - 2a_4 l_3 \dot{q}_3 \dot{q}_4 \sin(x_4) - a_4 l_2 \dot{q}_3^2 \sin(x_3 + x_4) - a_4 l_2 \dot{q}_4^2 \sin(x_3 + x_4)$$
$$-2a_4 l_2 \dot{q}_2 \dot{q}_3 \sin(x_3 + x_4) - 2a_4 l_2 \dot{q}_2 \dot{q}_4 \sin(x_3 + x_4) - 2a_4 l_2 \dot{q}_3 \dot{q}_4 \sin(x_3 + x_4) + l_1 l_2 \dot{q}_1^2 \sin(x_2)$$
$$+l_1 l_3 \dot{q}_1^2 \sin(x_2 + x_3) - 2l_2 l_3 \dot{q}_3 \dot{q}_1 \sin(x_3) - l_2 l_3 \dot{q}_3^2 \sin(x_3) - 2l_2 l_3 \dot{q}_2 \dot{q}_3 \sin(x_3)\Big\};$$

$$C3 = m_3\Big\{a_3 l_1 \dot{q}_1^2 \sin(x_2 + x_3) + a_3 l_2\left(\dot{q}_1 + \dot{q}_2\right)^2 \sin(x_3)\Big\} + m_4\{a_4 l_1 \dot{q}_1^2 \sin(x_2 + x_3 + x_4)$$
$$-2a_4 l_3 \dot{q}_4 \dot{q}_1 \sin(x_4) + a_4 l_2\left(\dot{q}_1 + \dot{q}_2\right)^2 \sin(x_3 + x_4) - a_4 l_3 \dot{q}_4^2 \sin(x_4) - 2a_4 l_3 \dot{q}_2 \dot{q}_4 \sin(x_4)$$
$$-2a_4 l_3 \dot{q}_3 \dot{q}_4 \sin(x_4) + l_1 l_3 \dot{q}_1^2 \sin(x_2 + x_3) + l_2 l_3 \dot{q}_1^2 \sin(x_3) + 2l_2 l_3 \dot{q}_2 \dot{q}_1 \sin(x_3) + l_2 l_3 \dot{q}_2^2 \sin(x_3)\Big\};$$

$$C4 = m_4\{a_4 l_1 \dot{q}_1^2 \sin(x_2 + x_3 + x_4) + a_4 l_3 \dot{q}_1^2 \sin(x_4) + 2a_4 l_3 \dot{q}_2 \dot{q}_1 \sin(x_4) + 2a_4 l_3 \dot{q}_3 \dot{q}_1 \sin(x_4)$$
$$+a_4 l_3 \dot{q}_2^2 \sin(x_4) + a_4 l_2\left(\dot{q}_1 + \dot{q}_2\right)^2 \sin(x_3 + x_4) + a_4 l_3 \dot{q}_3^2 \sin(x_4) + 2a_4 l_3 \dot{q}_2 \dot{q}_3 \sin(x_4)\};$$

$$G1 = g\{m_2(a_2 \sin(x_1 + x_2) + l_1 \sin(x_1)) + m_3(a_3 \sin(x_1 + x_2 + x_3) + l_1 \sin(x_1)$$
$$+l_2 \sin(x_1 + x_2)) + m_3(a_3 \sin(x_1 + x_2 + x_3) + l_1 \sin(x_1) + l_2 \sin(x_1 + x_2))$$
$$+l_2 \sin(x_1 + x_2) + l_3 \sin(x_1 + x_2 + x_3)) + a_1 m_1 \sin(x_1)\};$$

$$G2 = g\{m_3(a_3 \sin(x_1 + x_2 + x_3) + l_2 \sin(x_1 + x_2)) + m_4(a_4 \sin(x_1 + x_2 + x_3 + x_4)$$
$$+l_2 \sin(x_1 + x_2) + l_3 \sin(x_1 + x_2 + x_3)) + a_2 m_2 \sin(x_1 + x_2)\};$$

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$$G3 = g\{m_4(a_4 \sin(x_1 + x_2 + x_3 + x_4) + l_3 \sin(x_1 + x_2 + x_3)) + a_3 m_3 \sin(x_1 + x_2 + x_3)\};$$

$$G4 = a_4 g m_4 \sin(x_1 + x_2 + x_3 + x_4);$$

Similar to the motion equation of the two-link robot, Eq. (36) can be rewritten as follows.

$$\dot{x} = \begin{bmatrix} y \\ -M^{-1}(x)(C(x) + G(x)) \end{bmatrix} + \begin{bmatrix} 0 \\ M^{-1}(x)E \end{bmatrix} \begin{bmatrix} u_2 \\ u_3 \\ u_4 \end{bmatrix} \equiv f(x, u). \tag{37}$$

3.2. Multiprediction delayed feedback control

As is discussed in the reference [51], multiprediction delayed feedback control is based on a new discretization method to increase the control performance by introducing a notion of plural Poincaré maps, (P_i, P_2,..., P_N) which divide the first link angle $x_1 \in (-\pi, \pi)$ into N sections as shown in **Figure 4**.

By the ith ($i = 1, 2, ..., N$) Poincaré map, the four-link horizontal bar gymnastic robot system can be discretized into the following

$$x(k+1, i) = A_i x(k, i) + B_i u(k, i), \tag{38}$$

where k is the discrete time and $x(k, i)(i = 1, 2, ..., N) \in \mathrm{R}^n$, $A_i \in \mathrm{R}^{n \times n}(n = 8)$, $B_i \in \mathrm{R}^{n \times 3}$ denote, respectively, the state error, the error transfer matrix, and the input matrix in terms with the ith Poincaré map. Furthermore, $u(k, i)$ is defined as

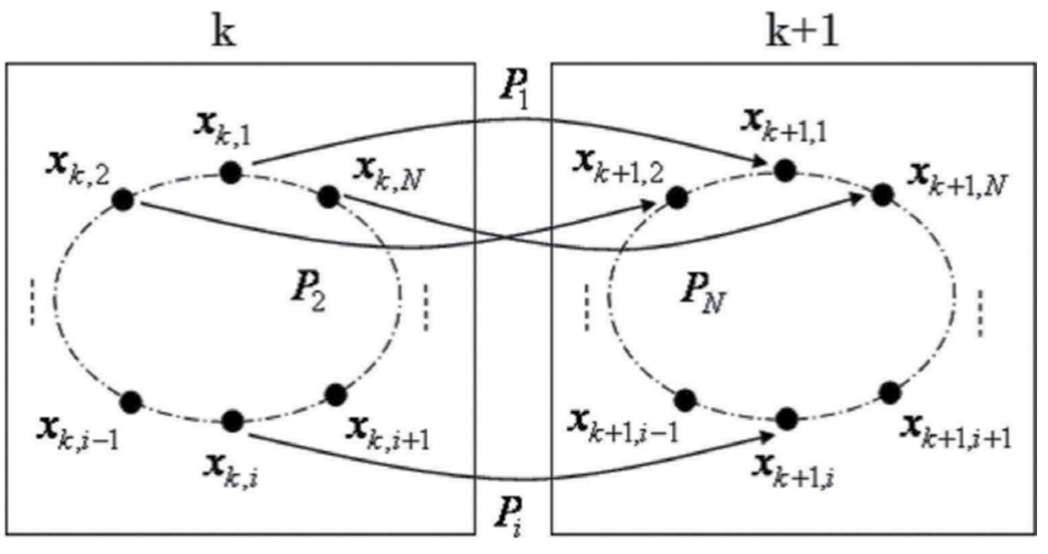

Figure 4. Image of Poincaré maps [51].

$$u(k,i) = K_i\{x(k,i) - x(k+1,i)\} = \widehat{K}_i x(k,i). \tag{39}$$

Here, the equivalence of $\widehat{K}_i \equiv K_i(I - A_i)$ and $K_i = K_{i+N} \in \mathrm{R}^{3\times n}$ are satisfied for each i. By introducing the variable of control period, τ, and defining u_0 as the control input to the system during (t_0, τ) while $x = x_0$, the input torque u is described as

$$u = \mathrm{rect}(t)u_0, \tag{40}$$

where rect(t) is a rectangular function as Eq. (41).

$$\mathrm{rect}(t) = \begin{cases} 1 & \text{if} \quad (kT + t_i) < t \leq (kT + t_i + \tau) \quad (k = 0, 1, 2, \ldots) \\ 0 & \text{otherwise} \end{cases} \tag{41}$$

Here, t_i is the time at ith Poincaré map $P_i(i = 1, 2, \ldots, N)$.

Summarize the state variables at each one of the ith Poincaré section into one vector as follows:

$$X(k,i) = [x(k,i), \ldots, x(k,N), x(k+1,1), \ldots, x(k+1,i-1)]^T \in \mathrm{R}^{nN} \tag{42}$$

Therefore, the close-loop system relating to X(k, i) can be stated as the following discrete-time system with periodic N.

$$X(k, i+1) = F(i)X(k,i), \tag{43}$$

where,

$$F(i) = \begin{bmatrix} 0 & I & \ldots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \ldots & 0 & I \\ A_i + B_iK_i & 0 & \ldots & 0 & 0 \end{bmatrix}. \tag{44}$$

As it is known, the local stability of such a system can be determined by the eigenvalue of the monodromy matrix as follows:

$$\Phi_F(i+N, i) \equiv F(i+N-1) \cdots F(i+1)F(i). \tag{45}$$

The solution of the error transfer matrix A_i and the input matrix B_i is similar to the determination of the two-link gymnastic robot, so only the difference is shown below.

3.3. Solution for obtaining the error transfer matrix A_i

Here, let $y_1 = \dot{x}_1$, $y_2 = \dot{x}_2$, $y_3 = \dot{x}_3$, $y_4 = \dot{x}_4$. Then the state vector of four-link gymnastic robot becomes

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$$x = (x_1, x_2, x_3, x_4, y_1, y_2, y_3, y_4). \tag{46}$$

Consider the objective system given by the equation of motion in Eq. (37). First, given the case of $u = 0$, the objective system becomes

$$\dot{x} = f(x(t)) \equiv [f_1, f_2, f_3, f_4, f_5, f_6, f_7, f_8]^T \tag{47}$$

Assume the state x to be the following vector function

$$x(t) = \varphi(t, x) \equiv [\varphi_1, \varphi_2, \varphi_3, \varphi_4, \varphi_5, \varphi_6, \varphi_7, \varphi_8]^T. \tag{48}$$

where $f_{\tilde{\imath}}$, $\varphi_{\tilde{\imath}}(\tilde{\imath} = 1 \sim 8)$ are the functions of x. Introducing the following definition,

$$\begin{gathered} \varphi^m_{x_{\tilde{i},0}} = \frac{\partial \varphi_m}{\partial x_{\tilde{i},0}} \quad (\tilde{i} = 1\sim 8), \\ f^m_{x_j} = \frac{\partial f_m}{\partial x_j}, \quad f^m_{y_j} = \frac{\partial f_m}{\partial y_j} \quad (m = 1\sim 8, j = 1\sim 4) \end{gathered} \tag{49}$$

the variational equation becomes

$$\frac{d}{dt}\begin{bmatrix} \varphi^1_{x_{\tilde{i},0}} \\ \varphi^2_{x_{\tilde{i},0}} \\ \varphi^3_{x_{\tilde{i},0}} \\ \varphi^4_{x_{\tilde{i},0}} \\ \varphi^5_{x_{\tilde{i},0}} \\ \varphi^6_{x_{\tilde{i},0}} \\ \varphi^7_{x_{\tilde{i},0}} \\ \varphi^8_{x_{\tilde{i},0}} \end{bmatrix} = \begin{bmatrix} f^1_{x_1} & f^1_{x_2} & f^1_{x_3} & f^1_{x_4} & f^1_{y_1} & f^1_{y_2} & f^1_{y_3} & f^1_{y_4} \\ f^2_{x_1} & f^2_{x_2} & f^2_{x_3} & f^2_{x_4} & f^2_{y_1} & f^2_{y_2} & f^2_{y_3} & f^2_{y_4} \\ f^3_{x_1} & f^3_{x_2} & f^3_{x_3} & f^3_{x_4} & f^3_{y_1} & f^3_{y_2} & f^3_{y_3} & f^3_{y_4} \\ f^4_{x_1} & f^4_{x_2} & f^4_{x_3} & f^4_{x_4} & f^4_{y_1} & f^4_{y_2} & f^4_{y_3} & f^4_{y_4} \\ f^5_{x_1} & f^5_{x_2} & f^5_{x_3} & f^5_{x_4} & f^5_{y_1} & f^5_{y_2} & f^5_{y_3} & f^5_{y_4} \\ f^6_{x_1} & f^6_{x_2} & f^6_{x_3} & f^6_{x_4} & f^6_{y_1} & f^6_{y_2} & f^6_{y_3} & f^6_{y_4} \\ f^7_{x_1} & f^7_{x_2} & f^7_{x_3} & f^7_{x_4} & f^7_{y_1} & f^7_{y_2} & f^7_{y_3} & f^7_{y_4} \\ f^8_{x_1} & f^8_{x_2} & f^8_{x_3} & f^8_{x_4} & f^8_{y_1} & f^8_{y_2} & f^8_{y_3} & f^8_{y_4} \end{bmatrix} \begin{bmatrix} \varphi^1_{x_{\tilde{i},0}} \\ \varphi^2_{x_{\tilde{i},0}} \\ \varphi^3_{x_{\tilde{i},0}} \\ \varphi^4_{x_{\tilde{i},0}} \\ \varphi^5_{x_{\tilde{i},0}} \\ \varphi^6_{x_{\tilde{i},0}} \\ \varphi^7_{x_{\tilde{i},0}} \\ \varphi^8_{x_{\tilde{i},0}} \end{bmatrix}, \tag{50}$$

where $x_{\tilde{\imath},0}$ refers to the solution at $t = 0$ of the $\tilde{\imath}$th state corresponding to the state vector x defined in Eq. (48).

