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OPTIMIZATION OF BIOPHYSICAL PROCESSES IN NANOBIOTECHNOLOGICAL SYSTEMS BASED ON COMPUTER MODELING

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Abstract
Nanobiotechnology is one of the rapidly developing scientific fields in recent years, particularly in medicine, pharmacy, and bioengineering. In this field, the interaction of nanoscale structures with biological systems occurs through complex biophysical processes. This article provides a comprehensive analysis of the study and optimization of biophysical processes in nanobiotechnological systems based on computer modeling. The capabilities of molecular dynamics, Monte Carlo methods, agent-based models, and Bayesian optimization approaches are analyzed. The use of computational models enables the enhancement of nanosystem efficiency, ensures biocompatibility, and significantly reduces experimental costs.

Keywords: Nanobiotechnology, biophysical processes, computer modeling, molecular dynamics, nanoparticles, optimization.

Introduction

The development of modern science and technology necessitates an in-depth study of nanoscale objects. Nanobiotechnology is a scientific discipline that investigates the interaction between nanomaterials and biological systems and is

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widely applied in medicine, pharmacy, ecology, and materials science. Nanoparticles actively participate at the cellular level, giving rise to complex biophysical processes.

Traditional experimental studies have limited capabilities in investigating nanoscale phenomena. Therefore, computer modeling has become an essential tool for analyzing biophysical processes. Computational models allow the prediction of nanosystem behavior and the identification of optimal parameters prior to experimental implementation.

Literature Review

International scientific literature contains numerous studies devoted to modeling nanobiotechnological systems. Researchers have employed molecular dynamics models to determine the energetic stability between biomolecules and nanoparticles. Such models play a crucial role in explaining the molecular mechanisms of biophysical processes.

Other studies demonstrate the effectiveness of Monte Carlo and probabilistic models in predicting biophysical processes. Several authors emphasize the advantages of *in silico* modeling approaches in the design of nano-drug delivery systems. Bayesian optimization methods are widely applied to enhance the biological activity of nanosurfaces.

Additionally, bioinformatics and computational chemistry occupy a significant place in nanobiotechnology, enabling the analysis of large-scale datasets.

Main Body

Biophysical Foundations of Nanobiotechnological Systems

Nanobiotechnological systems operate based on interactions between nanoscale particles and biological environments. In these systems, diffusion, molecular binding, electrostatic forces, and thermodynamic equilibrium play essential roles. During translocation across the cell membrane, nanoparticles overcome various biophysical barriers.

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Due to the complexity of biophysical processes, their complete mathematical description is challenging. Therefore, the application of computational modeling is of critical importance.

Computational Modeling Approaches

Molecular Dynamics Modeling

The molecular dynamics method calculates the time-dependent motion of atoms and molecules based on Newton's laws. This approach enables an in-depth analysis of nanoparticle interactions with biomolecules.

Monte Carlo Methods

MC methods are a class of computational algorithms that rely on repeated random sampling to obtain numerical results. These methods are particularly effective for solving problems that are deterministic in nature but analytically intractable due to their complexity. MC simulations are widely used in scenarios where the solution involves a large number of variables or uncertain inputs, making direct computation impractical.

MC methods were developed during the 1940s, largely in response to problems encountered in nuclear physics. The term "Monte Carlo" was coined by physicists Stanislaw Ulam and John von Neumann while working on the Manhattan Project, referencing the famous Monte Carlo Casino due to the method's reliance on randomness and chance. Their work was instrumental in solving neutron transport problems, which involve tracking the random interactions of particles in a medium. In physics, MC simulations have since become indispensable for studying systems with many degrees of freedom, such as molecular dynamics, statistical mechanics, and quantum field theory. They provide critical insights into phenomena like phase transitions, particle behavior, and radiation transport. In medicine, MC methods are extensively used for modeling the behavior of radiation in biological tissues, which is crucial in fields such as radiation therapy. and medical imaging. For example, in radiation therapy, MC simulations help optimize treatment plans by accurately predicting the dose distribution within the patient's body, ensuring maximum damage to cancerous tissues while sparing

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healthy ones. Similarly, in diagnostic imaging techniques like PET and CT scans, these simulations improve image reconstruction and enhance diagnostic accuracy illustrates the MC models for a cone-beam CT and PET detector system, along with their respective phantoms used for dosimetric measurements.

Models of Biophysical Processes in Nanobiotechnology

In nanobiotechnological systems, molecular-level processes exhibit stochastic behavior. Molecular motion, binding probability, and energetic changes are effectively modeled using the Monte Carlo approach.

