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REVIEW

Multiscale Modeling in Systems Biology

Modelado Multiescala en Biología de Sistemas

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ABSTRACT

Multiscale modeling in systems biology is a methodological approach designed to represent, integrate, and simulate complex biological phenomena occurring across various organizational levels, from the molecular to the tissue scale. In contrast to reductionist perspectives, this holistic framework acknowledges that biological processes emerge from dynamic interactions among components operating simultaneously in multiple spatial and temporal scales. Its development has been facilitated by the growing availability of omics data and the evolution of advanced computational tools, enabling the creation of realistic and predictive simulations. This article reviews theoretical foundations and current applications of multiscale modeling in key fields such as personalized medicine, computational pharmacology, tissue engineering, and clinical simulation. It covers integration strategies such as hierarchical and concurrent coupling, and highlights the use of specialized platforms like GROMACS, NAMD, SimBiology, and PhysiCell. The advantages of this modeling approach include the design of individualized treatments, virtual testing of biomaterials, and the optimization of clinical trials through simulated cohorts. Multiscale models allow not only a more accurate representation of biological systems but also enable the anticipation of pathophysiological dynamics, reduce drug development timelines, and enhance clinical decision-making. Their future effectiveness will depend on data interoperability, algorithmic refinement, and integration with artificial intelligence. Ultimately, multiscale modeling is a foundational tool for advancing toward a more predictive, contextual, and adaptive biology suited to the evolving challenges of contemporary medicine.

Keywords: Multiscale Modeling; Systems Biology; Computational Models.

RESUMEN

El modelado multiescala en biología de sistemas constituye una estrategia metodológica que permite representar, integrar y simular fenómenos biológicos complejos que ocurren en múltiples niveles de organización, desde lo molecular hasta lo tisular. En contraposición a enfoques reduccionistas, este modelo holístico reconoce que los procesos vitales emergen de la interacción dinámica entre componentes biológicos que operan simultáneamente en distintas escalas espaciales y temporales. Su implementación ha sido posible gracias al desarrollo de herramientas computacionales avanzadas y al acceso creciente a datos ómicos, lo que ha facilitado la construcción de simulaciones realistas y predictivas. Este artículo revisa enfoques teóricos y aplicaciones actuales del modelado multiescala en áreas como la medicina personalizada, la farmacología computacional, la ingeniería de tejidos y la simulación clínica. Se abordan metodologías de integración como el acoplamiento jerárquico y concurrente, así como el uso de plataformas como GROMACS, NAMD, SimBiology y PhysiCell. Además, se destacan sus beneficios en el diseño de tratamientos individualizados, evaluación virtual de biomateriales y optimización de ensayos clínicos mediante cohortes simuladas. Los modelos multiescala no solo permiten representar fenómenos biológicos con mayor fidelidad, sino también anticipar dinámicas fisiopatológicas, reducir tiempos de desarrollo terapéutico y mejorar la toma de decisiones clínicas. A futuro, su eficacia dependerá de la interoperabilidad de datos, el perfeccionamiento de los algoritmos y la integración con inteligencia artificial. En definitiva, el modelado multiescala representa una vía para consolidar una biología más predictiva, contextual y adaptada a los desafíos de la medicina contemporánea.

Palabras clave: Modelado Multiescala; Biología de Sistemas; Modelos Computacionales.

INTRODUCTION

In recent years, the view of biological systems has moved away from fragmented approaches to embrace a more integrative and holistic understanding. For many years, biology focused on analyzing its components in isolation, but it is now recognized that life processes arise from dynamic interactions between different levels of organization. From this new perspective, systems biology emerges as a key field that proposes to study organisms as a whole, analyzing how genes, proteins, cells, and organs interrelate to generate complex behaviors that cannot be explained separately or by linear models.(1,2)

Biological systems are, by nature, complex and multidimensional. They operate simultaneously on multiple spatial and temporal scales, from the molecular interaction of seconds to systemic processes that unfold over years. Attempting to explain their behavior using a single level of analysis profoundly limits the understanding of the phenomenon. Relationships between scales are determinant: a change in one molecular pathway can trigger a cascade of effects at the cellular level and, in turn, impact the functionality of a tissue or organ. The integration of scales is, therefore, an indispensable condition to achieve truly representative and functional models.(3)

A decisive element in the consolidation of this new approach has been the development of computational modeling, conceived not only as a tool to represent complex biological phenomena mathematically but also as a bridge between empirical data and virtual simulation. This type of modeling enables the structure of large volumes of biomedical information and, in addition, allows for experimentation with scenarios ranging from molecular dynamics to the physiology of complete organs, all within a reproducible, scalable, and predictive framework Environment.(4,5)

In that sense, multiscale modeling emerges as a robust methodological strategy that seeks to integrate different levels of molecular, cellular, tissue, and systemic biological organization within a coherent computational framework. This perspective not only enriches the understanding of biological processes but also broadens the possibilities for intervention in clinical and experimental contexts. By linking different levels of analysis, a more precise and detailed approach to the behavior of living systems is achieved, thus contributing to a more functional and contextualized biological knowledge.(6)