Note that the following equation holds.

$$\begin{gathered} A = [a_1 \quad a_2 \quad a_3 \quad a_4 \quad a_5 \quad a_6 \quad a_7 \quad a_8] \\ a\tilde{i} = \left[\varphi^1_{x_{\tilde{i},0}}, \quad \varphi^2_{x_{\tilde{i},0}}, \quad \varphi^3_{x_{\tilde{i},0}}, \quad \varphi^4_{x_{\tilde{i},0}}, \quad \varphi^5_{x_{\tilde{i},0}}, \quad \varphi^6_{x_{\tilde{i},0}}, \quad \varphi^7_{x_{\tilde{i},0}}, \quad \varphi^8_{x_{\tilde{i},0}}\right]^T (\tilde{i} = 1\sim 8)., \end{gathered} \tag{51}$$

Carrying out integrals in numerical integration to the variational equations of Eq. (50) over the interval $t \in [0, T]$ by eight times, each item of the error transfer matrix, $A_i(i = 1, 2,..., N)$, can be calculated.

3.4. Solution for obtaining the input matrix B_i

Note that Eq. (37) can be rewritten as

$$\dot{x} = \tilde{f}(x, u) = f(x) + g(x)u. \tag{52}$$

Here,

$$g(x) = \begin{bmatrix} 0_{4\times3} \\ M^{-1}(x)E \end{bmatrix} \equiv \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \\ g_{12} & g_{13} & g_{14} \\ g_{22} & g_{23} & g_{24} \\ g_{32} & g_{33} & g_{34} \\ g_{42} & g_{43} & g_{44} \end{bmatrix}. \tag{53}$$

Since the solution of equation at $x = x(0)$ can be written as

$$x(t) = \varphi(t, x_0, u_0). \tag{54}$$

The continuous system described by Eq. (53) will change to be a discrete system by mapping of $\tilde{P}_i$. Substituting Eq. (54) into Eq. (53), the following equation for the variable $\varphi(t, x_0)$ can be obtained.

$$\frac{d\varphi(t, x_0, u_0)}{dt} = f(\varphi(t, x_0, u_0)) + g(x)\,\mathrm{rect}\,(t)u_0 \tag{55}$$

Here, consider the case of differentiation at u_0, which can yield

$$\frac{\partial}{\partial u_0}\left(\frac{d\varphi}{dt}(t, x_0, u_0)\right) = \frac{\partial}{\partial u_0}(f(\varphi(t, x_0, u_0))) + g(x)\,\mathrm{rect}\,(t). \tag{56}$$

Let

$$\varphi^m_{u_{j,0}} = \frac{\partial \varphi_m}{\partial u_{j,0}} \quad (m = 1\sim8, j = 2, 3, 4). \tag{57}$$

Similar to previous subsection, Eq. (53) is equivalent to the following equation.

$$\frac{d}{dt}\begin{bmatrix} \varphi^1_{u_{j,0}} \\ \varphi^2_{u_{j,0}} \\ \varphi^3_{u_{j,0}} \\ \varphi^4_{u_{j,0}} \\ \varphi^5_{u_{j,0}} \\ \varphi^6_{u_{j,0}} \\ \varphi^7_{u_{j,0}} \\ \varphi^8_{u_{j,0}} \end{bmatrix} = \begin{bmatrix} f^1_{x_1} & f^1_{x_2} & f^1_{x_3} & f^1_{x_4} & f^1_{y_1} & f^1_{y_2} & f^1_{y_3} & f^1_{y_4} \\ f^2_{x_1} & f^2_{x_2} & f^2_{x_3} & f^2_{x_4} & f^2_{y_1} & f^2_{y_2} & f^2_{y_3} & f^2_{y_4} \\ f^3_{x_1} & f^3_{x_2} & f^3_{x_3} & f^3_{x_4} & f^3_{y_1} & f^3_{y_2} & f^3_{y_3} & f^3_{y_4} \\ f^4_{x_1} & f^4_{x_2} & f^4_{x_3} & f^4_{x_4} & f^4_{y_1} & f^4_{y_2} & f^4_{y_3} & f^4_{y_4} \\ f^5_{x_1} & f^5_{x_2} & f^5_{x_3} & f^5_{x_4} & f^5_{y_1} & f^5_{y_2} & f^5_{y_3} & f^5_{y_4} \\ f^6_{x_1} & f^6_{x_2} & f^6_{x_3} & f^6_{x_4} & f^6_{y_1} & f^6_{y_2} & f^6_{y_3} & f^6_{y_4} \\ f^7_{x_1} & f^7_{x_2} & f^7_{x_3} & f^7_{x_4} & f^7_{y_1} & f^7_{y_2} & f^7_{y_3} & f^7_{y_4} \\ f^8_{x_1} & f^8_{x_2} & f^8_{x_3} & f^8_{x_4} & f^8_{y_1} & f^8_{y_2} & f^8_{y_3} & f^8_{y_4} \end{bmatrix}\begin{bmatrix} \varphi^1_{u_{j,0}} \\ \varphi^2_{u_{j,0}} \\ \varphi^3_{u_{j,0}} \\ \varphi^4_{u_{j,0}} \\ \varphi^5_{u_{j,0}} \\ \varphi^6_{u_{j,0}} \\ \varphi^7_{u_{j,0}} \\ \varphi^8_{u_{j,0}} \end{bmatrix} + \mathrm{rect}\,(t) \times \begin{bmatrix} 0 & 0 & 0 & 0 & g_{1j} & g_{2j} & g_{3j} & g_{4j} \end{bmatrix}^T \tag{58}$$

Note that the following equation holds.

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$$B = [b_1 \quad b_2 \quad b_3],$$
$$b_{\tilde{i}} = \left[\varphi^1_{u_j,0}, \quad \varphi^2_{u_j,0}, \quad \varphi^3_{u_j,0}, \quad \varphi^4_{u_j,0}, \quad \varphi^5_{u_j,0}, \quad \varphi^6_{u_j,0}, \quad \varphi^7_{u_j,0}, \quad \varphi^8_{u_j,0}\right]^T (\tilde{i} = 1, 2, 3). \tag{59}$$

Carrying out integrals in numerical integration to Eq. (58) over the interval $t \in [0, T]$ by three times, it is not difficult to obtain the value of the input matrix $B_i(i = 1, 2,..., N)$.

4. Numerical simulations

This section shows some simulation results to verify the validity of the proposed prediction-based delayed feedback control for a two-link horizontal bar gymnastic robot. The parameters of the robot model are shown in **Table 1**. The stability of giant swing motion with period $T = 0.7$(s) was examined.

		1st link	2nd link
Mass	m_i (kg)	39.5	20.7
Moment of inertia	I_i (kgm^2)	3.25	1.56
Link length	l_i (m)	1.2	0.879
Offset of mass center	a_i (m)	0.756	0.377

Table 1. Link parameter values.

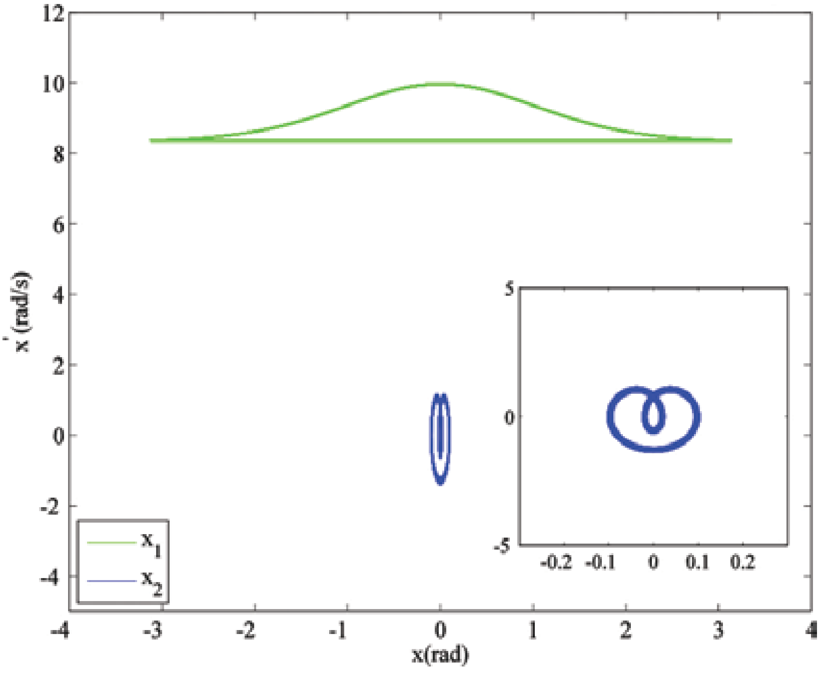

Figure 5. Phase portrait of X–$\dot{x}$ (no error).

By means of the shooting method, an initial condition was obtained such as $x(0) = (\pi, 0.0, 8.352, -1.19)$ that can achieve a free giant swing motion with a period of 0.7(s). During the first 30 s starting from this initial condition, the phase portrait of the uncontrolled system is depicted in **Figure 5** in the phase plane $(X, \dot{x})$ which refers to the angle and angular velocity of the link, respectively. It can be seen from **Figure 5** that the ideal phase plane orbit of the giant swing motions traces out a closed curve.

To see the stability of periodic orbits via delayed feedback control, numerical simulation was exercised from the initial condition $x(0) = (\pi, 0.1, 9.252, -2.39)$ that contained errors. First, consider the uncontrolled case, the 30 s trajectory of the orbits in the phase plane filled up a section of the phase space as in **Figure 6**. It can be confirmed that there was no periodicity without control.

