United States Patent Application Publication	20250259715
Kind Code	A1
Publication Date	August 14, 2025
Inventor(s)	Crabtree; Jason et al.

SYSTEM AND METHODS FOR AI-ENHANCED CELLULAR MODELING AND SIMULATION

Abstract

The AI-enhanced cellular modeling and simulation platform is a computational system designed to enhance biomedical research and development and personalized medicine and wellness. This platform integrates simulation modeling, machine learning and artificial intelligence, multi-omics data, and sophisticated data fusion and decision-support techniques to create comprehensive models of cellular systems and processes across multiple scales. It enables researchers and clinicians to simulate complex biological interactions, predict disease progression, and design or optimize treatment strategies or medical devices with improved accuracy and efficacy. The system's architecture allows for integration of various components, including real-time data processing, federated learning, and quantum computing enhancements. From personalized drug discovery and cancer therapies to synthetic biology and epidemiological analysis, this platform offers powerful tools for understanding and manipulating cellular systems and bioengineered systems. By bridging the gap between molecular-level interactions between cells and materials and organism-wide effects, it enables significant advancements in healthcare and biological sciences.

Inventors: **Crabtree; Jason (Vienna, VA), Kelley; Richard (Woodbridge, VA), Hopper; Jason (Halifax, CA), Park; David (Fairfax, VA)**

Applicant: **QOMPLX LLC** (Reston, VA)

Family ID: **96660058**

Appl. No.: **18/952932**

Filed: **November 19, 2024**

Related U.S. Application Data

parent US continuation-in-part 18900608 20240927 PENDING child US 18952932
parent US continuation-in-part 18801361 20240812 PENDING child US 18952932
parent US continuation-in-part 18662988 20240513 PENDING child US 18801361
parent US continuation-in-part 18656612 20240507 PENDING child US 18952932

Publication Classification

Int. Cl.: **G16C20/50** (20190101); **G16C20/30** (20190101); **G16C20/80** (20190101)

U.S. Cl.:

CPC   **G16C20/50** (20190201); **G16C20/30** (20190201); **G16C20/80** (20190201);

Background/Summary

CROSS-REFERENCE TO RELATED APPLICATIONS
[0001] Priority is claimed in the application data sheet to the following patents or patent applications, each of which is expressly incorporated herein by reference in its entirety: [0002] Ser. No. 18/900,608 [0003] Ser. No. 18/801,361 [0004] Ser. No. 18/662,988 [0005] Ser. No. 18/656,612 [0006] Ser. No. 63/551,328
BACKGROUND OF THE INVENTION
Field of the Art
[0007] The present invention is in the field of computational biology and artificial intelligence, and more particularly to artificial intelligence-enhanced cellular modeling and simulation for biomedical applications.
Discussion of the State of the Art
[0008] Cellular modeling and simulation have become indispensable tools in modern biological research, drug discovery, and increasingly personalized medicine. Traditional approaches to cellular modeling typically involve the use of differential equations to describe cellular processes, agent-based models to simulate cell-cell interactions, or statistical methods to analyze large-scale omics data. Single cell models and cell population models both have value, but single cell modeling techniques are often limited by physical contact or metabolite-based interaction between cells or insufficient consideration of factors such as limited space or resources. Probabilistic and deterministic models have both contributed to our understanding of local and broader tissue or organism level phenomena. While existing methods have provided valuable insights into cellular behavior and disease mechanisms, they are often limited in their ability to capture the sufficient complexity of real-world biological systems, especially when dealing with practical heterogeneous cell populations, dynamic microenvironments, and multi-scale interactions of interest.
[0009] Current state-of-the-art cellular modeling techniques face several limitations. First, they often struggle to integrate diverse data types, such as genomics, proteomics, metabolomics, and imaging data, into a cohesive model. Second, most existing models lack the ability to simulate cellular behavior across multiple scales, from molecular interactions to tissue-level phenomena. Third, traditional models are typically static or have limited capacity to adapt to new data in real-time, making it challenging to capture the dynamic nature of biological systems.
[0010] Furthermore, the increasing volume and complexity of biological data have outpaced the capabilities of conventional modeling approaches. The advent of single-cell technologies, high-throughput screening methods, and advanced imaging techniques has generated unprecedented amounts of data, which current modeling frameworks struggle to fully utilize. Additionally, existing models are often built to simulate either microscopic (relative to system size) detailed interactions and systems, or macroscopic (relative to the system in question) processes and

systems. Therefore, these models fail to account for, or improperly estimate, the effects and impact of processes at different scales, as well as the boundary and edge cases at the interface and emergent phenomena arising from complex cellular interactions. For example, while it is widely known that interface boundary values connected with different kinds of partial differential equations or systems may be used to represent a wide range of phenomena in biology, chemistry, engineering, and physics, the determination of appropriate boundary representations and harmonization of model outputs across detailed numerical models representing specific phenomena within each specialized domain remains a challenge, especially when variability or complexity of geometry, temperature, pressure, materials, fluids, or other composition elements inside the modeled system is high or uncertain. The field of computational biology is presently lacking comprehensive and customizable, usability focused, multiscale, computationally efficient cell simulators capable of detailed population modeling that combines specialized models across various subdomains such as models allowing for automatic quantification of key parameters of cell phenotype such as cell growth rate and doubling time, models for off-lattice simulation of growth and organization processes in multi-cellular systems in 2D and 3D, the Open Pharmacology Suite (which describes itself as a multiscale modeling and simulation of whole-body physiology, disease biology, and molecular reactions networks but has several shortcomings), or the CompuCell3D simulation environment (which describes itself as a flexible scriptable modeling environment, which allows the rapid construction of sharable virtual tissue in silico simulations of a wide variety of multi-scale, multi-cellular problems including angiogenesis, bacterial colonies, cancer, developmental biology, evolution, the immune system, tissue engineering, toxicology and even non-cellular soft materials). These systems today are designed primarily for local execution, not distributed systems, and are not optimized for production scale utilization or analysis needed to support personalized modeling and medical treatments of the future.

[0011] In the realm of personalized medicine and drug discovery, current cellular modeling approaches are limited in their ability to predict individual patient responses to treatments or to efficiently identify promising drug candidates. This is partly due to the difficulty in creating accurate, patient-specific models that account for the unique genetic and environmental factors influencing cellular behavior.

[0012] What is needed is an artificial intelligence (AI)-enhanced cellular modeling and simulation platform which leverages statistics, modeling simulation and advanced artificial intelligence and machine learning techniques to address many of the limitations of traditional modeling approaches. Such a platform can offer a comprehensive solution that integrates multi-omics data, imaging information, and clinical data into a unified analysis, simulation and modeling framework, providing a more accurate and comprehensive understanding of biological systems and informing healthcare, bioengineering and other disciplines.

SUMMARY OF THE INVENTION

[0013] Accordingly, the inventor has conceived and reduced to practice, an AI-enhanced cellular modeling and simulation platform designed to enhance biological system modeling to include biomedical research and engineering and personalized medicine or veterinary care. This platform integrates advanced artificial intelligence, multi-omics data analysis, and sophisticated simulation techniques to create comprehensive models of cellular processes across multiple scales. It enables researchers and clinicians to simulate complex biological interactions, predict disease progression, and optimize treatment strategies or medical device design utilization with improved relevance, accuracy and precision. The system's modular architecture allows for integration of various components, including real-time data processing, federated learning, and optional compatibility with advanced computing platforms and methodologies such as quantum computing. This system is also capable of modeling human altered cells. From drug discovery to personalized cancer therapies, from synthetic biology to epidemiological analysis, this platform offers powerful tools for understanding and manipulating cellular systems and pairing them with engineered materials or

devices. By bridging the gap between molecular-level interactions and organism-wide effects, it paves the way for significant advancements in healthcare and biological sciences and engineering.

[0014] According to a preferred embodiment, a computing system for designing personalized cancer therapies (e.g., including but not limited to vaccines) using AI-enhanced cellular modeling and simulation is disclosed, the computing system comprising: one or more hardware processors configured for: compiling cellular data comprising genomic, transcriptomic, proteomic, and metabolomic information from cancer cells and healthy cells; generating one or more cellular models based on the compiled cellular data; simulating interactions between potential vaccine candidates and the generated cellular models; visualizing and analyzing cellular responses to vaccine candidates across different cellular regions and time points; linking observed cellular responses to known biological pathways and previous research findings; quantifying uncertainty in vaccine efficacy predictions; iteratively optimizing vaccine design based on multiple factors including efficacy, cellular stress, and genetic stability; running multiple in silico experiments testing various combinations of vaccine components; and outputting a personalized cancer vaccine design based on the optimized vaccine design and in silico experiment results.