The relevance of this multiscale strategy becomes evident when considering that many biological phenomena span multiple orders of magnitude in both space and time. From the organization of atomic bonds in proteins to the three-dimensional architecture of a tissue, each level provides essential elements for a comprehensive understanding of the system. Reducing the analysis to a single scale is tantamount to omitting critical connections, such as the transduction of molecular signals that regulate cellular processes, or the formation of tissue patterns that condition overall physiological function. Only through multiscale integration can this complexity be adequately and usefully represented.(6)

The choice of approaching multiscale modeling in systems biology responds to a specific need: the need to move towards a more integrative and predictive science in a context of accelerated growth in biomedical knowledge and associated technologies. In contrast to traditional approaches, which analyze components separately, this strategy allows a more realistic articulation of simultaneous phenomena at different levels. Its applicability is particularly relevant in scenarios such as the design of personalized treatments, tissue engineering, or the simulation of multifactorial diseases. Therefore, a critical review of current approaches, their possibilities, and limitations is not only timely but also essential to guide new lines of research and clinical applications.

In this sense, the present article aims to explore the primary approaches, applications, and computational tools associated with multiscale modeling in systems biology, emphasizing its capacity to articulate different levels of biological organization within a single conceptual and mathematical framework. The most commonly used methodologies in this field, the theoretical frameworks that support them, and their impact on strategic areas such as personalized medicine, precision pharmacology, and bioengineering are addressed.

METHOD

This article is based on a scientific literature review that identifies, analyzes, and synthesizes theoretical and applied approaches to multiscale modeling in systems biology. A qualitative approach was adopted, where an analysis and synthesis of peer-reviewed academic publications available in recognized databases is performed. The selection included articles addressing both the methodological foundations of multiscale modeling and its applications in medicine, pharmacology, and tissue engineering. The systematization of the contents enabled us to identify current trends, classify the computational tools employed, and highlight the opportunities and challenges associated with implementing these models in advanced biomedical contexts.

DEVELOPMENT

The development and implementation of multiscale modeling in systems biology have become essential pillars for a comprehensive approach to biological complexity. From this perspective, it is recognized that vital functions cannot be explained from the isolated behavior of molecules or cells, but are the result of the structured and dynamic interaction between multiple organizational levels. Far from being a mere methodological alternative, the multiscale approach responds to a fundamental empirical need in contemporary life sciences: the need to integrate molecular signals, cellular processes, and physiological functions under both normal and pathological conditions. This type of modeling is a tool capable of simulating, analyzing, and predicting the evolution of complex biological systems from a systemic, coherent, and robust viewpoint.(7)

In the context of advanced research, several theoretical and applied lines of inquiry have been developed that converge in the construction of models with increasing fidelity to the structure and function of living organisms. These proposals range from mathematical modeling of biochemical processes, such as enzyme kinetics, to computational simulations based on massive omics data.(8,9,10,11,12)

This redefines biological analysis strategies and overcomes one-dimensional approaches, which favor a more nuanced reading of phenomena. The implementation of multiscale models not only allows for the study of processes at the micro level but also enables understanding of how these alterations have repercussions on larger-scale systems, establishing a direct link between the molecular, cellular, and tissue levels. This feedback between scales is a key element in anticipating pathophysiological trajectories and designing more specific and effective therapeutic interventions.(3,13)

In addition to its impact on basic research, multiscale modeling has a significant role in clinical practice and the formulation of public health policies. Due to its predictive capacity, it is incorporated into medical decision support platforms, where genetic, environmental, and social variables converge to provide answers tailored to the individual characteristics of each patient. In a scenario marked by demographic aging and the growing prevalence of chronic diseases, these models represent a strategic approach to optimizing the use of healthcare resources and moving towards a more personalized, efficient, and preventive medicine. Thus, multiscale modeling is projected as a transformative component in the paradigm shift of the contemporary healthcare system.(7,14,15,16,17,18,19)

The hierarchical nature of biological systems necessitates methodologies that can simultaneously represent processes occurring at vastly different scales. In this sense, multiscale modeling is configured as a strategy that enables the integration of compatible mathematical representations, thereby achieving a coherent description of biological functions across all levels, from the most elementary to the most complex.20-22 Unlike traditional approaches focused on a single scale, this type of modeling establishes coupling points between levels, using hybrid models that combine deterministic and stochastic elements, and establishes bidirectional information flows between the hierarchical layers. In this way, a more comprehensive and useful systemic view is achieved to address multifactorial biological issues. Phenomena.(7,20,21,22,23)