Next, consider the system controlled by the proposed method, with which the error transfer matrix A was obtained as follows:

$$A = \begin{bmatrix} 1.0054 & 0.0521 & 0.5986 & 0.0954 \\ -0.0377 & 0.7685 & -0.1017 & 0.0210 \\ 0.2982 & 1.8534 & 1.0041 & 0.0399 \\ -1.7310 & -10.6479 & -0.0170 & 0.7728 \end{bmatrix}.$$

The input matrix B in the case of $\tau = 10$(ms) is obtained as follows:

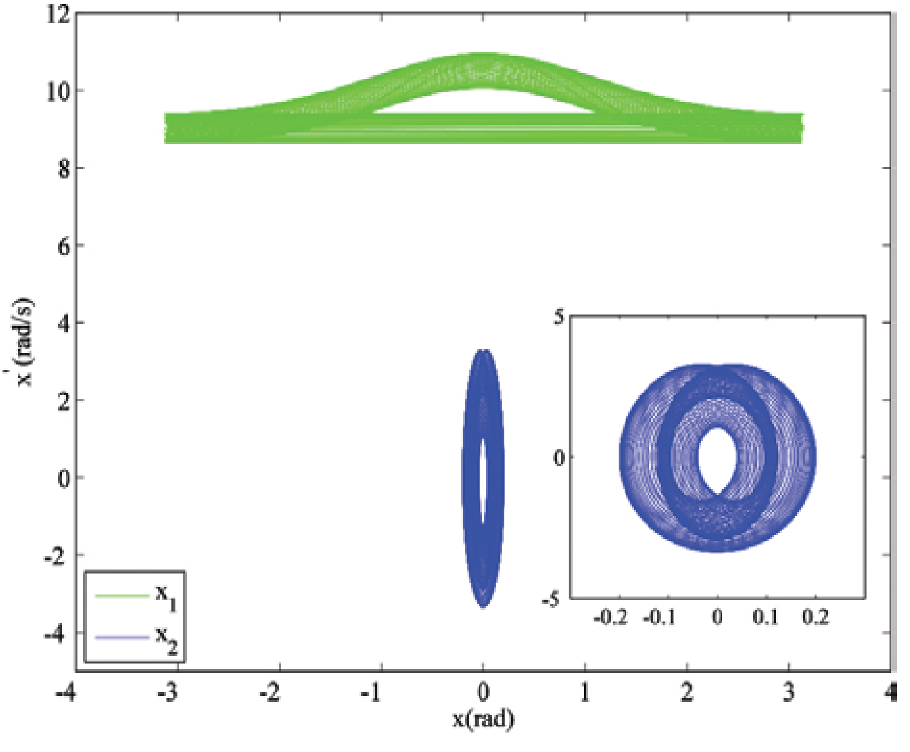

Figure 6. Phase portrait of X–$\dot{x}$ (with error).

$$B = \begin{bmatrix} -0.000167 \\ 0.000552 \\ -0.004464 \\ 0.024859 \end{bmatrix}.$$

Based on the value of the matrix A and B shown in the above, the feedback gain K was obtained by assigning all of its poles of the system matrix $A + B\widehat{K}$ in the unit disk. Generally, in a linear system, the poles of the system matrix $A + B\widehat{K}$ are assigned as close as possible to the origin in order to decrease the convergence time; however, in such a nonlinear system as gymnastic robot, it is found that it becomes to show the divergence while the poles of $A + B\widehat{K}$ is in the disk with ratio equals 0.6 approximately. Here, two cases were studied by assigning the poles larger than 0.6 as follows.

$$\begin{cases} Case\ I: & pole = (0.75, 0.73, 0.71, 0.69), \quad K = (-2242.7, -128.82, 48526, 8447.7), \\ Case\ II: & pole = (0.90, 0.88, 0.835, 0.815), \quad K = (-206.94, 354.01, 1577.1, 296.42). \end{cases}$$

In Case I, the numerical simulation results via calculated feedback gain K are shown in **Figure 7**. **Figure 7(a)** and **(b)** show the trajectory of the orbits in the phase plane (x, $\dot{x}$), of which **Figure 7(a)** depicts the trajectory of the first 50 s, while **Figure 7(b)** plots that of 50 ~ 60

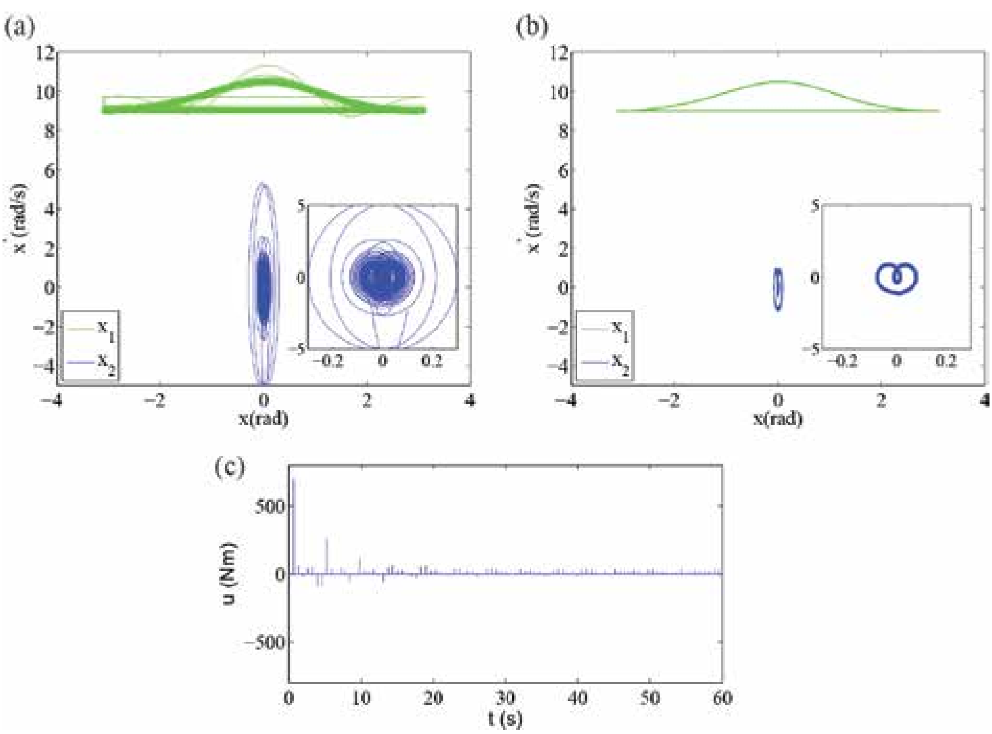

Figure 7. Phase portrait and joint torque (Case I): (a) Phase portrait of X–$\dot{x}$(t=0~50s); (b) Phase portrait of X–$\dot{x}$ (t=50~60s); (c) Joint torque.

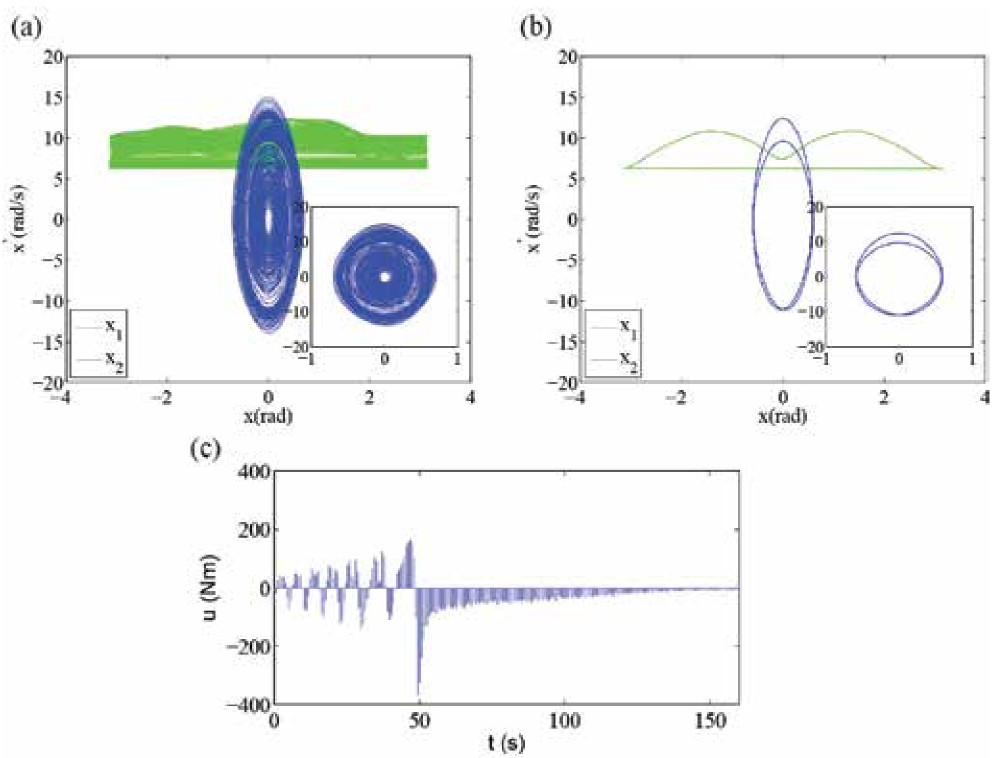

Figure 8. Phase portrait and joint torque (Case II): (a) Phase portrait of X–$\dot{x}$ (t=0~150s); (b) Phase portrait of X–$\dot{x}$ (t=150~160s); (c) Joint torque.

(s). Meanwhile, the time history of control input is shown in **Figure 7(c)** from which it can be seen that the control input diminished with time. It is obvious that from **Figure 7(c)**, the control input u began to vanish from about t = 30(s), and from **Figure 7(b)** the periodicity began to appear from approximately t = 50(s).

However, on further analysis conducted, it was found that one can change the type of giant swing type by changing the pole placement of the matrix $A + B\widehat{K}$. This phenomenon is shown in **Figure 8** which depicts the change histories of link angle, angular velocity, and input control with 160 s in Case II. The first 150 s trajectory of the orbits in the phase plane $(x, \dot{x})$ is depicted in **Figure 8(a)** and the remaining is shown in **Figure 8(b)**. Moreover, the time history of input torque is shown in **Figure 8(c)**.

It could be said that in Case II, the proposed method showed the ability of controlling the giant-swing motion to an unknown periodic orbit, which is known as one of the advantages of delayed feedback control.

Moreover, **Figures 9** and **10** depict the stick diagrams based on one period data after the giant swing motion converging to a stable orbit in Case I and Case II, in which the figures of (a), (b),

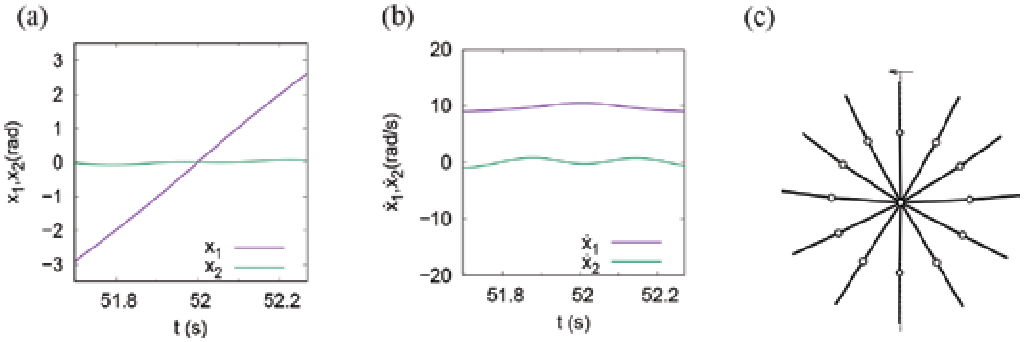

Figure 9. Angle, angular velocity, and stick (Case I).

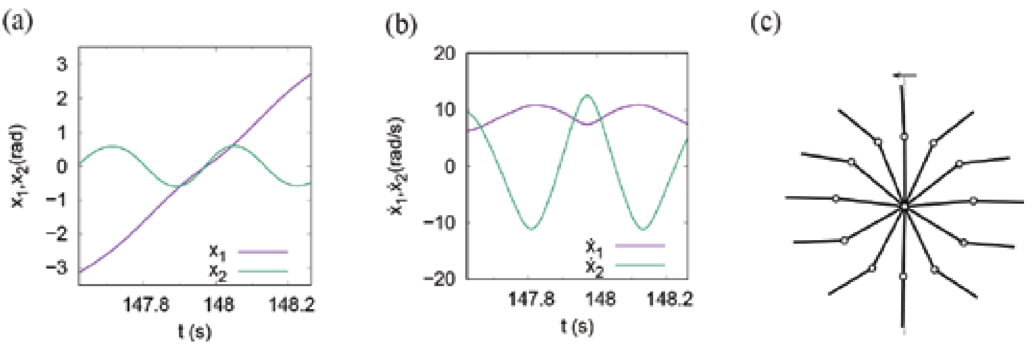

Figure 10. Angle, angular velocity, and stick (Case II).

and (c) plot, respectively, the angle, angular velocity, and stick figure. From the above two figures, it can be seen that the difference between the assigned poles caused periodic giant swing motion to change to a different type.

5. Conclusion

This chapter studied the behavior of the giant swing motions of a two-link and a four-link horizontal bar gymnastic robot systems via delayed feedback control. First, it has been discussed as a solution to calculate analytically the error transfer matrix and the input matrix by which the stability of DFC for the original two-link gymnastic robot system is equivalent to that of the corresponding discrete system. Moreover, it was introduced as a method by which a feedback gain to ensure the stability of original system can be determined. Second, a modified DFC method, MDFC, has been extended to a four-link gymnastic robot. Plural Poincaré maps were defined so that the stability of the close-loop system can be evaluated based on the theory of monodromy matrix. Finally, the simulation results showed its effectiveness.