[0015] According to another preferred embodiment, a computer-implemented method executed on a cellular modeling and simulation platform for designing personalized cancer vaccines using AI-enhanced cellular modeling and simulation is disclosed, the computer-implemented method comprising: compiling cellular data comprising genomic, transcriptomic, proteomic, and metabolomic information from cancer cells and healthy cells; generating one or more cellular models based on the compiled cellular data; simulating interactions between potential vaccine candidates and the generated cellular models; visualizing and analyzing cellular responses to vaccine candidates across different cellular regions and time points; linking observed cellular responses to known biological pathways and previous research findings; quantifying uncertainty in vaccine efficacy predictions; iteratively optimizing vaccine design based on multiple factors including efficacy, cellular stress, and genetic stability; running multiple in silico experiments testing various combinations of vaccine components; and outputting a personalized cancer vaccine design based on the optimized vaccine design and in silico experiment results.

[0016] According to another preferred embodiment, a system for designing personalized cancer vaccines using AI-enhanced cellular modeling and simulation is disclosed, comprising one or more computers with executable instructions that, when executed, cause the system to: compile cellular data comprising genomic, transcriptomic, proteomic, and metabolomic information from cancer cells and healthy cells; generate one or more cellular models based on the compiled cellular data; simulate interactions between potential vaccine candidates and the generated cellular models; visualize and analyze cellular responses to vaccine candidates across different cellular regions and time points; link observed cellular responses to known biological pathways and previous research findings; quantify uncertainty in vaccine efficacy predictions; iteratively optimize vaccine design based on multiple factors including efficacy, cellular stress, and genetic stability; run multiple in silico experiments testing various combinations of vaccine components; and output a personalized cancer vaccine design based on the optimized vaccine design and in silico experiment results.

[0017] According to another preferred embodiment, non-transitory, computer-readable storage media having computer-executable instructions embodied thereon that, when executed by one or more processors of a computing system employing a cellular modeling and simulation platform for designing personalized cancer vaccines using AI-enhanced cellular modeling and simulation, cause the computing system to: compile cellular data comprising genomic, transcriptomic, proteomic, and metabolomic information from cancer cells and healthy cells; generate one or more cellular models based on the compiled cellular data; simulate interactions between potential vaccine candidates and the generated cellular models; visualize and analyze cellular responses to vaccine candidates across different cellular regions and time points; link observed cellular responses to known biological pathways and previous research findings; quantify uncertainty in vaccine efficacy predictions;

iteratively optimize vaccine design based on multiple factors including efficacy, cellular stress, and genetic stability; run multiple in silico experiments testing various combinations of vaccine components; and output a personalized cancer vaccine design based on the optimized vaccine design and in silico experiment results.

[0018] According to an aspect of an embodiment, the one or more hardware processors are further configured for: identifying potential vaccine candidates based on specific cellular characteristics of a patient's cancer cells by inverting the simulation process.

[0019] According to an aspect of an embodiment, simulating interactions between potential vaccine candidates and the generated cellular models further comprises: predicting off-target interactions and influence on gene expression patterns over time for each vaccine candidate.

[0020] According to an aspect of an embodiment, the one or more hardware processors are further configured for: incorporating whole-slide imaging data for enhanced cancer subtyping and mutation prediction to refine the generated cellular models.

[0021] According to an aspect of an embodiment, the one or more hardware processors are further configured for: generating a comparative analysis of potential treatment options based on predicted health outcomes, quality of life considerations, and economic factors associated with the system produced personalized vaccine design.

Description

BRIEF DESCRIPTION OF THE DRAWING FIGURES

[0022] FIG. **1** is a block diagram illustrating an exemplary system architecture for an AI-enhanced cellular modeling and simulation, according to an embodiment.

[0023] FIG. **2** is a block diagram illustrating an exemplary system architecture for an artificial intelligence enhanced drug discovery platform, according to an embodiment.

[0024] FIG. **3** is a high-level architecture diagram of an exemplary personal health database (PHDB) platform, according to an aspect.

[0025] FIG. **4** is a block diagram illustrating an exemplary aspect of an embodiment of the AI-enhanced cellular modeling and simulation platform.

[0026] FIG. **5** illustrates a distributed embodiment of the system across a plurality of cloud and edge devices.

[0027] FIG. **6** is a block diagram illustrating an exemplary embodiment of AI-enhanced cellular modeling and simulation platform configured for federated learning.

[0028] FIG. **7** is a block diagram illustrating an aspect of the AI-enhanced cellular modeling and simulation platform, a real-time adaptive cellular modeling and treatment planning system.

[0029] FIG. **8** is a block diagram illustrating an exemplary system architecture for an AI-enhanced cellular modeling and simulation platform comprising a personalized medicine system, according to an embodiment.

[0030] FIG. **9** is a block diagram illustrating an aspect of the AI-enhanced cellular modeling and simulation platform, a personalized medicine system.

[0031] FIG. **10** is a block diagram illustrating an exemplary system architecture for an AI-enhanced cellular modeling and simulation platform comprising a drug discovery system, according to an embodiment.

[0032] FIG. **11** is a block diagram illustrating an aspect of an AI-enhanced cellular modeling and simulation platform, a drug discovery system.

[0033] FIG. **12** is a block diagram illustrating an exemplary system architecture for an AI-enhanced cellular modeling and simulation platform comprising a cellular engineering system, according to an embodiment.

[0034] FIG. **13** is a block diagram illustrating an aspect of an AI-enhanced cellular modeling and

simulation platform, a cellular engineering system.

[0035] FIG. **14** is a block diagram illustrating an exemplary system architecture for an AI-enhanced cellular modeling and simulation platform comprising a synthetic biology system, according to an embodiment.

[0036] FIG. **15** is a block diagram illustrating an aspect of an AI-enhance cellular modeling and simulation platform, a synthetic biology system.

[0037] FIG. **16** is a block diagram illustrating an exemplary system architecture for an AI-enhanced cellular modeling and simulation platform comprising a microbiome simulation and monitoring system, according to an embodiment.

[0038] FIG. **17** is a block diagram illustrating an aspect of an AI-enhanced cellular modeling and simulation platform, a microbiome simulation and monitoring system.

[0039] FIG. **18** is a block diagram illustrating an exemplary system architecture for an AI-enhanced cellular modeling and simulation platform comprising a phage dynamics analysis system, according to an embodiment.

[0040] FIG. **19** is a block diagram illustrating an aspect of an AI-enhanced cellular modeling and simulation platform, a phage dynamics analysis system.

[0041] FIG. **20** is a block diagram illustrating an exemplary system architecture for an AI-enhanced cellular modeling and simulation platform comprising an epidemiological analysis system, according to an embodiment.

[0042] FIG. **21** is a block diagram illustrating an aspect of an AI-enhanced cellular modeling and simulation platform, an epidemiological analysis system.

[0043] FIG. **22** is a block diagram illustrating an exemplary system architecture for an AI-enhanced cellular modeling and simulation platform configured for ecosystem-level analysis, according to an embodiment.

[0044] FIG. **23** is a block diagram illustrating an aspect of an AI-enhanced cellular modeling and simulation platform, an ecosystem-level analysis system.

[0045] FIG. **24** is a block diagram illustrating an exemplary system architecture for an AI-enhanced cellular modeling and simulation platform configured for AI-enhanced image analysis in histology and pathology, according to an embodiment.

[0046] FIG. **25** is a block diagram illustrating an aspect of an AI-enhanced cellular modeling and simulation platform, an AI image analysis system.

[0047] FIG. **26** is a block diagram illustrating an exemplary system architecture for an AI-enhanced cellular modeling and simulation platform configured for quantum computing in advanced applications of cellular modeling, according to an embodiment.

[0048] FIG. **27** is a block diagram illustrating an aspect of an AI-enhanced cellular modeling and simulation platform, a quantum computing cellular modeling system.

[0049] FIG. **28** is a block diagram illustrating an exemplary system architecture for an AI-enhanced cellular modeling and simulation platform configured for quantum computing in advanced applications of cellular modeling, according to an embodiment.

[0050] FIG. **29** is a block diagram illustrating an aspect of an AI-enhanced cellular modeling and simulation platform, an AI predictive oncology system.