Brownian motion of a molecule is described as:

$\Delta x = \sqrt{(2D\Delta t)} \cdot \xi$

where:

D — diffusion coefficient,

Δt — time interval,

ξ — normally distributed random variable.

Monte Carlo Optimization (Metropolis Algorithm)

In optimization problems, the objective function is defined as:

$F = F(x_1, x_2, \ldots, x_n)$

In the Metropolis algorithm, the probability of accepting a new state is given by:

$P = \min(1, \exp(-\Delta E / kT))$

If $\Delta E < 0$, the state is always accepted; otherwise, it is accepted probabilistically. This method is essential for finding the global energetic minimum of the system.

Practical Significance of Monte Carlo Methods in Nanobiotechnology

— determination of optimal size and shape of drug-delivery nanoparticles;
— calculation of nanoparticle translocation probability across cell membranes;
— identification of energetically stable conformations of proteins and enzymes;
— probabilistic modeling of DNA–ligand binding processes;
— enhancement of nanosensor sensitivity;
— design of targeted nano-drug systems for cancer therapy;

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— evaluation of ion channel permeability in biomembranes;
— prediction of toxicological risks.
Monte Carlo optimization significantly reduces the number of experiments, saving time and material resources.

Agent-Based Models (ABM)

Agent-based models represent complex systems through individual, autonomous, and interacting elements—agents. Each agent possesses its own state, behavioral rules, and decision-making mechanisms. The global behavior of the system emerges from local interactions among agents.
In nanobiotechnological systems, agents include biomolecules (proteins, DNA, RNA), nanoparticles, cellular components, ligands, receptors, and ions. The state of each agent is expressed as a vector:
$s_i(t) = \{x_i(t), v_i(t), E_i(t), \sigma_i(t)\}$
where:
$x_i(t)$ — spatial position of the agent,
$v_i(t)$ — velocity,
$E_i(t)$ — energetic state,
$\sigma_i(t)$ — internal biological state.

Modeling Biophysical Processes via Agents

Due to the stochastic and nonlinear nature of biophysical processes in nanobiotechnological environments, agent-based models ensure high accuracy. Molecular diffusion is expressed through agent motion as:
$x_i(t + \Delta t) = x_i(t) + v_i\Delta t + \sqrt{(2D\Delta t)}\cdot\xi$
where:
D — diffusion coefficient,
Δt — time interval,
ξ — normally distributed random variable.
Interactions between agents are determined by an energetic potential:
$E_{ij} = f(r_{ij})$
where r_{ij} is the distance between agents.

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Agent-Based Optimization

The main objective of optimization is to enhance system efficiency or minimize energetic costs. The objective function is defined as:

$F = \Sigma\, w_i \cdot g(s_i)$

The probability of an agent selecting a new state is based on statistical mechanics principles:

$P_i = \exp(-\Delta E_i / kT) / \Sigma \exp(-\Delta E_j / kT)$

This approach facilitates convergence toward the global optimal state of the system.

Practical Applications in Nanobiotechnology

Agent-based models are applied to solve the following tasks:

— modeling nanoparticle transport across cell membranes;
— optimization of ligand–receptor binding kinetics;
— evaluation of biological efficiency of nano-drug systems;
— analysis of ion channel activity in biomembranes;
— amplification of signal transmission in nanosensors;
— prediction of toxicological risks;
— development of nanotherapy strategies targeting tumor cells.

Optimization Methods for Biophysical Processes

Computer-based optimization of nanosystems is carried out in the following directions:

— enhancement of nano-drug delivery system efficiency;
— improvement of biocompatibility of nanosurfaces;
— reduction of toxicity levels;
— optimization of energy and resource consumption.

Bayesian optimization and artificial intelligence algorithms are used to tune nanosystem parameters to their optimal values.

Conclusion

Optimization of biophysical processes in nanobiotechnological systems based on computational modeling represents one of the key research directions in modern

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biomedicine, pharmacy, and nanomedicine. The study demonstrates that stochastic and discrete approaches, such as Monte Carlo and agent-based models, exhibit high efficiency in modeling complex biological systems. These approaches allow realistic representation of molecular-level randomness, nonlinear interactions, and multiparametric processes under physical conditions close to reality.

The results indicate that computational modeling reduces the number of experimental studies, saves time and material resources, and enables prior assessment of the safety and efficiency of nanobiotechnological systems. These methods have significant scientific and practical importance in the design of nano-drug delivery systems, development of targeted therapy strategies, enhancement of nanosensor sensitivity, and prediction of toxicological risks. Therefore, the integrated application of Monte Carlo and agent-based models is considered a promising direction for the future innovative development of nanobiotechnology.

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