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Quantitative Methods in System-Based Drug Discovery

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Additional information is available at the end of the chapter

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Abstract

Modern pharmaceutical industries have faced significant challenges to deliver safe and effective medicines because of significant toxicity and severe side effects of discovered drugs. On the other hand, recent developments and advances in system-based pharmacology aim to address these challenges. In this chapter, we provide an overview of quantitative methods for system-based drug discovery. System-based drug discovery integrates chemical, molecular, and systematic information and applies this knowledge to the designing of small molecules with controlled toxicity and minimized side effects. First, we discuss current approaches for drug discovery and outline their advantages and disadvantages. Next, we introduce basic concepts of systems pharmacology with an emphasis on ligand-based drug discovery and target identification. This is followed by a discussion on structure-based drug design and statistical tools for pharmaceutical research. Finally, we provide an overview of future directions in systems pharmacology that will guide further developments.

Keywords: systems pharmacology, drug discovery, chemoinformatics

1. Introduction

The discovery of effective medicines has been a long-term human endeavor aimed at curing illnesses and improving physiological conditions. Early drug discovery methods often relied on serendipitous findings. For example, penicillin, a substance released by mold, was accidentally discovered to inhibit bacterial growth. However, with the advances of molecular cloning techniques, X-ray crystallography, robotics, and computational aided technology, drugs can now be rationally designed. Additionally, the marriage of combinatorial chemistry and robotics has also created a new drug discovery approach called "high-throughput screening." In a high-throughput screening campaign, a library consisting of millions of molecules is tested against a disease-relevant target to identify potential drug candidates.

However, the application of modern drug discovery methods has not directly translated into increases in the output of new drugs. Although many of these "designer" drugs have been optimized for binding and specificity, they are all low-weight molecular ligands and are likely to interact with multiple off-targets, which contribute to severe side effects in patients taking these medicines. Consequently, a system drug discovery approach that simultaneously optimizes drug binding, target promiscuity, and safety profile has been proposed. In particular, "poly-pharmacology" is a new drug discovery paradigm that aims to study the interactions of many drugs to many targets as many body problems. The binding profile of a compound can be used to modify a ligand structure to maximize on-target binding while minimizing off-target interactions. More recently, "structural poly-pharmacology" has also been proposed, which utilizes the structural data of proteins or drugs to gain a mechanistic understanding of drug action and side effects [1, 2].

System-based drug discovery can be classified as ligand-based and structure-based drug discovery approaches. In the ligand-based drug discovery approach, ligand structure information takes center stage, and only ligand information is used to derive its multitude of chemical and biological properties. On the other hand, the structure-based approach utilizes the structure of the receptor to identify shape-complementary ligands with optimal interactions. Given a validated disease target with a known crystal structure, the structure-based approach can be utilized to discover ligands that bind to the receptor of interest. On the other hand, the ligand-based approach is useful when the target structure is unknown or when the crystal structure of the target is difficult to obtain. In some cases, the system-based drug discovery approach combines both ligand-based and structure-based approaches to facilitate the drug design and discovery process [3].

2. Ligand-based approaches to drug design

2.1. Introduction

Ligand-based drug design, also known as "knowledge-based" drug design, extracts essential chemical features from drugs to construct a learning model to predict drug properties. It has been proposed that a ligand structure contains all the necessary information to accurately infer its mechanism of action. Several chemical descriptors such as molecular weight and lipophilicity are predictors of important pharmacodynamic and pharmacokinetic properties of ligands. A well-known example is Lipinski's rule of five, which describes a set of chemical properties and rules that can be used to differentiate drugs from nondrug molecules [4]. Likewise, the chemical similarity principle has been widely applied in similarity-based drug design. The chemical similarity principle assumes that if two molecules share similar structures, then they will likely have similar biological properties [5]. This concept is the underlying principle of modern chemical database search techniques used to identify similar compounds with improved bioactivities.

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2.2. Outline of ligand-based drug design

The chemical similarity search is an established approach for ligand-based drug discovery. Given a compound with known biological properties, it is possible for a drug designer to identify similar compounds with improved biological properties. To compare two ligand structures, it is essential to develop appropriate data structure representations for chemical structure comparisons. Mathematically, the chemical structure can be represented by graphs where atoms represent vertices and edges represent chemical bonds [6]. Several chemoinformatics algorithm can be used to extract essential characteristic from the chemical graph such as the number of vertices, the number of bonds, path, connectivity, and others. These properties then become chemical features that can be used in feature engineering using complex machine learning techniques for similarity comparison.

The most direct chemical search approach is the nearest neighbor where the chemical feature of a ligand, also known as a "chemical fingerprint," is used to search a compound database to identify the most similar compounds using a predefined distance measure [7]. The most commonly used chemical fingerprints include path-based and substructure-based fingerprints. Using path-based fingerprints, such as Daylight fingerprints or Obabel FP2 fingerprints, potential paths at different bond lengths in a molecular graph of a molecule are used as features for the similarity comparison. On the other hand, substructure-based fingerprints such as MACCS keys use predefined substructures and characterize each molecule based on the presence or absence of a particular substructure using a binary array. Overall, path-based fingerprints offer higher search specificity due to the unique path dependency of the molecular graph. However, substructure-based fingerprints can be used to identify scaffold hopping ligands since the fingerprints do not impose requirements on the connectivity of the scaffolds and functional groups [8]. To quantify the chemical similarity between two fingerprints, several distance metrics have been proposed. The most commonly used chemical similarity metric is the Tanimoto index, which computes the shared feature bits between two fingerprints in the range of 0–1. Although there is no predefined threshold to define the similarity level, a value of 0.7–0.8 has been commonly adapted in many chemical similarity search programs.

2.3. Ligand-based drug design (LBDD) process

The similarity-based drug design process is as follows (**Figure 1**):

1. The target molecule is used as a query for the chemical search.
2. Similar ligands with similar biological properties are identified.
3. Original ligands are modified to suggest new molecules with improved activities.

The advantages of LBDD are as follows:

1. Does not necessitate receptor structures.
2. Low computational intensity and fast database searching.
3. Allows for large-scale similarity drug design and target prediction.

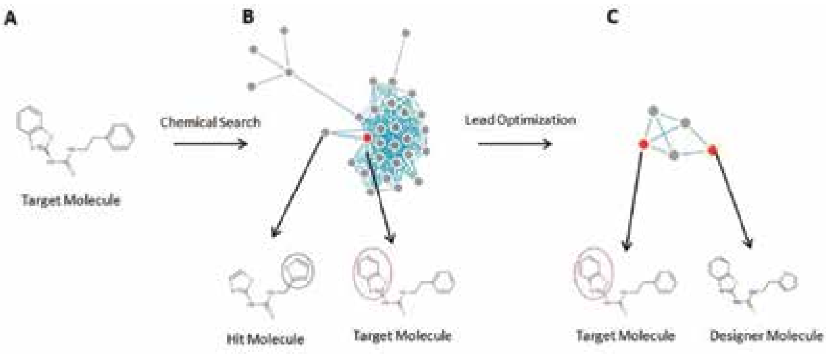

Figure 1. Ligand-based drug design (LBDD) process.

2.4. Target prediction of drugs

While similarity-based methods are prevalently applied in modern drug discovery programs as an efficient way to transition a hit to a lead, the molecular mechanism of the drug is often unknown, and the adverse reaction cannot be predicted. Consequently, drug-target prediction becomes an important follow-up step. Drug-target prediction can be classified as ligand-based or structure-based methods [9]. In ligand-based target prediction, the molecular target of a drug can be inferred from the target-annotated ligand sharing the highest chemical similarity. Chemical bioactivity databases such as ChEMBL, PubChem and DrugBank, and BindingDB have been developed for this application [10]. However, one major limitation of ligand-based target prediction is that there is no natural cutoff for chemical similarity that clearly defines biological similarity, also known as bioactivity cliffs. Approaches such as similarity ensemble approach (SEA) aim to remedy this by calculating similarity values against a random background using an algorithm similar to BLAST [11]. On the other hand, structure-based target prediction methods identify molecular targets based on the structure of the receptor binding sites. For example, panel docking is a common structure-based approach to identify the most probable target based on the docking score. Alternatively, binding site similarity methods that compare the receptor environment of the target ligand to a database of receptor pockets have also proven to be an effective target prediction approach [12].

More recently, network poly-pharmacology has been proposed as a more comprehensive approach to analyze drug-target interactions. Network pharmacology goes beyond the one drug one target hypothesis to multiple drugs multiple targets hypothesis [13]. The goal of this new paradigm is not only to accurately identify on-targets but also other off-targets. One such approach is the drug-target network, which utilizes a bipartite network to analyze complex drug gene interactions. Alternatively, drug-drug networks or chemical similarity networks have also been proposed [8]. The chemical similarity network clusters drugs based on their structure similarity. This approach can be applied for large-scale compound analysis by clustering diverse chemical structures into distinct scaffolds known as chemotypes. Consequently, each chemotype can be correlated with specific molecular targets. Using a consensus statistics scheme similar to that used for functional prediction in protein-protein interaction networks, chemical similarity networks have proven useful for target identification from chemical screening campaigns. In addition, structural poly-pharmacology has also gained substantial attention due to the possibility of correlating structural variations to clinical side effects. One example is CSNAP3D, which uses 3D ligand structure similarity to identify simplified scaffold hopping compounds of complex natural products to suggest new drugs with improved pharmacokinetic properties [1].

2.5. Side effect prediction of drugs

Since severe clinical side effects have contributed to drug failure in the late stages of clinical trials, side effect prediction will need to become an integrated part of the drug design process. Knowing the binding affinity of a drug to an array of proteins makes it possible to predict side effects using several statistical methods such as canonical component analysis (CCA), which identify a set of parameters that optimize the correlation between drug binding features and side effect features [14]. In addition, side effect predictions based on chemoinformatics analysis of the compound structures have also been developed. Many of these approaches provide an accurate prediction of the drug side effects and have been applied in the early stages of clinical drug development.

3. Structure-based approaches to drug design

Modern medicinal chemistry methods and molecular modeling have been employed as powerful tools for the study of structure-activity relationships (SAR) [15]. Structure-based drug design is a drug discovery approach by which synthetic compounds are designed from detailed structural knowledge of the active sites of protein targets associated with particular diseases. This field has involved the integrated application of traditional biology and medicinal chemistry along with advances in biomolecular spectroscopic methods such as X-ray crystallography, nuclear magnetic resonance (NMR), combinatorial chemistry, computer modeling of molecular structure, and protein biophysical chemistry, to focus on the three-dimensional molecular structure and active site characterization of the proteins that control cellular biology. Structure-based drug design is an improvement over traditional drug screening techniques. By identifying the target protein in advance and by discovering the chemical and molecular structure of the protein, it is possible to design a more optimal drug to interact with the protein.

3.1. Basic concept of structure-based drug design

Enzymes are a subset of receptor-like proteins that are directly responsible for catalyzing the biochemical reactions that sustain life. For example, digestive enzymes act to break down the nutrients of our diet. DNA polymerase and related enzymes are crucial for cell division and replication. Enzymes are genetically programmed to be specific for their appropriate molecular targets. Any errors could have grave consequences. Enzymes ensure the specificity of their targets by forming a molecular environment that excludes interactions with inappropriate molecules. The analogy most often mentioned is that of a lock and key. The enzyme is a molecular lock, which contains a keyhole that exhibits a very specific and consistent size and shape. This molecular keyhole is termed the active site of the enzyme and allows interaction with only the appropriate molecular targets. Just as a typical lock is much bigger than the keyhole, the receptor is usually much larger than the active site. The receptor, as specified by our DNA, is a folded protein whose major purpose is to form and maintain the size and shape of the active site.

The most important concept in drug design is to understand the methods by which the active site of the receptor selectivity restricts the binding of inappropriate structures. Any potential molecules that can bind to a receptor are called ligands. In order for a ligand to bind, it must contain a specific combination of atoms that present the correct size, shape, and charge composition needed to bind and interact with the receptor. In brief, the ligand must possess the molecular key that binds the receptor lock.

Computer-aided drug design has played an important role in drug discovery and drug development and has become an indispensable tool in the drug industry. For the purposes of discovering and optimizing biologically active compounds, various types of computer-aided drug design software and resources have been used by computational medicinal chemists. Unsurprisingly, many chemical compounds were discovered and optimized by computer-aided drug design methodologies and have reached the late stages of clinical trials.