[0051] FIG. **30** is a block diagram illustrating an exemplary system architecture for an AI-enhanced cellular modeling and simulation platform configured for simulating basal cognition with oncology and regenerative medicine applications, according to an embodiment.

[0052] FIG. **31** is a block diagram illustrating an aspect of an AI-enhanced cellular modeling and simulation platform, an oncology simulation and regenerative medicine system.

[0053] FIG. **32** is a block diagram illustrating an exemplary system architecture for an AI-enhanced cellular modeling and simulation platform configured for advanced image analysis and simulation, according to an embodiment.

[0054] FIG. **33** is a block diagram illustrating an aspect of an AI-enhanced cellular modeling and

simulation platform, an advanced image analysis and simulation system.

[0055] FIG. **34** is a flow diagram illustrating an exemplary method for designing personalized cancer vaccines, according to an embodiment.

[0056] FIG. **35** is a flow diagram illustrating an exemplary federated learning process for training a cellular model across one or more separate institutions, according to an embodiment.

[0057] FIG. **36** is a flow diagram illustrating an exemplary method for real-time adaptive modeling, according to an embodiment.

[0058] FIG. **37** is a flow diagram illustrating an exemplary method for providing uncertainty quantification, according to an embodiment.

[0059] FIG. **38** is a flow diagram illustrating an exemplary method for personalized treatment optimization, according to an embodiment.

[0060] FIG. **39** is a flow diagram illustrating an exemplary method for cellular imaging analysis, according to an embodiment.

[0061] FIG. **40** is a flow diagram illustrating an exemplary method for providing personalized medicine, according to an embodiment

[0062] FIG. **41** is a flow diagram illustrating an exemplary method for providing drug discovery using an AI-enhanced cellular modeling and simulation platform, according to an embodiment.

[0063] FIG. **42** is a flow diagram illustrating an exemplary method for providing cellular engineering using the AI-enhanced cellular modeling and simulation platform, according to an embodiment.

[0064] FIG. **43** is a flow diagram illustrating an exemplary method for providing synthetic biology design and simulation, according to an embodiment.

[0065] FIG. **44** is a flow diagram illustrating an exemplary method for microbiome simulation and monitoring, according to an embodiment.

[0066] FIG. **45** is a flow diagram illustrating an exemplary method for phage dynamics analysis, according to an embodiment.

[0067] FIG. **46** is a flow diagram illustrating an exemplary method for applying epidemiological analysis, according to an embodiment.

[0068] FIG. **47** is a flow diagram illustrating an exemplary method for ecosystem-level analysis in cancer, according to an embodiment.

[0069] FIG. **48** is a flow diagram illustrating an exemplary method for ecosystem-level analysis in endometriosis, according to an embodiment.

[0070] FIG. **49** is a flow diagram illustrating an exemplary method for AI-image analysis in histology and pathology, according to an embodiment.

[0071] FIG. **50** is a flow diagram illustrating an exemplary method for quantum computing cellular modeling, according to an embodiment.

[0072] FIG. **51** is a flow diagram illustrating an exemplary method for facilitating AI predictive oncology, according to an embodiment.

[0073] FIG. **52** is a flow diagram illustrating an exemplary method for simulating basal cognition, according to an embodiment.

[0074] FIG. **53** is a flow diagram illustrating an exemplary method for advanced image analysis and simulation, according to an embodiment.

[0075] FIG. **54** is a block diagram illustrating an exemplary system architecture for an AI-enhanced cellular modeling and simulation platform configured for enhanced patient communication, according to an embodiment.

[0076] FIG. **55** is a block diagram illustrating an aspect of an AI-enhanced cellular modeling and simulation platform, a patient communication system.

[0077] FIG. **56** illustrates an exemplary computing environment on which an embodiment described herein may be implemented.

DETAILED DESCRIPTION OF THE INVENTION

[0078] The inventor has conceived, and reduced to practice, an AI-enhanced cellular modeling and simulation platform designed to enhance biomedical research and personalized medicine which integrates advanced artificial intelligence, multi-omics data analysis, and sophisticated simulation techniques to create comprehensive models with multiple collaborative models using a variety of techniques including simulation modeling and machine learning of cellular processes across multiple scales and finite time periods.

[0079] The platform's ability to perform multi-scale simulations, from molecular to tissue levels, provides a more holistic understanding of cellular systems. Its use of AI algorithms enables the platform to adapt and learn from new data in real-time, creating dynamic models that evolve as more information becomes available. This adaptability is particularly useful in capturing the complexity of biological systems and in personalizing models for individual patients across a range of healthcare and veterinary care stages from preventative medicine and wellness to therapeutics or medical device selection and implantation.

[0080] Moreover, the AI-cellular modeling system's advanced computational capabilities allow it to process and analyze vast amounts of heterogeneous data, extracting meaningful patterns and relationships that might be missed by conventional methods. The platform's incorporation of both deterministic and stochastic modeling approaches and its ability to simulate emergent behaviors provide a more realistic representation of cellular processes at single cell, group of cells, local tissue, regional multi-tissue, tissue and engineered object(s), or whole organism levels.

[0081] In the context of drug discovery and personalized medicine, the platform offers additional predictive power. It can simulate drug responses at local (e.g. the cellular), regional e.g. tissue, or patient levels (both singular or group), potentially accelerating the drug development and certification process and enabling more precise, personalized treatment strategies. The system's ability to integrate real-time data from various sources, including wearable devices and continuous monitoring systems, further enhances its utility in clinical settings.

[0082] By addressing the limitations of current cellular modeling techniques and leveraging the power of modeling simulation alongside AI techniques, e.g. as verification, approximation, explanation, error estimation, or as empirical vs theoretical approach comparison tools, the AI-enhanced cellular modeling and simulation platform represents a significant advancement in the field. It has the potential to enhance the understanding of cellular biology, accelerate scientific discovery, and improve patient outcomes through more accurate and personalized modeling approaches.

[0083] According to various embodiments, the AI-enhanced cellular modeling and simulation platform also optionally integrates the Expansion in situ genome sequencing (ExIGS) technique and its findings to significantly enhance its capabilities across multiple application domains. By incorporating the high-resolution spatial genomics and protein imaging data from ExIGS, the platform can refine its existing multi-scale modeling and 'omics mapping framework, allowing for more precise representation of nuclear structures and chromatin organization and tracking 'omics data with spatio-temporal details and linking gene expression to specific cells and tissue(s). The platform's data integration layer can be expanded to handle the rich, multi-modal data generated by ExIGS, combining genomic sequences, protein localizations, and spatial information into a unified data model. This enhanced data integration enables the platform to create more detailed and accurate cellular digital twins, particularly in modeling nuclear dynamics and gene regulation processes.

[0084] The platform's AI and machine learning core can be updated to leverage the insights gained from ExIGS studies, particularly in understanding the relationship between nuclear morphology and chromatin organization. The platform can also incorporate the additional data sources into its data comparison and selection and dimensionality reduction (e.g. PCA vs ICA vs InformationSieve) techniques during machine learning or AI method model training and tuning activities for a given patient, group or disease/phenomenon modeling initiative. New algorithms

may be implemented to detect and analyze lamin abnormalities and their associated euchromatin repression hotspots, allowing the platform to more accurately model how structural changes in the nucleus affect gene expression and cellular function, with awareness of surrounding tissue and changes over time within a patient or related to disease progression or healing from a disease or injury. This improved modeling of nuclear dynamics enhances the platform's ability to simulate cellular aging processes and disease and healing progressions, especially for conditions involving nuclear envelope proteins like progeria. The platform's ability to help patients, providers, researchers and payers understand more of the progression dynamics can aid in expectation management, supplemental treatment and support optimization and superior health and mental health outcomes in addition to economic efficiencies.

[0085] The simulation capabilities of the platform can be expanded to include more detailed models of chromatin-lamin interactions, incorporating the stochastic nature of disruption hotspots observed in the ExIGS data. This may allow for more realistic simulations of how cellular stressors or genetic variations might lead to changes in nuclear organization and gene regulation. The system's ability to not only model systems which have inherent complex system characteristics but also exhibit reflexive phenomena is critical here, for example, in this case the lamina-associated domains that are shaped by, and shape, epigenomic states and high-order genome architecture in eukaryotes. The platform's personalized medicine module may be significantly enhanced, using the high-resolution, single-cell data from ExIGS to create more accurate patient-specific models that address LAD heterogeneity from relevant cell ensemble and single-cell data. This improvement enables better predictions of individual responses to treatments, particularly for therapies targeting nuclear processes or age-related disorders.