The emergent dynamics that characterize biological processes demand tools capable of representing both discrete and continuous interactions. In this framework, multiscale models enable the simulation of phenomena with high accuracy, such as the activation of molecular signaling pathways, specific cellular responses, and the functional effects these generate at the tissue or organ level.(24,25) This ability to integrate processes at different levels has made multiscale modeling a central tool for disciplines such as personalized medicine, tissue engineering, and computational pharmacology. Moreover, its predictive potential has been leveraged in the development of computational diagnostic systems for studying complex diseases, such as cancer, pulmonary fibrosis, or neurodegenerative disorders, where pathological mechanisms operate across multiple scales of organization simultaneously.(26,27)

From a structural perspective, multiscale modeling is organized around five fundamental levels: molecular, cellular, tissue, organ, and whole organism. Each represents a level of complexity with emergent properties that must be modeled using specific approaches, but which can also be integrated into global models. Along these lines, Michael et al.(28) propose a methodological framework that links molecular receptor activation with systemic immune response in virtual cohorts of patients, allowing for the simulation of complex immunological phenomena with a high degree of realism, including antigen-antibody interaction, lymphocyte activation, and cytokine secretion at the systemic level.(29,30)

Regarding methods of cross-scale integration, two main approaches stand out: hierarchical coupling and concurrent coupling. The first consists of transferring data from a lower to a higher scale, which enables the modeling of the influence of molecular events on cellular or tissue processes. The second, more sophisticated approach allows simultaneous interaction between scales throughout the simulation. Michael et al.28 illustrate the utility of concurrent coupling in therapeutic models that integrate molecular, cellular, and tissue variables in real time. These schemes have favored the development of hybrid models adjustable to different levels of resolution, broadening their applicability in biomedical research and clinical simulation scenarios.(31,32,33,34)

The advancement of multiscale modeling has been made possible thanks to highly specialized computational tools, such as GROMACS,(35) NAMD(36), or SimBiology,(37) that enable the representation of mechanochemical processes using ordinary differential equations, molecular dynamics simulations, and gene regulatory networks. The versatility of these platforms enables the development of simulations ranging from the kinetics of molecular interactions to nutrient transport in tissues, generating computational representations with a high degree of similarity to the real behavior of biological systems.(28,38,39)

Cook et al.(40) demonstrate the successful application of multiscale models in processes such as bone remodeling, which integrate biomechanical data with molecular signaling pathways. The study by Jeżnach et al.(41) highlights how the combination of machine learning and multiscale modeling provides solutions in tissue engineering. Tools such as PhysiCell or Chaste are used in the implementation of hybrid models that combine cellular agents with mechanical networks. These applications are beneficial in simulating processes such as tumor growth, angiogenesis, and tissue regeneration under various biomechanical conditions.(42)

The integration of omics databases, such as transcriptomics, metabolomics, and proteomics, enriches models with experimental information and generates more accurate and contextualized simulations. This approach favors the development of clinical simulation platforms that incorporate artificial intelligence and high-performance computing, consolidating multiscale modeling as the backbone of current predictive biology.(42,43)

In the field of personalized medicine, this strategy enables the tailoring of treatments to the genomic and phenotypic profiles of each individual. Personalized simulations not only help to optimize doses and reduce adverse effects, but also improve overall therapeutic efficacy. Additionally, these models are utilized in the preclinical stage to validate pharmacological strategies, thereby reducing costs and development times. They are also used to simulate clinical trials in virtual cohorts, allowing more specific and representative inclusion criteria to be established.(28,42,44)

Post et al.(45) state that multiscale computational modeling allows virtual evaluation of biomaterial behavior before clinical implantation. These models consider both physicochemical properties, such as elasticity, porosity, and stiffness, as well as biological variables, including cell adhesion and degradation. This model recreates a safe and effective environment for experimentation before its real use.(45,46)

The combination of cellular and tissue models enables the prediction of the immune response to biomaterials, thereby improving biocompatibility. This capability extends to the design of innovative materials, capable of controlled drug release. In addition to responding to changes in the environment, it dynamically adapts to the host tissue.(47)

Multiscale platforms have been utilized to simulate the degradation of biodegradable polymers and bone regeneration, serving as valuable tools in the design of customized implants. These simulations enable the anticipation of complications, such as inflammation or rejection, and allow for the adjustment of material properties to optimize functionality after implantation.

CONCLUSIONS

Multiscale modeling in systems biology has been examined as an essential methodological approach to more faithfully represent the hierarchical complexity of living organisms. This approach, through constant consolidation, articulates molecular, cellular, and tissue levels in integrative computational frameworks that enable the prediction of biological behaviors and the design of advanced biomedical solutions. Its strategic value lies not only in its ability to represent complex phenomena but also in its transformative potential in areas such as personalized medicine, tissue engineering, and computational pharmacology. The effectiveness of multiscale modeling will depend on its integration with omics data, its technical interoperability, and its effective translation to the clinical setting. Ultimately, multiscale biological modeling is a scientific, technological, and ethical endeavor that demands an interdisciplinary vision, a commitment to accuracy, and a willingness to guide knowledge toward a more predictive, contextual, and humanly meaningful biology.

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CONFLICT OF INTEREST

The authors declare that there is no conflict of interest.

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