3.2. Outline of structure-based drug design

Structure-based drug design is a cyclic process which consists of stepwise procedures (**Figure 2**). It begins with a known target structure, and then, *in silico* studies are conducted in order to identify potential ligands. These molecular modeling procedures are followed by the synthesis of the most promising compounds [16]. Next, using diverse experimental platforms, biological properties such as potency, affinity, and efficacy are evaluated [17]. In the end, given that active compounds are identified, the three-dimensional structure of the ligand-receptor complex can be solved. The available structure allows the visualization of the intermolecular features that support the process of molecular recognition. Structural descriptions of ligand-receptor complexes are useful for the investigation of binding conformations, characterization of key intermolecular interactions, characterization of unknown binding sites, mechanistic studies, and the elucidation of ligand-induced conformational changes [18].

3.3. Process of structure-based drug design (SBDD)

The structure-based drug design process is as follows:

1. An enzyme that is important in a particular pathological condition is chosen.
2. The three-dimensional structure of the active site of the enzyme is determined, often by X-ray crystallography.
3. A chemical is prepared to fit the active site of the enzyme, which can alter the properties of the enzyme, that is, inactivate the enzyme.

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The advantages of structure-based drug design are as follows:

1. Useful results are obtained faster than by traditional drug design methods.

2. The process is less expensive than other drug design methods.

3. The compounds are more specific for the active site and potentially less toxic than compounds prepared by other approaches.

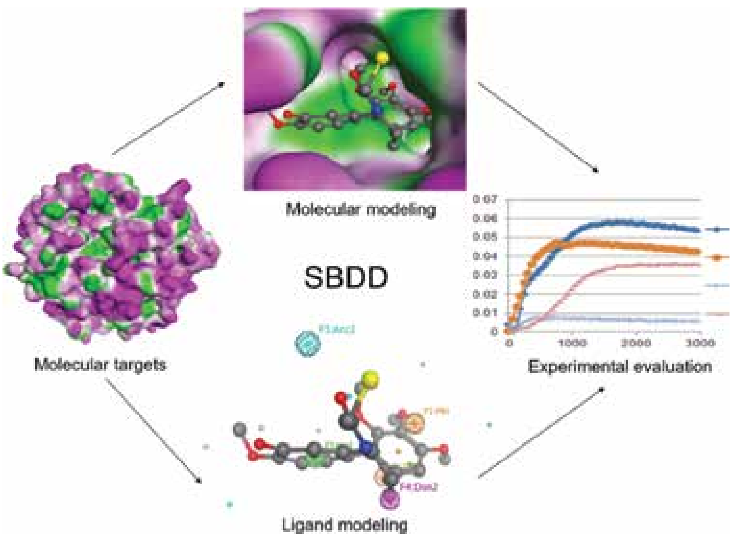

Figure 2. Structure-based drug design (SBDD) process.

3.4. Synthesis of lead compound

The initial drug design phase is followed by the synthesis of the lead compound, quantitative measurements of its ability to interact with the target protein, and X-ray crystallographic analysis of the compound-target complex. This analysis reveals important, empirical information on how the compound actually binds to the target, and the nature and extent of changes induced in the target by the binding. These data, in turn, suggest ways to refine the lead compound to improve its binding to the target protein. The refined lead compound is then synthesized and complexed with the target, and further refined in a reiterative process. If lead compounds are available from other studies, such as screening of combinatorial libraries, these compounds may serve as starting points for this optimization cycle using structure-based drug design.

Once a sufficiently potent compound has been designed and optimized, its activity is evaluated in a biological system to establish the compound's ability to function in a physiological environment. If the compound fails at any stage of the biological evaluation, the design team reviews the structural model and uses crystallography to adjust structural features of the compound to overcome the difficulty. This process continues until a designed compound exhibits the desired properties. The compound is then evaluated in an experimental disease model. If the compound fails, the reasons for failure (e.g., adverse metabolism, plasma binding, distribution, etc.) are determined, and again new modified compounds are designed to overcome the deficiencies without interfering with their ability to interact with the active site of the target protein. The experimental drug is then ready for conventional drug development (e.g., studies in safety assessment, formulation, clinical trials, etc.). This reiterative analysis and compound modification are possible because of the structural data obtained by X-ray crystallographic analysis at each stage. This capability renders structure-based drug design, a powerful tool for rapid and efficient development of drugs that are highly specific for particular protein target sites.

3.5. Docking methodologies

Several docking procedures exist in the literature, from the use of interactive graphics to manipulate the position of the ligand to completely automated procedures, which are becoming increasingly powerful to screen databases of molecules. Many docking algorithms follow a similar pattern. Usually, the first stage is to represent the molecules by their solvent-accessible surfaces. Beginning with a number of different relative orientations, the two molecules can then be brought together. More sophisticated methods carry out their moves by using a Monte Carlo algorithm to direct both rotations and translations. Rapid convergence to a minimum can be achieved by gradually cooling the simulation temperature as the molecule appears to be descending into a potential well.

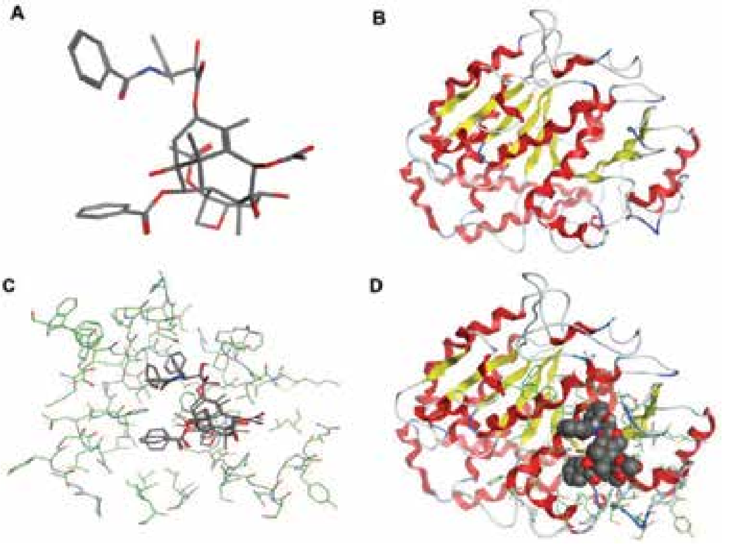

Figure 3. The molecular docking methodology. (A) Prepare the ligand structure, (B) Prepare the receptor structure, (C) Dock the ligand into the receptor surface with multiple potential conformations. (D) The most likely binding mode was identified based on intermolecular interaction between the ligand and the receptor surface. The protein backbone is represented as a cartoon. The ligand and active site residue are shown in stick representation.

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Molecular docking is one of the most frequently used methods in structure-based drug design because of its ability to predict, with a substantial degree of accuracy, the conformation of small-molecule ligands within the appropriate target binding site (**Figure 3**) [19]. Following the development of the first algorithms in the 1980s, molecular docking became an essential tool in drug discovery [20]. Highly intensive investigations involving crucial molecular events, including ligand-binding modes and the corresponding intermolecular interactions which stabilize the ligand-receptor complex, could be conveniently performed. Furthermore, molecular docking algorithms execute quantitative predictions of binding energetics, given docked compounds, based on the binding affinity of ligand-receptor complexes [21].

3.6. Computer simulation in drug design

The development of a new drug starts with the design of suitable candidate compounds so-called "ligands" that are selected according to observations about how these compounds are recognized by the target protein and how they bind to it. It is important to know that proteins have dynamic properties: they change their shape in much the way as a machine tool needs to in order to fulfill its function. Now, it is being realized how important it is to have techniques available for studying protein dynamics. Performing experiments is not only expensive but also very time-consuming and, moreover, cannot answer all relevant questions. An alternative is computer-aided simulation of the dynamics of molecules [molecular dynamics (MD) simulations], which is becoming increasingly important to identify the molecular properties that are important and to determine the detailed molecular interactions that are critical for binding.

In some instances, high-performance computing (HPC) is required to cross the threshold where MD simulation becomes a valuable tool for industry. However, in most pharmaceutical companies, HPC is something very new, and supercomputers are simply not available to industrial researchers. With the arrival of affordable high-performance multiprocessor machines and corresponding developments of parallel software, it now becomes possible for industrial researchers to undertake more realistic calculations that were previously out of reach. Scientists at Novo Nordisk, a large Danish pharmaceutical company, are convinced that this new capability will dramatically change the acceptance of MD simulation as a tool in the design of new ligands. During Europort-D, they, for the first time, studied the dynamics of the complex molecular interactions critical for recognition of ligands by their target proteins.

4. Statistical tool for drug design

4.1. Introduction to SPASS for pharmaceutical research

As a sophisticated statistical software, Statistical Package for Social Science (SPSS) can help researchers and users realize their complex statistical tests with result interpretation and the access to data figures, tables, and graphs, which can be quickly and easily displayed in the output view. Even though additional training is usually required before users can maximize its features and the graphing feature is not as simple as an excel spreadsheet, SPSS is still being used by more and more researchers from other fields for applications specific to their research areas, for example, the application of SPSS in clinical trials, with power and sample size calculation functions, comprehensive statistical tests and graphical tools, such as predictive data trends, forecasting and report generation, and the analysis of complex drug assays, etc. [22].

SPSS is being used majorly in pharmaceutical and medical research, where it can provide techniques for the design, implementation, and development of drug campaigns that are important to pharmaceutical research organizations and also provides data mining solutions based on their existing data on quality control and manufacturing, regulatory safety testing, clinical trials, data mining in drug discovery, compliance, and validation [23]. As many pharmaceutical research organizations have experienced that even small improvements in research or processing affect the efficiency and success of the project, SPSS provides a sophisticated analytical platforms to decrease development costs and unnecessary preclinical and clinical trials by integrating with existing data sources.

Overall, the tools in SPSS provide an efficient mechanism to automatically validate the routine analysis reports. In other words, SPSS empowers researchers with tools, which might bring the rapid and solid return on investments in the near future.

4.2. Outlines of the SPASS package

SPSS is a Windows-based program, which can be used to perform data entry and data analysis by tables and graphs (**Figure 4**). Because SPSS is capable of dealing with huge amounts of data with different modules, it is commonly used in the business world and in the Social Sciences [24]. Familiarity with this software will be useful in the field of drug research where big data,

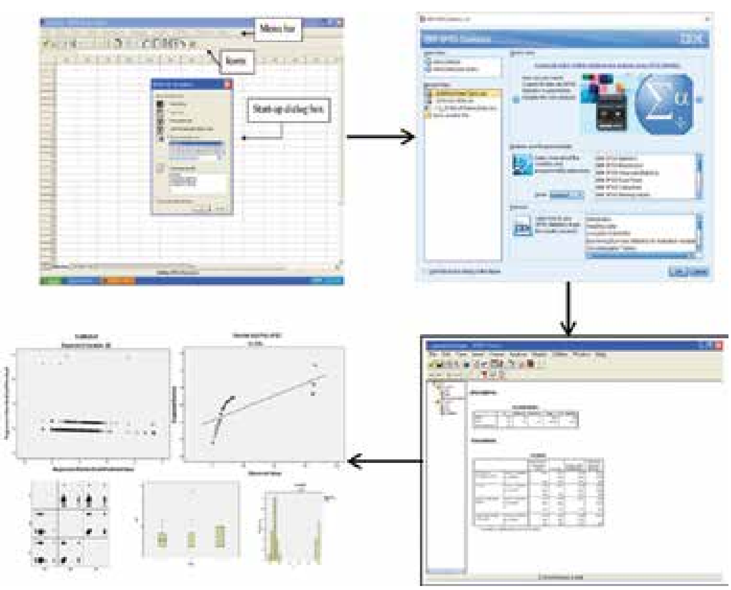

Figure 4. SPSS package in pharmaceutical data analytics application.

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such as clinical trials data ranging from simple bioassays and dose-response experiments to long-term survival, and carcinogenicity studies need to be integrated. Unlike Excel, SPSS software can support screen transfers between the data entry view and the output view, which display the results and summarize the data.

4.3. Features of SPSS package

Whether its small and medium enterprises (SME) or large-scale enterprises (LSE), the application of SPSS can provide data accessing in rational data sets, which allows accessing inflexible resources and practices and real-time processing, and mapping of the database [25]. Although other commercial softwares, such as SAS, MATLAB, and others, can also perform such functions, SPSS is a more sophisticated application in statistics analysis. SPSS conducts statistical analysis from basic data, descriptive statistics, such as average and prevalence, and advanced inferential statistics, such as t test, regression model, one-way and factorial analysis of variance (ANOVA), one-way and factorial analysis of covariance (ANCOVA), one-way and factorial multivariate analysis of variance (MANOVA), one-way and factorial multivariate analysis of covariance (MANCOVA), factor analysis, path analysis, and logistic regression [26].