[0086] Furthermore, the platform's tissue modeling capabilities may be refined based on the ExIGS observations of lamin variations in different cell types and tissues. This allows for more nuanced simulations of tissue-specific cellular behaviors and interactions. The visualization component of the platform can be upgraded to render the super resolution data provided by ExIGS, offering researchers and clinicians more detailed and intuitive visual representations of cellular structures and processes.

[0087] The AI-enhanced cellular modeling and simulation platform integrates the ExIGS technique to significantly enhance its capabilities, particularly in the realm of intact cell analysis. The platform's data acquisition module can be expanded to incorporate the ExIGS methodology, enabling the simultaneous sequencing of DNA and precise localization of proteins within intact cells. This integration allows the platform to generate highly detailed, spatially resolved genomic and proteomic data without disrupting cellular structures. The platform's AI algorithms can be updated to process and interpret this rich, multi-modal data, creating more accurate 3D models of cellular interiors, with a specific focus on nuclear organization and chromosome territories.

[0088] The platform's simulation engine can be refined to leverage this high-resolution data, enabling more precise modeling of DNA packaging, protein-DNA interactions, and their effects on gene regulation. This enhancement may allow for more accurate predictions of how cellular processes are affected by changes in nuclear architecture, particularly in the context of aging and disease. The platform may be configured with advanced machine learning algorithms that can identify subtle patterns in protein localization and DNA organization, providing insights into cellular states that were previously undetectable. Furthermore, the system's ability to model cell-to-cell variability is significantly improved, as it can now account for fine-scale differences in nuclear organization and protein distribution among individual cells within a population.

[0089] The platform's disease modeling capabilities can be expanded to include more detailed representations of conditions like progeria, leveraging the ExIGS findings on lamin protein abnormalities and their effects on gene suppression. This allows for more accurate simulations of disease progression and potential treatment outcomes. An aging simulation module may be enhanced, incorporating the observed changes in nuclear protein interactions and gene activity

suppression over time. These improvements enable the platform to provide more nuanced and personalized predictions of cellular behavior in response to various stimuli, aging processes, and therapeutic interventions. By integrating the ExIGS technique, the AI-enhanced cellular modeling platform significantly advances its ability to provide comprehensive, high-resolution insights into cellular function, offering researchers and clinicians a powerful tool for understanding complex biological processes and developing targeted therapeutic strategies.

[0090] One or more different aspects may be described in the present application. Further, for one or more of the aspects described herein, numerous alternative arrangements may be described; it should be appreciated that these are presented for illustrative purposes only and are not limiting of the aspects contained herein or the claims presented herein in any way. One or more of the arrangements may be widely applicable to numerous aspects, as may be readily apparent from the disclosure. In general, arrangements are described in sufficient detail to enable those skilled in the art to practice one or more of the aspects, and it should be appreciated that other arrangements may be utilized and that structural, logical, software, electrical and other changes may be made without departing from the scope of the particular aspects. Particular features of one or more of the aspects described herein may be described with reference to one or more particular aspects or figures that form a part of the present disclosure, and in which are shown, by way of illustration, specific arrangements of one or more of the aspects. It should be appreciated, however, that such features are not limited to usage in the one or more particular aspects or figures with reference to which they are described. The present disclosure is neither a literal description of all arrangements of one or more of the aspects nor a listing of features of one or more of the aspects that must be present in all arrangements.

[0091] Headings of sections provided in this patent application and the title of this patent application are for convenience only, and are not to be taken as limiting the disclosure in any way.

[0092] Devices that are in communication with each other need not be in continuous communication with each other, unless expressly specified otherwise. In addition, devices that are in communication with each other may communicate directly or indirectly through one or more communication means or intermediaries, logical or physical.

[0093] A description of an aspect with several components in communication with each other does not imply that all such components are required. To the contrary, a variety of optional components may be described to illustrate a wide variety of possible aspects and in order to more fully illustrate one or more aspects. Similarly, although process steps, method steps, algorithms or the like may be described in a sequential order, such processes, methods and algorithms may generally be configured to work in alternate orders, unless specifically stated to the contrary. In other words, any sequence or order of steps that may be described in this patent application does not, in and of itself, indicate a requirement that the steps be performed in that order. The steps of described processes may be performed in any order practical. Further, some steps may be performed simultaneously despite being described or implied as occurring non-simultaneously (e.g., because one step is described after the other step). Moreover, the illustration of a process by its depiction in a drawing does not imply that the illustrated process is exclusive of other variations and modifications thereto, does not imply that the illustrated process or any of its steps are necessary to one or more of the aspects, and does not imply that the illustrated process is preferred. Also, steps are generally described once per aspect, but this does not mean they must occur once, or that they may only occur once each time a process, method, or algorithm is carried out or executed. Some steps may be omitted in some aspects or some occurrences, or some steps may be executed more than once in a given aspect or occurrence.

[0094] When a single device or article is described herein, it will be readily apparent that more than one device or article may be used in place of a single device or article. Similarly, where more than one device or article is described herein, it will be readily apparent that a single device or article may be used in place of the more than one device or article.

[0095] The functionality or the features of a device may be alternatively embodied by one or more other devices that are not explicitly described as having such functionality or features. Thus, other aspects need not include the device itself.

[0096] Techniques and mechanisms described or referenced herein will sometimes be described in singular form for clarity. However, it should be appreciated that particular aspects may include multiple iterations of a technique or multiple instantiations of a mechanism unless noted otherwise. Process descriptions or blocks in figures should be understood as representing modules, segments, or portions of code which include one or more executable instructions for implementing specific logical functions or steps in the process. Alternate implementations are included within the scope of various aspects in which, for example, functions may be executed out of order from that shown or discussed, including substantially concurrently or in reverse order, depending on the functionality involved, as would be understood by those having ordinary skill in the art.

Conceptual Architecture

[0097] FIG. **1** is a block diagram illustrating an exemplary system architecture for an AI-enhanced cellular modeling and simulation, according to an embodiment. This figure provides a bird's-eye view of the overall AI-enhanced cellular modeling and simulation platform **100**. According to the embodiment, platform **100** comprises a data integration layer **110**, a visualization and user interface **115**, an AI model layer **120**, a distributed computational graph (DCG) platform **125**, an AI drug discovery platform **130**, and a personal health database (PHDB) computing platform **135**. The diagram illustrates how these components interact with each other and connect to external data sources **140**. It also depicts different user types, such as researchers **151**, healthcare professionals **152**, and PHDB users **153**, interacting with the system.

[0098] The AI-enhanced cellular modeling and simulation platform, with its integrated capabilities from the AI drug discovery **130**, PHDB **135**, and DCG platforms **125**, can support a wide range of cellular modeling and simulation types, spanning from single cell to cellular ensemble, from the microscopic to the macroscopic levels of biological organization, and from empirical observation to hybrid empirical and simulated to full in silico simulation modeling. At the most fundamental level, the platform excels in single-cell modeling, simulating the intricate internal processes, gene expression patterns, protein interactions, and responses to stimuli within individual cells, be they simple prokaryotes or complex eukaryotic cells. This capability extends seamlessly into multi-cellular modeling, where the platform can simulate the complex interactions between multiple cells, including cell-cell communication, tissue formation, and collective cell behavior, ranging from simple bacterial colonies to intricate human tissues. The platform's versatility allows it to tackle more specialized modeling tasks, such as organ-on-a-chip simulations that mimic physiological conditions of organs in microfluidic devices, whole-organ modeling that integrates multiple tissue types, and even multi-organ system modeling to study the intricate interactions between different organs.

[0099] The platform's capabilities extend to developmental modeling, simulating the complex cellular processes during embryonic development, including cell differentiation, morphogenesis, and organogenesis. It can also handle sophisticated cancer modeling, simulating tumor growth, metastasis, and the complex tumor microenvironment. The immune system, with its myriad cell types and intricate interactions, can be modeled to study inflammation processes and responses to pathogens or cancer cells. Neuron and neural network modeling capabilities allow for the simulation of individual neurons and their connections, as well as larger neural networks, providing insights into brain function and neurological disorders. Stem cell behavior, including self-renewal and differentiation processes, can be simulated to study their potential in tissue regeneration. The platform can even model the complex microbiome communities in various body sites, simulating their interactions with host cells and their impact on health and disease.

