National Committee of Ukraine by Theoretical and Applied Mechanics
Taras Shevchenko National University of Kyiv
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XVIII International Conference

DYNAMICAL SYSTEM MODELLING AND STABILITY INVESTIGATION

MODELLING & STABILITY

ABSTRACTS OF CONFERENCE REPORTS
Kiev, Ukraine

May 24-26, 2017

ВІСНИК
Київського національного університету імені Тараса Шевченка

The various aspects of theoretical and applied researches are represented in abstracts of conference reports. Problems of adequate mathematical model of studied processes are considered.
Problems of control synthesis and stability investigation of movements are separately allocated. Significant numbers of papers are devoted to modeling of economic problems, biological and social phenomena. Big quantity of reports presented at the conference is devoted to the problems of applied mechanics.Logic-mathematical methods of modeling are considered.
Prepared by A.V.Shatyrko

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В тезисах докладов конференции представлены различные аспекты теоретических и прикладных исследований. Рассмотрены вопросы создания математических моделей, адекватно описывающих исследуемые объекты.
Отдельно рассмотрены проблемы синтеза управления и исследования устойчивости движения. Значительное количество работ связано с моделированием экономических, биологических и социальных процессов. Большое количество работ посвящено проблемам теоретической и прикладной механики. Рассмотрены логико-математические методы моделирования.
Подготовлено А.В.Шатырко

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В тезах доповідей конференції представлено різні аспекти теоретичних та прикладних досліджень. Розглянуто питання створення математичних моделей, що адекватно описують об’єкти.
Окремо розглянуто проблему синтезу керування та дослідження стійкості руху. Значна кількість праць пов’язана із моделюванням економічних, біологічних та соціальних процесів. Велика кількість праць присвячена проблемам теоретичної та прикладної механіки. Розглянуті логіко-математичні методи моделювання.
Підготовлено А.В.Шатирко

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The Conference covers the following topics:

1. **Mathematical methods of system investigation.**
   - Investigation of differential, functional-differential and difference systems.
   - Investigation of system stability, controllability and optimization.
   - Bifurcations and chaos in dynamical systems.
   - Lyapunov's methods in system investigation.
2. **Methods and technologies of computer modeling.**
   - Numerical Methods of Mathematical Physics.
   - Method and Technology computer calculations.
   - Specialized software and systems.
   - Software and Systems Modeling
3. **Modeling and investigation of processes in mechanics.**
   - Mathematical modeling in composite materials of mechanics.
   - Modeling and investigation of dynamical processes in elastic and hydroelastic systems.
   - Mathematical modeling in connected fields of mechanics.
4. **Method of control and complex systems research**
   - Methods of control and optimization.
   - The continuous-discrete systems
   - Methods of differential games.
   - Fuzzy modeling and systems with uncertainty.
   - Modelling in economy and ecology.
5. **Logic-mathematical methods of modeling.**
   - Methods and tools of subject domains specifications.
   - Methods and tools of software systems description.
   - Modal and temporal formalisms of systems modeling

Також в цей же період відбулася

КОНФЕРЕНЦІЯ-СУПУТНИК

ВСЕУКРАЇНСЬКА НАУКОВО-ПРАКТИЧНА КОНФЕРЕНЦІ МОЛОДИХ ВЧЕНИХ

«Теоретичні та прикладні аспекти застосування інформаційних технологій в галузі природничих наук»

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Секції конференції:

- Математичні основи інформаційних технологій
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- Інформаційні технології в системах моніторингу навколишнього середовища
- Технології вбудованих і мобільних систем

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MATHEMATICAL MODELLING OF CONFORMATIONAL DYNAMICS OF DNA BY DIELECTRIC SPECTROSCOPY

Batyuk L.V., Astapovich D.F., Berest V.P., Kizilova N.N.,

Between the different forms of DNA, with changing external conditions, conformational transitions occur. Conformational transitions have both cooperative and noncooperative nature. Cooperative conformational transitions are associated with the need to overcome the energy barrier. Besides, there is a boundary of conformations, for example, “A-B junction”, which, without breaking the stacking, leads to the bending of the double helix of DNA, which is important for the processes of DNA supercoiling and its interaction with proteins [1]. One of the factors determining the conformation of DNA is its hydrated environment. The water molecules sorbed on the surface of the biopolymer form a multilayered hydrated shell with a regular structure of hydrogen bonds [2]. Such water bridges contribute significantly to the stabilization of DNA double helices, up to 70% in the enthalpy of B-DNA melting in moistened films and gels. The influence of the hydration shell on the conformational state of DNA causes the researchers' interest in studying the properties of water molecules in a hydrated shell. It is difficult to conduct such an analysis in solution, because, for example, at usual DNA concentrations used in the study of UV spectra (10^{-6}-10^{-5} g/ml), the amount of water bound to DNA is 10^{-4}-10^{-5} % of the total amount of water in the solution, which leads to unrealistic requirements for the accuracy of measuring devices. Therefore, a convenient model object for studying the properties of the hydrate shell is moistened DNA samples, such as films and fibers. In addition, according to modern concepts in biological systems, there are no free water molecules, so DNA in them, apparently, are not in solution, but, on the contrary, compete for hydrated water with other substances.

In this paper we consider a model of bounded volume that describes the conformational transitions of a DNA molecule induced by a change in the relative humidity of a sample. The conformation of DNA is determined by its ion-hydrate environment. The DNA molecule is modeled by a sequence of monomer units, of a certain length. The DNA molecules commonly used in the experiment include 10^5 pairs of nucleotides, which allow us to use the methods of thermodynamics in the description of DNA. The chain links can be in one of three conformational states: a disordered form, and two conformations, between which reversible cooperative conformational transitions are possible. Water molecules that are directly connected to the double helix of DNA form an impermeable cationic primary hydrate shell, which includes 11-12 water molecules per nucleotide. The water molecules associated with the primary hydrated shell due to hydrogen bonds form a secondary hydrated DNA envelope. There are also tertiary, etc. hydrate shells, however, the properties of the water molecules that form them, differ little from the properties of water molecules far from DNA. The inclusion of DNA in the consideration of the hydrate environment requires the

use of a device designed to describe open thermodynamic systems [3], using stochastic methods of analysis, DNA exchanges water with the environment when the external conditions change. Numerical modeling makes it possible to obtain a system of differential equations that describes processes of sorption of water molecules and associated conformational transitions of nucleic acids. The increase in relative humidity leads to an increase in the change in free energy during the sorption of water moles due to the increase in the number of sorbed water molecules, which changes the ratio of the minima and makes the conformational transition energetically favorable.

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