Normally, researchers use SPSS as a tool to collect and analyze data. The data entry screen in SPSS looks like an excel spreadsheet, and users can input variables and quantitative data and save the file as a data file [27]. After data are collected and entered into the data sheet in SPSS, users can also create an output file from the data they used. Then, the users can edit or organize the data in SPSS to check the running results after they choose the module they want. For example, users can check out the frequency distributions of the data to see whether the data set is normally distributed. Furthermore, the researchers can download the tables or graphs directly from the data output view. Because SPSS has the statistical tests built-in to the program, users do not need to do any math calculation or equations to get the results.

5. Conclusion and future direction

Systems pharmacology represents a new paradigm in drug research where ligand and protein information are combined to produce new methods for drug discovery and design. Traditionally, ligand-based approaches utilize information contained within the chemical structure to predict the biological properties of the drug. In particular, chemical similarity database searches can be used to identify molecules with improved activity. However, to be able to design compounds with satisfactory safety profiles, the drug targets will also need to be determined. Target prediction can be performed using ligand or structure data. Both of these approaches require a bioactivity database with pre-characterized activities or functions. If the target structure of the ligand is known, then the structure-based drug discovery approach can be applied. Computer-aided drug design techniques such as molecular docking and molecular dynamic simulation are capable of accurately predicting the binding sites of ligand, docking pose, and binding affinity based on the geometry of the receptor surface. The prediction can then be validated using *in vitro* biochemical assays and X-ray crystallography to validate ligand binding. Thus, a cyclic drug design process is then continued until the strongest binder is found.

Currently, drug discovery has been mainly focused on in vitro optimization. One future direction in system-based drug discovery will necessarily shift to ADMET prediction to assess drug performance *in vivo*. Although several ADMET properties such as drug-likeness can be predicted by simple rules, a more detailed classification of drug properties can be achieved by more advanced machine learning techniques. Likewise, a holistic drug design process that simultaneously optimizes the drug properties based on *in vitro* and *in vivo* data will also hold promise to optimize drug safety and minimize adverse reactions. Consequently, integration of multilevel data from structure, tissue, and the whole organism will be required to achieve a more accurate prediction. In conclusion, we have presented the essential quantitative methods in system-based drug discovery, and the approaches presented here will stimulate further efforts in the progress of drug discovery and design to engineer safer and more effective drugs.

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Chapter 6

Stochastic Agent-Based Simulation of the Role of Labor in the Economy

Alexander Kindler , Natasa Golo and Sorin Solomon

Additional information is available at the end of the chapter

http://dx.doi.org/10.5772/64698

Abstract

We present a platform for stochastic agent-based simulation of the role of labor in the economy (SABLE). The platform facilitates heterogeneous agents: a large number of firms, workers, and banks are represented as individual agents. It allows the agents to have fixed or random reactions to the other agents and to pursue goals through decisions with bounded rationality. Its purpose is to clarify the feedback effects between the individuals as workers and consumers in a complex environment. SABLE is meant to be a quantitative precise tool to express classical, neoclassical and heterodox scenarios and to document their outcomes. In particular, questions regarding policies dealing with minimum wages, unemployment wages, hiring regulation, and the role of finance on unemployment can be studied in a new, interactive, and transparent way, inspired among others by the critical thoughts in.

Keywords: unemployment, complex systems, agent-based model, stochastic process, econophysics

1. Introduction

Unemployment is one of the main concerns of any society, because of its effect on economic, social, and political stability of countries. One of its aspects that is relatively well known and explained is job search. The main approach to understand job search is known as search and matching modeling [1, 2]. Search and matching models represent a stochastic process of joining of unemployed individuals and firms. In the existing literature, this joining is called the aggregate matching function [1], which proved successful at predicting quantitative and qualitative features of employment. The assumption of aggregate matching functions in labor markets has tested using a network configuration model for directed multigraphs in [3] and the results suggest the need for theoretical frameworks that take into account the structure of labor market frictions.

Also, the models of aggregate matching are often based on a number of assumptions that are specific to a certain case and related with specific market conditions. For example, in [4], the assumption is that newly created jobs are the most profitable in the market. Such an assumption is less valid if job creation is by new start-ups. Our approach, stochastic agent-based simulation of the role of labor in an economic system (SABLE) is unique in the sense that it allows for testing of any such assumption with relative ease and high efficiency.

Our agent-based stochastic macroeconomic model also includes the interaction between credit and labor markets. Under the assumption that the investment is dependent on the credit, and that the access to credit is dependent of firms performance, it is expected that the credit market plays a very important role in the dynamics of the labor markets. In this respect, particularly the new firms can be credit constrained, as in [5].

To describe the underlying concept of stochastic agent-based simulations, and its design concepts specific to our method of implementation, we wrote the paper along the general guidelines of [6]. We conclude with several examples of obtained output and their short discussion.

1.1. General approach

Economic heterogeneous interactive agents are on the workbench of an ever-increasing community for already 20 years (at least the age of the Workshop with the same name WEHIA). In parallel with the finance-focused platforms of the LLS [7] and Santa Fe type [8], they have been used to create stylized facts in business cycles, power laws of wealth distribution, fractal time series, etc. as shown in [9–11].

In spite of the limitations of agent-based simulations, they are recognized as a new mathematical tool to tackle concrete problems and connect them easily with the data.

The agent-based platform SABLE offers a standard environment for implementing and comparing specific mechanisms focused on problems in the labor market suggested by the empirical observations or the theoretical discourse within the academic or practitioner economics community.

Moreover, SABLE can be perceived as a neutral scaffold to express in a quantitative precise way various scenarios of current or generic economic situations and processes. In particular, it allows illustrating the possible outcomes of implementing the solutions proposed by various neoclassical and heterodox schools to current economic debates.

1.2. Agents

The basic groups in the current version of the SABLE platform are workers and firms. Each firm and each worker is represented individually, having a bank account, income, and some

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other specifications. Further entities such as banks, government, and external markets are implemented in the current version as single/representative agents.

The main interactions between real sector firms are supplier-client ones. As such, the firms are related through a "transactions matrix," which is a microeconomic similar of the Leontief matrix. It is an antisymmetric matrix representing money transfer between firms (in return to products/services).

The speed by which this matrix changes has a crucial effect on the dynamics and resilience of the economy. Too fast changing of the matrix makes the economy unstable, too slow—it makes it vulnerable to external (e.g., financial sector) change, as seen in [12].

The next important interaction is between firms and workers. It includes two aspects:

- Workers as employees: receiving money from the employer firm;
- Workers as customers spending their income on buying products.

As such, the workers are crucial in closing the flow/causal chain in the economic system.

Among other things, the double role of the workers allows for very significant feedback loops that dominate the SABLE system: these feedback loops may stabilize or destabilize the system and are a key to understanding how capitalist economy works.

1.3. Activities

Workers, firms, the bank, and the government interact through a set of routines that include the following:

- Workers are employed in firms or unemployed. Correspondingly,
    - they get a salary from the firm where they work in return for the labor they produce for the firm, or
    - they get an unemployment wage from the government (for "free").
- Workers spend their income in the market, thus returning money back to the firms.
- Firms pay workers in exchange for the labor they get from them.
- Besides, they do business with other firms, paying for services and products.
- Firms draw income from the sales to their market.
- Firms also compete between themselves over their share of the whole market.
- Firms get loans from banks and repay them back later.
- Taxes are paid by firms and workers to the government.

These relations are summarized in **Figure 1**.

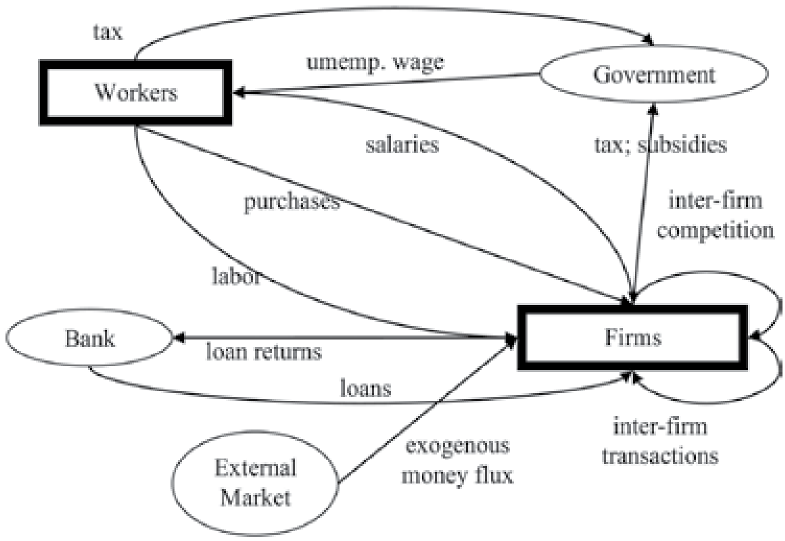

Figure 1. The major activities that are modeled in the basic version of SABLE.

2. Design concepts

In this section, we describe the previously introduced general features in more detail and we introduce the specifications of the code underlying the platform.

2.1. Time, activity patterns, and activation schemes

The basic sequence of events consists of several operations performed by agents as outlined in **Figure 1**:

- Create new firms.
- Initialize/update related parameters (e.g., the "transaction matrix (TM)").
- Update income of each firm according to its market share.
- Update the loan portfolios of the firms.
- Update the bankruptcy status of firms.
- Rescale the relative market shares of the remaining firms accordingly.
- Enforce the limits on the effective market share on each firm according to the maximal amount of products and services that it can receive from suppliers.
- Introduce new workers and initialize their respective parameters.
- Firms hire or fire workers, according to labor requirements and the salaries level.

- Enforce the limits on the effective market share on each firm according to its current available labor.
- Update workers' wages: workers get raises or cuts in their wages (according to their employment history and status).
- Pay salaries (and unemployment wages).
- Workers spend a certain fraction of their income in the market.
- Their aggregate spending generates the income for firms at the next time step.
- Firms compete between themselves over market share potential (not their effective hold on the market, which is limited by required labor and services of other firms).
- Update interest rate.
- Other events may take place, such as government intervention at different stages of the above dynamics, according to the desired effect.

According to the above list, one iteration of the platform corresponds to roughly a month of "real-world" economy progress, since salaries and loan returns are paid monthly.

2.2. Interaction protocols and information flows

Generally, interactions between agents are on the individuals' level, meaning that different decisions and actions are made by each firm and by each worker (on some occasions, the whole pool of firms or workers acts in coordination; e.g., collective labor contracts):

- Pairs of firms may agree to particular transactions.
- Loans are decided by pairs of firms or banks (according to a set of rules which takes into account the firm's features, the interest rate, etc.).
- The hiring and firing of workers is decided by the firms that employ them.
- In the present implementation, workers do not resign of their own volition.
- Initial wages are determined by labor initial capability (a given parameter).
- Further wages are fixed by previous wages and seniority.

In the present implementation, the end consumer market equals the total labor income (after taxes and interest).

2.3. Levels of randomness

SABLE has a core of random processes, which govern the dynamics of the entire economy as follows:

- The initial wealth of the new companies is random.
- For each firm, the relevant elements of the transaction matrix may evolve through a random process.

- Loans are granted with a certain probability depending on firm income, firm wealth, interest rate, etc.
- Hiring, firing, and offered wages have a random element too.
- The competition between companies for market shares is decided in a random way (with bias toward the larger companies).

3. Functional specifications

In this section, we describe in detail the implementation of the features discussed above, specifically agents and their interactions. We abstain from giving a full parametric description of each entity since that would flood the reader with a multitude of minor details, and instead we will give a general description, supported with mathematical formulation when essential only.

We will not list the different parameters and their uses, but rather give a more detailed description of the mechanisms underlying the interaction protocols and activities listed earlier.

In **Table 1**, we list these actions, interactions, and calculations.

Name	Type	Description
Determines whether employed workers get raises, or whether unemployed workers lower their wage.	Action	Get raise and drop wages
Updates the interest rate.	Action	Update interest
Generates new firms and workers.	Action	Create new firms and workers
Determines whether a firm gets a loan. Size is a fraction of the firm's cash.	Interaction	Get loan
Determines if and how much labor a firm hires or fires.	Interaction	Hire and fire
Varies the amount of money transferred between firms.	Interaction	Vary transaction matrix
Determine which firms compete over market shares potential, and determine the outcome of the competition.	Interaction	Competition
Calculate how much of the market share potential a firm effectively utilizes.	Calculation	Effective market share
Calculate how much income firms get.	Calculation	Firm income

Table 1. Actions, interactions, and important calculations.