[0100] Furthermore, platform's **100** integration with drug discovery capabilities enables advanced pharmacokinetic/pharmacodynamic (PK/PD) cellular modeling, combining cellular models with

drug distribution and effect models to predict how drugs interact with cells and tissues over time. It can simulate cellular aging processes, epigenetic modifications in response to environmental factors, and complex metabolic pathways. Signal transduction modeling focuses on how cells process and respond to external signals, while cell cycle and division modeling simulates the processes of cell growth, DNA replication, and cell division. The platform can also model cellular stress responses to various stressors, interactions with the extracellular matrix, and cellular transport processes. These diverse modeling capabilities can be combined and integrated as needed to create comprehensive, multi-scale models that capture the full complexity of biological systems. The platform's advanced AI capabilities, coupled with its ability to integrate diverse data types and perform distributed computations, make it exceptionally well-suited to handle these complex modeling tasks and generate insights that can significantly advance our understanding of cellular biology and its applications in medicine and biotechnology.

[0101] Data integration layer **110** is responsible for ingesting, preprocessing, and harmonizing diverse types of data from various sources, creating a unified and coherent data model that can be leveraged by other components of the platform. The complexity of this layer stems from the heterogeneity of data types involved in cellular modeling, ranging from molecular-level information to tissue-level observations. At its core, the data integration layer employs a distributed computing architecture, utilizing technologies such as Apache Spark, Apache Flink, or Apache Beam for scalable data processing. This allows the system to handle large volumes of data efficiently, which is important when dealing with high-throughput omics data or time-series data from cellular simulations. According to an aspect, the system implements a flexible, schema-on-read approach using data lake technologies like Delta Lake or Apache Hudi, allowing it to ingest and store raw data in its original format while providing structure and consistency for downstream analysis.

[0102] For data ingestion, the ingestion layer may employ a variety of connectors and application programming interfaces (APIs) to interface with different data sources. This can comprise RESTful APIs for web-based data retrieval, JDBC/ODBC connectors for relational databases or equivalents for various NoSQL systems, and specialized connectors for scientific instruments and IoT devices. The system may also incorporate a data streaming component, using technologies like Apache Kafka and Apache Flink or Apache Beam, to handle real-time data streams from ongoing experiments or continuous cellular or sensor monitoring.

[0103] Once data is ingested, it undergoes a series of preprocessing steps. This may comprise data cleaning to handle missing values and outliers, using techniques like multiple imputation or anomaly detection algorithms. Data normalization can be performed to bring different data types to comparable scales, which is important when integrating data from diverse sources. Schematization, normalization, quality checks and semantification steps may all be taken by system and synthetic data (e.g. at a sensor or spatial or temporal resolution) may be created and analyzed or persisted in addition to or in lieu of the original reported, sensed, inferred, or synthetically constructed data. For omics data, this might involve techniques like quantile normalization for gene expression data or total ion current normalization for metabolomics data.

[0104] The AI-enhanced cellular modeling and simulation platform is designed to integrate with a wide variety of external data sources **140** such as databases, Internet-of-Things (IoT) devices, sensors, real-time data streams, external computational resources, collaborative platforms, and other data sources. Databases may comprise, but are not limited to, protein databases, large chemical databases, drug and target databases, structural databases, biological context databases, virtual screening databases, tissue databases, bioengineered or medical device databases, materials science databases, and clinical and toxicology databases. IoT devices may comprise, but are not limited, lab instruments (e.g., automated cell culture systems, high-throughput screening systems, etc.), environmental sensors (e.g., for monitoring laboratory conditions or exposure history), wearable devices (e.g., for collecting real-time physiological data in clinical trials or radiation

exposure over time), smart pills and drug delivery systems, implantable sensors (e.g., for real-time pharmacokinetic monitoring or kinesiology). Sensors can include, but are not limited to, microfluidic devices (e.g., for monitoring cellular processes), mass spectrometers, imaging systems (e.g., microscopes, MRI, CT scanners, etc.), biosensors, continuous glucose monitors or blood monitors, oxygen or heart rate monitors, breathing or heart rate monitors, kidney or liver function monitors, pancreas monitors or artificial pancreas, and temperature sensors, to name a few. Real-time data streams may comprise continuous monitoring devices in clinical settings, real-time sequencing data, and/or live cell or cellular ensemble or tissue imaging or sensing feeds. External computational resources can include, but are not limited to, high-performance computing clusters, cloud computing services, and specialized AI and machine learning services. Collaborative platforms can include research data sharing platforms, open science initiatives, and federated learning systems for multi-institutional collaborations. Other data sources can include, but are not limited to, electronic health records (EHRs) genomic sequencing data, multi-omics data (e.g., proteomics data, metabolomics data, transcriptomics data, etc.), imaging data (e.g., cellular imaging, tissue samples, etc.), literature databases (e.g. for natural language processing or LLM based extraction or analysis of scientific publications), clinical trial data or simulated trial data, environmental data sources (e.g. for studying environmental impacts on cellular processes for biological or anatomical modeling), and biobanks or tissue repositories.

[0105] The platform's data integration layer is designed to handle this diverse range of data sources **140**, using various connectors, APIs, and data harmonization techniques to create a unified data model. This comprehensive integration of diverse data sources enables the platform to provide a holistic view of cellular processes and supports more accurate modeling and simulation capabilities.

[0106] Platform **100** may comprise a visualization and user interface **115** which can incorporate functionalities from AI drug discovery platform **130** to enhance the way researchers interact with cellular models and data. This interface can provide intuitive, interactive visualizations of complex cellular processes, allowing researchers to explore multi-dimensional datasets and simulation results. It may incorporate advanced 3D rendering techniques for visualizing molecular and cellular structures, and use techniques like dimensionality reduction and t-SNE plots for visualizing high-dimensional omics data. For example, when studying the process of embryonic development, this system could provide an interactive 4D visualization of a developing embryo, allowing researchers to zoom in from the organism level to specific tissues, down to individual cells and even molecular interactions. Users could track the expression of specific genes over time and space, visualize morphogen gradients and their effects on cell fate decisions, and interactively perturb the system to see the effects of various experimental manipulations. The interface can also provide real-time visualizations of running simulations, allowing researchers to monitor and interactively adjust parameters as the simulation progresses.

[0107] The AI model layer **120** is a modular, scalable architecture designed to support a wide range of AI and ML techniques. The layer may be built on a distributed computing framework, such as TensorFlow on Kubernetes or PyTorch on Ray, allowing it to scale across multiple GPUs and nodes for training large, complex models. This architecture supports both synchronous and asynchronous training paradigms, enabling efficient utilization of computational resources for different types of models.

[0108] The AI model layer incorporates a diverse set of machine learning algorithms, ranging from traditional statistical methods to advanced deep learning models. This includes options such as supervised learning algorithms (e.g., random forests, support vector machines, gradient boosting machines) for tasks like cellular classification and regression, semi-supervised learning (e.g. training), unsupervised learning methods (e.g., clustering algorithms, dimensionality reduction techniques) for exploring data structure and identifying cellular subtypes, and reinforcement learning algorithms for optimizing cellular processes or experimental designs or improving model

or data set selection.

[0109] A component of this layer is its deep learning subsystem, which includes architectures specifically tailored for cellular and molecular data. In one embodiment, system may include graph neural networks (GNNs) for modeling molecular structures and cellular interaction networks, recurrent neural networks (RNNs) and transformers for capturing temporal dynamics in cellular processes, and convolutional neural networks (CNNs) for analyzing cellular imaging data. The system also incorporates advanced architectures like variational autoencoders (VAEs) for generating and modeling cellular states, and generative adversarial networks (GANs) for simulating cellular behaviors and generating synthetic data. Such techniques may also be combined with finite element analysis of structures, computational fluid dynamics of fluid flows (e.g. blood or air), and fluid-structure analysis or discrete event simulation. Here we note that examples may include whole organism or cardiovascular system health or heart health or more localized modeling—e.g. where finite element analysis of a stent device is combined with artery modeling using optimized boundary condition parameter and model selections to optimize the design or selection of a stent to minimize re-stenosis occurrence and development based on the specific artery, plaque conditions and types, lifestyle and diet history and future expectations and other anatomical and biological factors of the patient. This can aid in relative value discussions with patients (such as Cobalt Chromium vs Stainless Steel) based on age, cost, and other biomechanical suitability factors including stent shape, design and placement methodologies. The distributed computational graph computing platform **125** can enhance the functionality of the AI-enhanced cellular modeling and simulation platform by providing a robust, scalable, and flexible framework for managing complex computational workflows of immense scale and with substantial variability. The DCG's ability to represent computational tasks as nodes in a graph and data flows as edges allows for efficient orchestration of the diverse and often interconnected processes involved in cellular modeling and simulation. This graph-based approach enables the platform to dynamically allocate computational resources, parallelize tasks where possible, and optimize data movement, which is important when dealing with the computationally intensive and data-rich nature of advanced cellular modeling. It also ensures auditability of all data and analytic processes used to inform specific healthcare decisions or recommendations made by versioned models, record states, or providers over time.

[0110] The DCG's distributed architecture can be leveraged to scale cellular simulations across multiple computing resources, from local clusters to cloud environments. This scalability is particularly valuable for handling large-scale cellular models or running multiple simulations simultaneously, such as in parameter sweeps or sensitivity analyses. The platform's ability to handle heterogeneous computing environments can be utilized to optimize different aspects of cellular modeling (e.g., using GPUs for computationally intensive tasks like molecular dynamics simulations while leveraging CPUs for data preprocessing or analysis tasks).

[0111] Moreover, the DCG's fault-tolerance and resilience features can significantly improve the reliability of long-running cellular simulations. By automatically handling node failures and redistributing work, the platform can ensure that complex, time-consuming model runs or simulations are not lost due to hardware issues or network problems or limitations. The DCG's support for checkpointing and state persistence can be adapted to allow cellular simulations to be paused, resumed, or even migrated between different computing environments, providing flexibility in how researchers manage their computational resources.

[0112] The DCG's ability to represent and manage complex dependencies between computational tasks can be particularly beneficial for multi-scale cellular modeling. It can efficiently orchestrate the flow of information between models operating at different biological scales, from molecular interactions to cellular behaviors to tissue-level effects, ensuring that updates at one scale are propagated appropriately to other scales. This capability can enable more holistic and realistic cellular simulations that capture the complex interplay between different biological processes.

[0113] Furthermore, the DCG's support for dynamic workflow modification can be leveraged to

implement adaptive simulation strategies. For example, the platform could automatically refine the resolution of a simulation in regions of interest or dynamically adjust the simulation parameters based on intermediate results. This adaptivity can lead to more efficient use of computational resources and enable more sophisticated exploration of cellular behaviors.

[0114] The DCG's inherent support for data provenance tracking can be utilized to enhance the reproducibility and transparency of cellular modeling experiments. By maintaining a complete record of all computational steps and data transformations, the platform can provide researchers with detailed insights into how simulation results were obtained, facilitating validation and peer review processes.

[0115] Additionally, the DCG's ability to integrate with various data sources and external services can be exploited (e.g., via data integration layer or data integration tasks such as schematization, normalization or semantification or database specific transformations **110**) to incorporate real-time data feeds into cellular simulations. This allows for optional dynamic updating of cellular models based on incoming experimental data or even real-time physiological data from patients, enabling more responsive and relevant simulations or predictive analysis closely tailored to potential healthcare decisions including but not limited to prescriptions, therapies, imaging, or scheduling.

[0116] In some implementations, the use of federated DCG's that support federated computing can be leveraged to enable collaborative cellular modeling efforts across multiple institutions or entities or users. This can facilitate the sharing of data, models, computational resources and expertise while maintaining data privacy and security, which is particularly important when working with sensitive genetic or clinical data in cellular modeling applications. Narrowly tailored data exchange and computational process consistency and interoperability via DCG publication (or DCG specified components or tasks or jobs in an interoperable fashion) or federation supports more predictable, understandable and ultimately usable analysis to inform medical processes and modeling for patients, providers, payers and regulators.

[0117] For more detailed description of the operation and functionality of the DCG computing platform and variants thereof, please refer to U.S. patent application Ser. No. 18/656,612, which is incorporated herein by reference.

[0118] By integrating these capabilities of the DCG computing platform, the AI-enhanced cellular modeling and simulation platform can achieve scalability, flexibility, and sophistication in its computational workflows. This integration can enable researchers to tackle more complex and realistic cellular modeling challenges, run larger-scale simulations, and more efficiently explore the vast parameter spaces involved in cellular biology, ultimately accelerating progress in our understanding of cellular processes and their implications for health and disease.

[0119] The AI drug discovery platform **130** can significantly enhance the functionality of AI-enhanced cellular modeling and simulation platform **100** by providing a suite of advanced tools and capabilities specifically tailored to drug-related aspects of cellular biology. The drug discovery platform's sophisticated AI and machine learning algorithms can be integrated into the cellular modeling platform to improve predictive capabilities, especially in areas related to drug-cell interactions, pharmacokinetics, and pharmacodynamics. For instance, the drug discovery platform's ability to predict drug-target interactions at the molecular level can be incorporated into cellular simulations, allowing for more accurate modeling of how potential drug candidates might affect specific cellular processes or pathways.

[0120] The multi-scale modeling capabilities of the drug discovery platform can be leveraged to bridge the gap between molecular-level interactions and cellular-level effects in the cellular modeling platform. This integration may allow researchers **151** to simulate and visualize how changes at the molecular level, such as the binding of a drug to a target protein, propagate through cellular networks and ultimately affect cell behavior. The drug discovery platform's advanced simulation capabilities, including quantum-classical hybrid computing for molecular dynamics simulations, can be incorporated to enhance the accuracy and scale of cellular simulations,

particularly in modeling complex phenomena like protein folding or membrane transport processes.

[0121] Moreover, the drug discovery platform's data integration and knowledge graph components (e.g., implemented using one or more systems such as Neptune, Neo4j, Apache Hugegraph, Apache GraphAR, etc.) can significantly enrich the cellular modeling platform's data ecosystem. By incorporating drug-related data and knowledge, including information about known drug effects, off-target interactions, and drug metabolism, the cellular modeling platform can provide more comprehensive and context-aware simulations. This integration can be particularly valuable for studying drug effects on cellular processes, predicting potential side effects, and identifying new therapeutic targets.

[0122] The AI drug discovery platform's capabilities in personalized medicine and combination therapy optimization can be adapted to enhance the cellular modeling platform's ability to model patient-specific cellular responses. This may comprise integrating genetic and phenotypic data to create personalized cellular models, which could then be used to predict individual responses to different drugs or combinations of drugs. The platform's ability to model environmental factors and their impact on drug efficacy may also be incorporated, allowing for more realistic simulations that take into account the complex interplay between cells, drugs, and the extracellular environment.

[0123] Furthermore, drug discovery platform's **130** advanced visualization tools can be integrated to enhance the cellular modeling platform's user interface **115**, providing researchers with more intuitive ways to interact with and interpret complex cellular data and simulations at snapshots in time or across time for both empirical data, space-time stabilized representations of empirical data, or synthetic data or combinations of empirical and synthetic data, such as differences between observations or models. Common uses for such comparative visualization include model parameter selection and model type selection to aid users in better understanding or selecting parameter sets or model types or structures being used in downstream decision-making or approvals or automated actions and responses from people or robots. This system is designed to send resulting anatomical and biological system models into robotics planning and control processes or precursor equivalents such as computer aided manufacturing processes for toolpath definitions and validation in advance of a surgery, on an ongoing bases such as during a surgery, or to additive manufacturing processes for tissues or hardware (e.g., a mechanical heart or a 3-d printed liver) that benefit from precise calibration and conditioning to maximize compatibility with a patient. Features like interactive 3D visualizations of molecular docking or cellular pathway activations could be incorporated, making it easier for researchers to understand and explore the results of their cellular models.

[0124] The regulatory compliance and ethics modules from the drug discovery platform can be adapted to ensure that cellular modeling and simulations adhere to relevant guidelines and ethical standards, particularly when working with sensitive data or modeling processes with potential clinical applications. This integration can help ensure that the cellular modeling platform remains compliant with evolving regulations in biomedical research and drug development.

[0125] Additionally, the drug discovery platform's capabilities in designing and optimizing clinical trials, including the creation of digital twins for virtual trials, can be leveraged to enhance the cellular modeling platform's ability to translate in silico findings to in vitro and in vivo studies. This may comprise using cellular models to design more effective experiments, predict potential challenges in translating cellular-level findings to organism-level effects, and optimize the design of preclinical and clinical studies.

[0126] By integrating these advanced capabilities from the AI drug discovery platform, the AI-enhanced cellular modeling and simulation platform can become a more powerful and versatile tool for researchers. It would not only provide more accurate and comprehensive cellular models but also bridge the gap between basic cellular biology and practical applications in drug discovery and development, potentially accelerating the translation of cellular-level insights into new therapeutic strategies.