Now, we briefly describe the mathematics behind each action, interaction, and calculation as applied in our model.

Get raise and drop wages: An employed individual has a probability to increase his wage each step he is employed by a certain percentage of his current wage (get a raise). Vice versa, an

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unemployed individual has a probability to decrease the wage for which he is willing to work each step that he is unemployed, in order to help himself get a job that is better paying than the unemployment wage.

Update interest: Interest rates may also rise and fall with respect to demand in loans. We apply a single interest rate among all firms in this version of SABLE. Every given time period, the proportion of the total debt is used to rescale the interest rate: if debt is growing, then interest rates will fall and vice versa.

Create new firms and workers: Both growth effects are assumed to be Poisson processes, with a mean related to the initial amount of workers and firms.

Get loan: **Table 2** lists a means for determining the likelihood of a firm getting a loan.

	Low income	High income
Low cash Low debt	Likely	Very likely
High cash Low debt	Unlikely	Likely
Low cash High debt	Unlikely	Likely
High cash High debt	Very unlikely	Unlikely

Table 2. Likelihood of a loan.

This could be conveniently formulated in probability terms, P_{cash} and P_{income}, which represent the probability of a firm to get a loan regarding its cash and income, respectively.

Since we would like a probability function that rises with income and falls with increase in cash, we propose as follows:

$$P_{\text{cash}} = \left\{ \tan^{-1}\left[A - \text{cash} \right] + \pi / 2 \right\} / \pi \tag{1a}$$

and similarly

$$P_{\text{income}} = \left\{ \tan^{-1}\left[B - \text{income} \right] + \pi / 2 \right\} / \pi \tag{1b}$$

where A and B are parameters. Since P_{cash} and P_{income} should be independent, in general, we begin constructing the probability for a loan with

$$P''_{\text{loan}} = 1 - \left(1 - P_{\text{cash}}\right) \cdot \left(1 - P_{\text{income}}\right) \tag{2}$$

Next, we must account for the interest rate—when it is high, all firms are less likely to loan money, and so we multiply Eq. (2) by a factor of (1-conf·I), where conf is a "confidence" parameter and I is the interest rate. Certainly, conf·$I < 1$, and the smaller conf is the less impact interest rate has on the probability of getting loans. This results in the following step in the loan probability function:

$$P_{\text{loan}}^{'} = 1 - \left(1 - P_{\text{cash}}\right) \cdot \left(1 - P_{\text{income}}\right) \cdot \left(1 - \text{conf} \cdot I\right) \tag{3}$$

The last argument to be added is the current debt, since the more indebted the firm, the less likely it is for a bank to increase that debt. Plainly, we multiply Eq. (3) by $[C/(C + \text{debt})]^D$ where C and D are parameters. This gives us the definitive loan probability function:

$$P_{\text{loan}} = 1 - \left(1 - P_{\text{cash}}\right) \cdot \left(1 - P_{\text{income}}\right) \cdot \left(1 - \text{conf} \cdot I\right) \cdot \left[C / \left(C + \text{debt}\right)\right]^{D} \tag{4}$$

This formula allows for achieving the desired control over the financing mechanism we have created (by scaling the parameters), through a random process.

Hire and fire: Firms need labor in order to utilize their market share, and do business with other firms. On the other hand, the salaries they pay are a burden, therefore resulting in a search for optimality. We assume that firms attempt to increase or decrease a percentage of currently paid salaries for each step, since the salaries they pay are the only objective measure firms usually have of their labor effectiveness. This too is a random process, where the probability of hiring, firing, or doing neither is controlled through a similar mechanism as in Eqs. (1a) and (1b):

$$P_{\text{hire}} = 1 - \tan^{-1}\left(\frac{\text{Salaries}_i}{E_i}\right) \cdot 2 / \pi \tag{5}$$

where E_i is a firm-specific parameter. Firing will happen in a similar fashion, leaving a probability for neither effect occurring as well.

Vary transaction matrix: We remind that the transaction matrix represents the trade of products and services between firms. To account for changes in firm behavior, we assume that the absolute values of the transaction matrix vary over time with some probability. However, we maintain the client-supplier relations fixed.

Competition: We model competition between firms through exchange in market shares, MS. Currently our model permits only one-on-one competition between firms.

The larger the market share of the firm, the less likely it is to lose to a smaller firm. So, if we have $MS_i > MS_j$ as respective market shares, the probability of shares going from firm j to firm i is as follows:

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$$P_{j \to i} = 1 - 0.5 \cdot \exp\left(-\left|\mathrm{MS}_i - \mathrm{MS}_j\right| / T\right) \tag{6}$$

where T is a coefficient. The amount of shares traded is a function of the difference in respective market shares, $\delta = |\mathrm{MS}_i - \mathrm{MS}_j|$. Certainly, the total shares of a smaller firm may be traded this way, leaving it totally out of the market. Not all firms compete at any given time step, and the amount of competing firm pairs is a parameter of the model. New firms start without market shares, but to compensate, they always compete when they are created.

Effective market share: If a firm has a certain MS_i, then it could only fully exploit a percentage of it due to not having enough products and services traded from other firms, or enough labor. Thus, all firms reach their potential market shares only asymptotically. Here, we implement the feedback between the transferring of money from firms to its peers and to its workers on its effectiveness to draw income from sales. The following equation shows the effective market share of a firm:

$$\mathrm{MS}_i^{\mathrm{eff}} = \mathrm{MS}_i \cdot \tan^{-1}\left(\frac{\text{Employed Labor}_i}{E_i}\right) \cdot \tan^{-1}\left(\frac{\text{Products Services}_i}{F_i}\right) \cdot \left(2/\pi\right)^2 \tag{7}$$

The measures of Employed Labor$_i$ and Products Services$_i$ are just as they appear—the amount of them a given firm has paid for. E_i and F_i are parameters of efficiency. We should stress here that firms hire and fire labor according to the salaries paid, and not according to the labor procured from each worker, but what really counts on efficiently utilizing market shares is the labor itself.

Firm income: Firms earn (and spend) money through a total of five features, best shown through an equation:

$$\text{Income}_i = (\text{Market} \cdot \mathrm{MS}_i^{\mathrm{eff}} - \text{Salaries}_i + \Sigma_j \mathrm{TM}_{ij} - \text{Loan Returns}_i) \cdot (1 - \text{Tax}) \tag{8}$$

The Market represents the entire flux of money in the economy, either from consumer spending (again, the feedback) or from exogenous sources, such as external markets or government spending. This way, each firm utilizes a certain fraction of the entire economic input. Salaries are straightforward such as the loan returns and the tax reduction. The sum on the transaction matrix represents the trade balance of the firm.

This ends the description of the core features of SABLE.

4. Results

First, let us show the number of total and active firms at each time step. We see that at first the number of active firms will drop to a semi-stable (or slowly varying) amount, since the initialization is unstable. This result is valid when counting all firms, and when counting only firms that have been active at least several time steps Results are plotted after the initialization of the system is complete (about 50 time steps) (**Figure 2**):

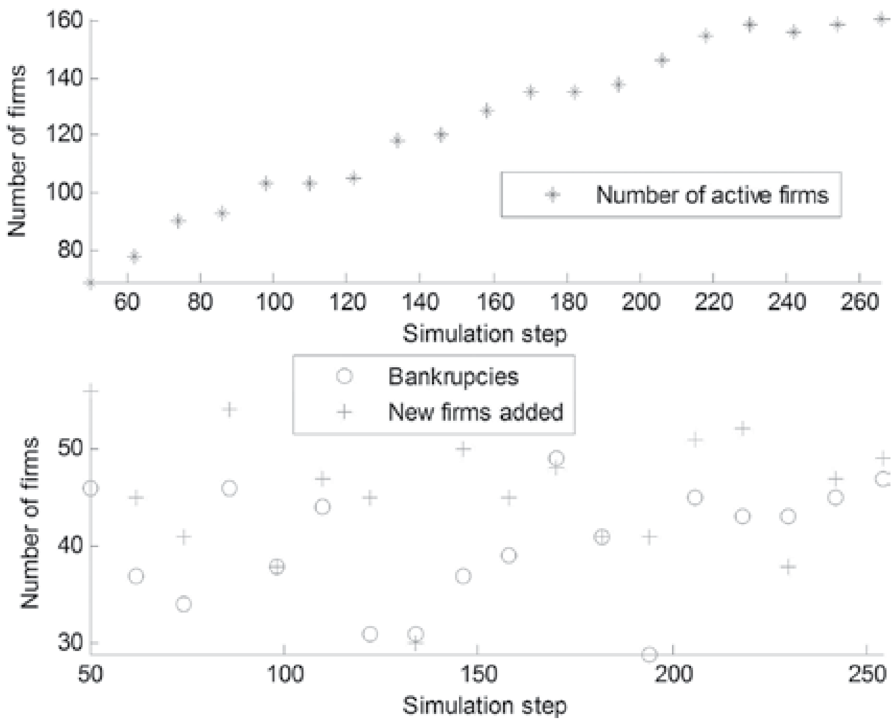

Figure 2. Top: The active number of firms (black asterisks), measured each 12 steps. Bottom: The change in bankruptcies (blue circles) and the added new firms (red pluses) between each 12 steps.

We plot the results on a 12-step interval to indicate yearly changes.

This result is reasonable enough: if economy is growing, it does not necessarily mean that every firm succeeds, but that the overall number of firms increases. If economy is receding, then new firms may still emerge though their chances of success are low, since even established firms are closing.

Moreover, almost any realistic set of parameters produces more or less the same variation in the number of active firms, while sometimes that number grows or recedes. This is a very robust product of SABLE.

We see that changes in the amount of firms vary mostly in the range between ±5% of the total amount of active firms at that step, meaning that these changes are rather stable: the median is 1.5%, the 80 percentile is 3% (absolute values of change).

For different parameter sets, economy can either grow or shrink, but changes in the amount of active firms remain similar to those depicted above.

We sort the firms according to their capital (cash), earnings (the positive figures from Eq. (**8**)), the relative amount of employees, and employed labor, at the final step of the simulated run. In order to study that distribution, we plot the results on a log-log scale (**Figure 3**).

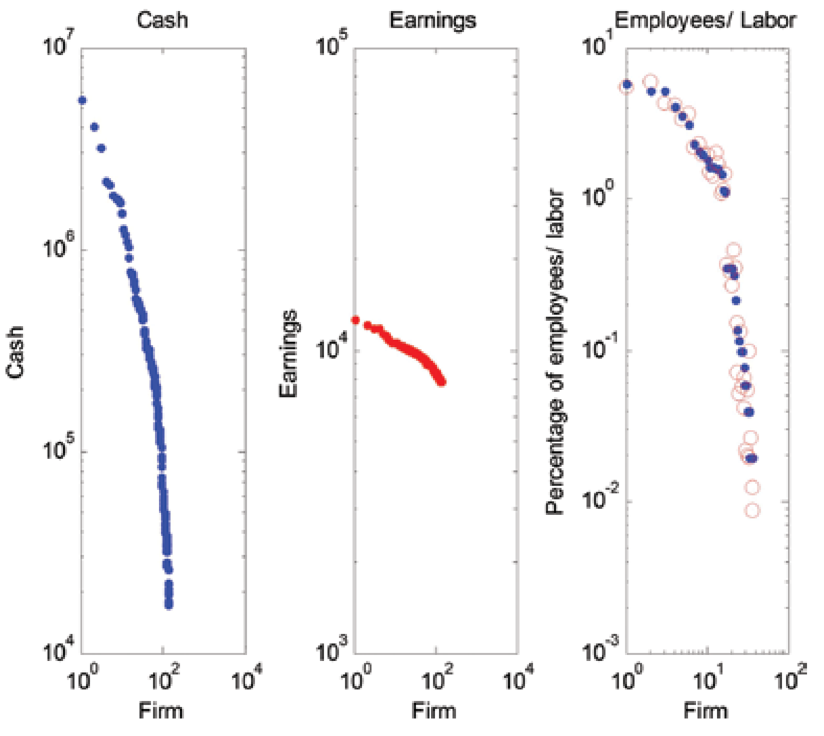

Figure 3. Left: Money distribution in between active firms at the end of the simulation run, on a log-log scale. Middle: Earnings distribution in between active firms at the end of the simulation run, on a log-log scale. Right: Employees (blue dots) and labor (red circles) distribution in between active firms at the end of the simulation run, on a log-log scale.

We see that the distribution of the above variables roughly satisfies a power-law distribution. That is reasonable since the large capital accumulation is unavoidable for large firms: our model does not include either shareholders or a financial market where the cash could have been reinvested (except in the expansion of production). The dependence in the lower part might be characterized by another power law: the splitting of the distribution into two parts is expected [13] but largely exaggerated: most firms are indeed small (in all aspects) and only a few firms should be able to have large funds, income, and labor.

Also, we see that the relative amount of employees (blue dots) and employed labor (red circles) on the right-most plot are strongly correlated in this example.

It is a reassuring feature of SABLE, since this power law in capital accumulation is expected. Similar power-law dependencies in the firms' financial indicators have been often empirically validated by various authors [14–16] and were spontaneously achieved.

We inspect unemployment rates, and see that it is in the rational vicinity of up to 10% most of the time. There are, however, crises (besides the initialization effects), where unemployment soars, but then returns to low values (**Figure 4**).

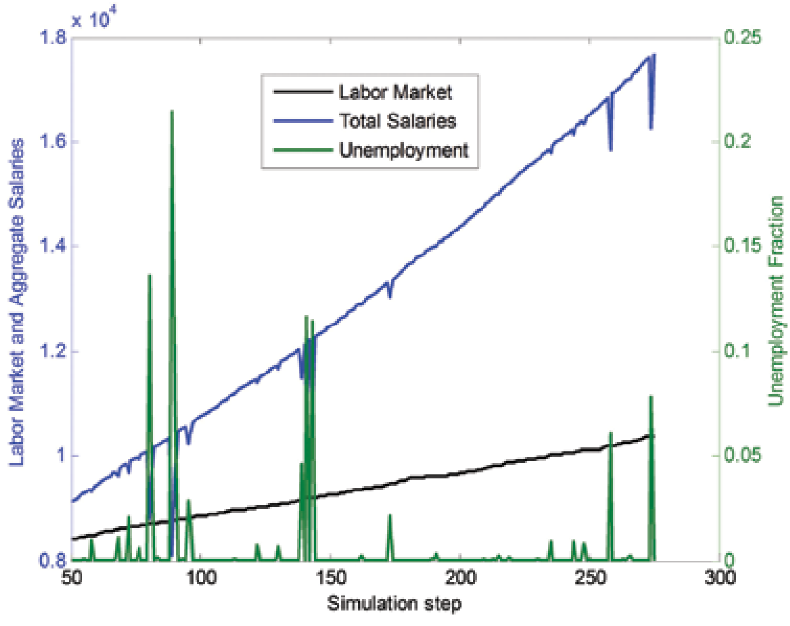

Figure 4. The total labor available (labor market—black line), total salaries paid (blue line), and unemployment ratio (green line) at each step, cropping the initialization phase.

The "peaks" in unemployment result from two effects, which may overlap: a wave of bankruptcies causing several firms to close and fire their workers during the same step, or the closing of major firms.

We see that these crises are highly correlated with the dips in aggregate salaries as expected.

We have truncated the initialization steps, since the unemployment is extremely high and, respectively, very confusing when visualized.

Although it may seem that at some intervals unemployment is going down to zero (when not discussing the peaks), it is in fact just a low percentage: firms constantly go bankrupt and lose their workers, and firms may sometimes fire workers due to financial problems. However, when small firms go bankrupt the global effect on unemployment is usually insignificant because these firms hold a very low percentage of labor.

This small percentage is, however, important because in periods of growth when unemployment is very low new firms still emerge with man-power requirements, which cannot be met without available labor that has been released from current firms.

The slope of the rise in aggregate salaries is a product of input parameters, mainly the probability of giving raises, the raise amount relative to current employee wage, and the growth of new workers. Also, since we have a maximum wage (in the default setting equals 20 times the minimum wage), should that wage be achieved for all current workers further raises would become impossible, and the only growth in the aggregate salaries would be due to the introduction of new workers. This effect is inevitable when regarding sensible labor procedures: if unemployment is low, most people stay at their jobs (or move mostly to better-paying jobs, though it is not part of SABLE). Eventually, a person who stays employed will get a raise, though his/her productive ability remains more or less the same on the scope in which we deal. After enough such raises, his/her salary will exceed his/her labor capability.

Next, we discuss the variation in firms' debt. In the current version of SABLE, we do not deal with firms' debt in great detail. In particular, the debt of the firms that are going bankrupt is not being dealt with: it is simply being ignored. This approximation is satisfying for the current level of implementation when our goal is to test the basic functions of economy; however, for a more profound result that can be compared with the empirical analysis [17], it will be necessary to refine the model. The light blue color indicates bankruptcy, as opposed to the dark blue color which indicates no debt (trivially true for nonexistent firms). The end of initialization is indicated by a thick red horizontal line (**Figure 5**).

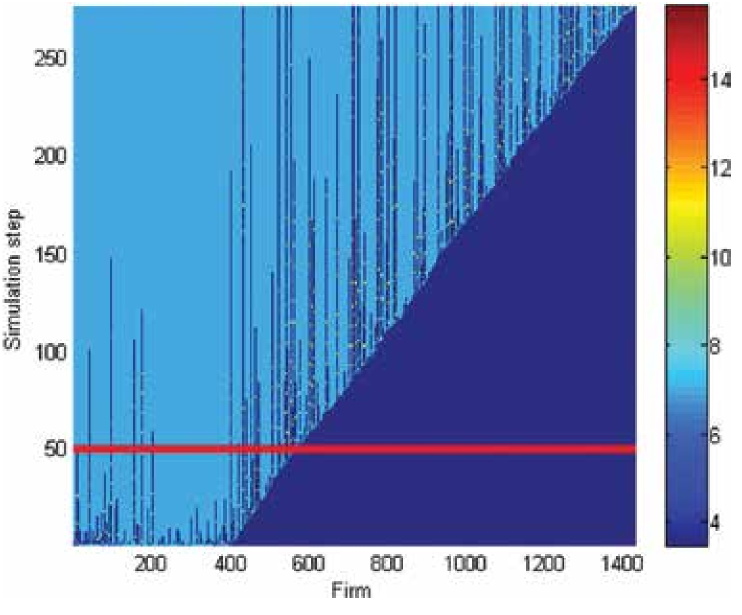

Figure 5. The logarithm of the debt of each firm (x-axis) at each time step (y-axis, red line signifies the end of initialization). The light blue color represents the time when firms are bankrupt.

Overall, debt per firm slowly grows in this example (more frequent loans). This happens mostly due to the fact that interest is low, so that firms are expected to get loans. This allows the firms who get loans better chances of success. Then, new firms emerge and get loans before older firms have paid off their current debts, so that momentarily the total debt increases.

Moreover, since more firms are active at each time, the chances that they would loan additional money increase, causing an increase in the normalized debt.

Correlation between behavior in debt and other features has not yet been thoroughly established. However, a preliminary analysis indicates that economy and debt grow together, meaning that when unemployment is low and firms succeed more than they fail—debt increases—and vice versa.

We are also inspecting the number of time steps that firms have been active before going bankrupt. We see that most firms are active for only a single step, and that a very small number of firms live more than 20 steps. This is also quite expected: we do not distinguish between the entrepreneurs and firms; thus the model makes the decision on which of the entrepreneurs starting new businesses will develop until the level of real firms. The growth opportunities are equal for all new firms and not related with the products they are bringing to the market, that is, we are neglecting any industrial classification in this version of the model, that is, the luck is the main ingredient needed to the survival of the small firms and entrepreneurs (similar as in the model of [18]) (**Figure 6**).

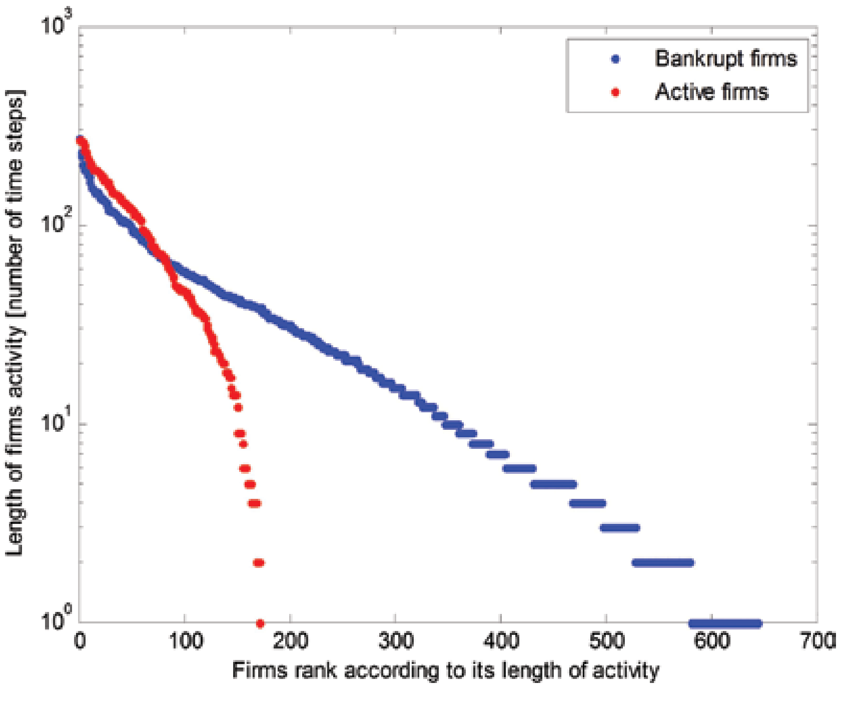

Figure 6. The distribution of firms' life span: blue dots represent bankrupt firms, and red dots represent active firms at the end of the simulation run.

This result is sensible enough, since most firms eventually will close, and most firms will be short-lived. Generally, it does not mean that older firms are more powerful in terms of available cash or income.

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5. Discussion

The generic runs we performed until now show that a series of properties of the economic systems and of their models are very nonspecific and do not depend on the details of the implementation:

- We obtain relatively stable economies with a number of active firms in the market that fluctuates around an average value corresponding to the economy size, and yet have firms go bankrupt and new firms are created. This is a rather realistic feature of the economy [16].
- The power-law distribution, in particular in the distribution of wealth of the firms, their life span, and the labor they employ, emerges spontaneously without any fine-tuning of the parameters (in particular, this means that most firms are small, and only a few are large).
- We reach sensible unemployment levels, with fluctuations in unemployment coupled to the market fluctuations.
- In particular, when unemployment is low, wages are higher than the labor they buy, meaning that workers work for more than they are actually worth.
- The life span of firms also agrees with the empirical known facts. We obtain a power-law distribution, meaning that most firms are very short-lived, and only a few may stay active for long time periods.
- The current ratio of active firms that resulted from the default run agrees with the typical empirical data [19].

Representing economic reality in a simple computer platform seems to be quite a torturous path toward an elusive target.

However, this effort to capture the essentials of the economic system in a quantitative, intuitive, and conceptually meaningful way is not a void academic exercise. Rather, it offers an interactive and transparent way of revealing the mechanisms that make an economy function, such as the emergence of collective macroscopic phenomena out of individual interactions.

The fact that this is not a barren effort is proven daily by the strong controversies in the news between different economist schools about virtually every social and policy item.

We may hope at some stage to have the quantitative platforms such as SABLE as central participants to these debates by "commenting numerically" and supporting quantitatively the various proposals and verbal arguments raised in the media.

One does not expect a machine to be a definitive judge between the views and principles introduced by different schools or interest groups. Conversely, one can positively expect to check whether the logical conclusions and quantitative relations within a certain theory of narrative add up: presenting simulations that parallel a verbal/policy argument and confirm or contradict a certain position/prediction.

As such, we expect SABLE to contribute to an informed, precise, yet not "academic jargon" analysis: exactly what the society is yearning for in the last years!

At the conceptual level, one may hope to repeat in the economic field the success of natural sciences in the last century: understanding and predicting the macroscopic world (including this time society, economics, collective human behavior) in terms of "microscopic" simple rules acting at the level of the individual agent.

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Edited by Ciza Thomas

The book on complex systems, sustainability, and innovation explores a broad set of ideas and presents some of the state-of-the-art research in this field concisely in six chapters. In a complex system, it is difficult to know exactly how the individual components contribute to an observed behavior and the extent of each component's contributions. It is the interactions of the individual components that determine the emergent functionalities. This makes it difficult to understand and predict the behavior of complex systems and hence the effects of any innovations in this field. This necessitates for the emergence of a new age of innovations with the main focus on user orientation and sustainability. This book explores some of the complex systems and their dependence on the environment to provide a long-term perspective, aiding innovations and supporting a sustainable society. The intended audience of this book will mainly consist of researchers, research students, and practitioners in the field of complex systems and sustainability.

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