[0127] The PHDB computing platform **135** can enhance the functionality of AI-enhanced cellular

modeling and simulation platform **100** by providing a rich, personalized context for cellular models. The PHDB platform's ability to integrate diverse types of health data, including genomic, proteomic, metabolomic, clinical, and real-time health metrics, can provide a comprehensive foundation for creating more accurate and personalized cellular models. This integration allows the cellular modeling platform to incorporate individual-specific data, enabling the creation of digital twins at the cellular level that reflect the unique biological characteristics of individual patients.

[0128] The PHDB platform's spatiotemporal modeling subsystem can be leveraged to enhance the cellular modeling platform's ability to represent and simulate cellular processes in both space and time. This can lead to more sophisticated 4D models of cellular behavior that account for spatial heterogeneity within tissues and temporal changes in cellular states. The real-time data processing capabilities of the PHDB platform, particularly its ability to handle data from IoT devices and wearables, can be used to continuously update cellular models with current physiological data, allowing for dynamic, real-time simulations of cellular processes in response to changing environmental conditions or interventions.

[0129] Moreover, the PHDB platform's advanced data integration techniques can be utilized to harmonize cellular-level data with higher-level physiological and clinical data. This multi-scale data integration can provide a more holistic view of how cellular processes relate to overall health outcomes, enabling researchers to study the connections between cellular mechanisms and disease manifestations more effectively. The platform's ability to handle multi-modal data can also enhance the cellular modeling platform's capacity to incorporate diverse data types, from molecular-level omics data to tissue-level imaging data, creating more comprehensive and realistic cellular models.

[0130] The PHDB platform's robust security and privacy features, including its encryption capabilities and blockchain-based data integrity measures, can be applied to the cellular modeling platform to ensure the protection of sensitive cellular and genetic data. This is particularly important when working with personalized cellular models that may contain identifiable genetic information. The federated learning capabilities of the PHDB platform can be adapted to platform **100** to enable collaborative cellular modeling efforts across multiple institutions while maintaining data privacy, allowing researchers to build more robust and generalizable cellular models without centralizing sensitive data.

[0131] Furthermore, the PHDB platform's advanced visualization and user interface **115** components can be integrated into the cellular modeling platform to provide more intuitive and interactive ways for researchers to explore and analyze cellular models. This could include features for visualizing cellular processes in the context of whole-body physiology, or tools for exploring the relationships between cellular-level events and clinical outcomes.

[0132] The PHDB platform's AI and machine learning capabilities, particularly its ability to handle large-scale, heterogeneous health data, can be leveraged to enhance the predictive power of cellular models. This may comprise, for example, using machine learning algorithms to identify patterns in cellular behavior that correlate with specific health outcomes, or to predict how cellular processes might respond to various interventions based on an individual's health profile.

[0133] The PHDB platform's emphasis on personalized medicine can be extended to the cellular level through cellular modeling platform **100**. This integration can enable the development of personalized cellular models that account for an individual's unique genetic makeup, environmental exposures, and health history. These personalized cellular models can be used to predict individual responses to treatments, identify personalized drug targets, or develop tailored therapeutic strategies at the cellular level.

[0134] By incorporating these capabilities from the PHDB computing platform, the AI-enhanced cellular modeling and simulation platform can become a more powerful tool for personalized, context-aware cellular modeling. This integration would enable researchers to create more realistic and clinically relevant cellular models, potentially accelerating the translation of cellular biology insights into personalized therapeutic strategies and advancing the field of precision medicine.

[0135] AI-enhanced cellular modeling and simulation platform **100** can be effectively employed for real-time monitoring and prediction of cellular responses in laboratory settings, significantly enhancing experimental procedures and guiding therapeutic interventions. In this use case, the platform integrates advanced AI models with a network of high-precision sensors deployed in laboratory environments. These sensors continuously capture a wide array of cellular parameters, including but not limited to gene expression levels, protein concentrations, metabolite profiles, cell morphology changes, and various physiological indicators. The real-time data streams from these sensors are fed into the platform's AI models, which have been trained on vast datasets of cellular behavior and are capable of recognizing complex patterns and predicting cellular responses with high accuracy.

[0136] As an experiment progresses, the platform's AI models analyze the incoming sensor data in real-time, comparing it against predicted cellular behaviors and identifying any deviations or unexpected responses. This immediate analysis allows researchers to monitor cellular reactions to experimental conditions or therapeutic agents as they occur, rather than waiting for end-point measurements. The system can alert researchers to significant changes or anomalies, suggesting potential adjustments to experimental parameters or highlighting areas that require closer examination. For instance, in a drug screening experiment, the platform might detect subtle changes in cellular metabolism that indicate an adverse reaction to a compound long before visible signs of toxicity appear, allowing researchers to adjust dosages or terminate the exposure promptly.

[0137] Moreover, the platform's predictive capabilities enable it to forecast how cellular responses might evolve over time based on current trends and historical data. This predictive insight can be invaluable in guiding the course of long-term experiments or in optimizing therapeutic interventions. For example, in a stem cell differentiation experiment, the system might predict the optimal timing for introducing specific growth factors to maximize the yield of desired cell types. In a clinical setting, when monitoring patient-derived cells exposed to personalized treatments, the platform can provide early indications of treatment efficacy or resistance, allowing for timely adjustments to therapeutic strategies.

[0138] The platform's ability to integrate data across multiple scales, from molecular interactions to cellular behaviors to tissue-level effects, allows for a comprehensive understanding of cellular responses in context. This multi-scale integration enables researchers to connect microscopic cellular changes to macroscopic effects, providing a more holistic view of biological processes. Furthermore, the platform's machine learning algorithms continuously refine their predictive models based on new data, improving accuracy over time and adapting to the specific characteristics of different cell lines or experimental setups. This adaptive learning ensures that the platform becomes increasingly attuned to the nuances of each laboratory's unique experimental environment.

[0139] By providing this real-time monitoring and predictive capability, AI-enhanced cellular modeling and simulation platform **100** transforms the way cellular experiments are conducted. It enables a more dynamic, responsive approach to research, where experiments can be adjusted on the fly based on emerging data. This not only increases the efficiency of research by reducing the need for repeated experiments but also opens up new possibilities for discovering subtle cellular behaviors that might be missed in traditional end-point analyses. Ultimately, this real-time monitoring and prediction capability can accelerate the pace of scientific discovery, enhance the development of targeted therapies, and provide a powerful tool for personalized medicine approaches that require rapid, accurate assessment of individual cellular responses to treatments.

[0140] According to an embodiment, AI-enhanced cellular modeling and simulation platform **100** offers a powerful approach to personalized medicine by leveraging individual patient data to create highly specific cellular models that can predict treatment responses. In this use case, platform **100** integrates a patient's multi-omics data including, but not limited to, genomic, transcriptomic, proteomic, and metabolomic profiles, along with their clinical history, lifestyle factors, and real-

time physiological data from wearable devices. This comprehensive dataset can be used to construct a detailed, personalized cellular model that accurately represents the patient's unique biological characteristics. The platform's advanced AI algorithms, trained on vast datasets of cellular behaviors and treatment outcomes, then analyze this personalized model to predict how the patient's cells are likely to respond to various treatment options.

[0141] For instance, in the case of a cancer patient, the platform could simulate how different chemotherapy regimens or targeted therapies might affect the patient's tumor cells, taking into account the specific genetic mutations driving the cancer and the patient's overall health status. The AI models may predict not only the efficacy of each treatment but also potential side effects based on the patient's cellular characteristics. This could help oncologists choose the most effective treatment with the least adverse effects for each individual patient. In the context of immune disorders, the platform could model how a patient's immune cells might respond to various immunomodulatory therapies, considering factors like the patient's Human leukocyte antigen (HLA) type, cytokine profiles, and previous immune responses. This can be particularly valuable in complex conditions like rheumatoid arthritis or multiple sclerosis, where treatment responses can vary widely between individuals.

[0142] The platform's ability to integrate real-time data allows for continuous refinement of these predictions. As the patient undergoes treatment, data from regular blood tests, imaging studies, and other clinical assessments can be fed back into the model, allowing the AI to update its predictions and suggest treatment adjustments if necessary. This creates a dynamic, adaptive treatment approach that can respond to changes in the patient's condition over time. Moreover, the platform can simulate combination therapies, predicting how different drugs might interact at the cellular level in the context of the patient's unique biology. This could lead to the development of personalized combination treatments that are more effective than standard protocols.

[0143] In addition to guiding treatment selection, the platform can also assist in predicting potential disease progression or recurrence. By simulating cellular behaviors over extended periods, it can identify early warning signs of disease advancement or resistance to current treatments, allowing for proactive interventions. The platform's predictive capabilities extend beyond just choosing existing treatments; it can also guide the development of personalized therapies. For example, in the rapidly advancing field of cell therapies, the platform could be used to optimize the engineering of CAR-T cells for individual cancer patients, simulating how different receptor designs might perform given the patient's specific tumor characteristics and immune system status.

[0144] By providing these highly personalized predictions and treatment strategies, the AI-enhanced cellular modeling and simulation platform has the potential to significantly improve patient outcomes across a wide range of diseases. It enables a shift from the traditional "one-size-fits-all" approach to a truly personalized medicine paradigm, where treatments are tailored to the unique cellular characteristics of each individual. This not only increases the likelihood of treatment success but also helps in avoiding unnecessary treatments and reducing adverse effects, ultimately leading to better quality of life for patients and more efficient use of healthcare resources. As the platform continues to learn from each case it analyzes, its predictive power grows, promising an ever-improving ability to personalize and optimize medical treatments at the cellular level.

[0145] According to an embodiment, AI-enhanced cellular modeling and simulation platform **100** can be applied to accelerate drug discovery by enabling researchers to simulate drug-cell interactions at unprecedented scale and detail. In this use case, researchers investigating new treatments for a complex disease like Alzheimer's could leverage the platform's multi-omics data integration capabilities to create comprehensive cellular models incorporating genomic, transcriptomic, proteomic, and metabolomic data from both healthy neurons and those affected by Alzheimer's. The platform's AI models, trained on vast datasets of known drug-cell interactions, can then simulate how thousands of potential drug compounds might interact with these cellular

models. This may include predicting how drugs bind to specific protein targets, their effects on cellular pathways, potential off-target interactions, and even how they might influence gene expression patterns over time. The spatiotemporal modeling subsystem can visualize these interactions in 4D, allowing researchers to observe simulated drug effects across different regions of neurons and at various time points. Meanwhile, the platform's knowledge graph can provide context by linking observed effects to known biological pathways and previous research findings. This approach can allow researchers to rapidly screen a vast number of compounds, identifying the most promising candidates for further investigation. The stochastic modeling capabilities can also quantify uncertainty in these predictions, helping researchers prioritize compounds with the highest probability of success. By simulating drug interactions in silico before moving to laboratory testing, this use of the platform may significantly reduce the time and cost associated with early-stage drug discovery, potentially accelerating the development of new treatments for Alzheimer's and other complex diseases.

[0146] According to an embodiment, AI-enhanced cellular modeling and simulation platform **100** can enable synthetic biology and cellular engineering by providing powerful tools for designing and optimizing synthetic biological systems. In this use case, researchers aiming to engineer, for example, bacteria for efficient biofuel production may leverage the platform's advanced capabilities. The multi-omics data integration module would first compile comprehensive data on the target bacterial strain, including its genome, transcriptome, proteome, and metabolome. The AI models, trained on vast datasets of genetic circuits and metabolic pathways, can then simulate the effects of various genetic modifications on the bacteria's biofuel production capacity. The platform's knowledge graph would provide context, linking proposed modifications to known biological pathways and previous research in metabolic engineering. Using the spatiotemporal modeling subsystem, researchers could visualize how these genetic changes might alter cellular processes over time, such as metabolic flux distributions or protein expression patterns. The stochastic modeling capabilities can account for cellular variability, helping to design robust genetic circuits that perform consistently across a population of cells. As the AI suggests genetic modifications, the platform could simultaneously optimize for multiple factors, such as maximizing biofuel yield, minimizing cellular stress, and ensuring genetic stability. The simulation computing platform could run thousands of in silico experiments, testing different combinations of genetic elements like promoters, ribosome binding sites, and coding sequences to find optimal designs. Throughout this process, the platform's machine learning algorithms would continuously refine their predictions based on experimental feedback, improving the accuracy of future designs. By enabling rapid, iterative design-build-test cycles largely in silico, this use of the platform could dramatically accelerate the development of highly efficient, engineered bacteria for biofuel production, potentially revolutionizing the field of sustainable energy.

[0147] FIG. **2** is a block diagram illustrating an exemplary system architecture for an artificial intelligence (AI) enhanced drug discovery platform, according to an embodiment. One or more of the components or functionality described herein with respect AI drug discovery platform **200** may be implemented in various aspects of AI-enhanced cellular modeling and simulation platform **100**. For more detailed information regarding the operation of the AI drug discovery platform and variants thereof, please refer to U.S. patent application Ser. No. 18/900,608 which is incorporated herein by reference. The models, tools, and processes provided by AI drug discovery platform **200** may be used to support various AI-enhanced cellular modeling and simulation capabilities.

[0148] The AI drug discovery platform **200** may be configured to enable multi-scale drug design. In such a configuration platform **200** may receive, retrieve, or otherwise obtain a plurality of data from various data sources **230** and databases **220**. For example, for multi-scale drug design the plurality of data can include, but not limited to, molecular, cellular, tissue, and organism-level data associated with a complex disease (i.e., Alzheimer's disease, cancer, autoimmune disorders, etc.). Platform **200** may parse the obtained data to select one or more modules (e.g., computing

platforms, systems, and/or subsystem components of AI drug discovery platform **200**) for multi-scale drug design. Platform users **240** (e.g., scientist and researchers) may input a prompt for the selected modules. In some implementations, platform **200** may engineer one or more prompts for the selected one or more modules for multi-scale drug design and input the engineered prompts for the selected modules. Platform **200** can output drug design recommendations based on the submitted prompts, wherein the recommendations may address multiple aspects of complex disease pathology across different biological scales.

[0149] To support the multi-scale drug design process, platform **200** may be configured with one or more components (e.g., computing platforms, systems, modules, and/or subsystems) to assist with the large scale data ingestion, processing, and simulating which occurs during. As illustrated, platform **200** comprises a data integration computing platform **201**, an AI and machine learning (ML) core **202**, a simulation computing platform **203**, an integration and application programming interface (API) manager **204**, a visualization and user interface (UI) system **205**, a knowledge graph and reasoning computing platform **206**, a regulatory compliance and ethics computing platform **207**, a drug discovery computing platform **208**, and one or more data storage systems **209**. These platform components are merely exemplary and do not represent all possible combinations of systems which may be present. More or less components may be present in various implementations of AI drug discovery platform **200** and its variants described herein. The processes and functionality of platform **200** may be applied to other embodiments of the platform and vice versa, even if not explicitly stated.

[0150] According to the embodiment, AI drug discovery platform **200** may be configured to receive, retrieve, or otherwise obtain a plurality of information from diverse data sources **230** and databases **220**. By integrating these diverse data sources, AI drug discovery platform **200** can leverage a wealth of information across multiple biological scales and modalities. This comprehensive approach allows for more accurate predictions, better understanding of drug mechanisms, and the potential for truly personalized medicine approaches in drug development and therapy.

[0151] Multi-omics data **231** integrates information from multiple "omics" fields, including (but not limited to) genomics, transcriptomics, proteomics, metabolomics, metagenomics, spatial omics, and epigenomics. Each provides a different layer of biological information. Genomics data may comprise deoxyribonucleic acid (DNA) sequence data and genetic variants. Transcriptomics data may comprise ribonucleic acid (RNA) expression levels. Proteomics data may comprise protein abundance and post-translational modifications. Metabolomics data may comprise information about small molecule metabolites. Metagenomics data may comprise information obtained from direct genetic analysis of genomes contained with an environmental sample. Epigenomics data may comprise information associated with a set of epigenetic modifications on the genetic material of a given cell. According to an embodiment, the platform may implement one or more machine or deep learning models for multi-omics data analysis.

[0152] Spatial omics technologies (and data) serve as powerful tools for understanding tissue organization and function at unprecedented molecular detail. In cancer research, these technologies are particularly valuable for studying the tumor microenvironment, where they can help identify and localize rare immune cell subtypes that play roles in tumor response and treatment efficacy. The platform enables the ability to analyze tissue architecture in spatial context for understanding how cellular interactions influence tumor behavior and progression. Spatial omics (e.g., spatial proteomics) can also enable researchers to examine disease-relevant structures and their molecular organization, which has direct implications for diagnosis, treatment selection, and outcome prediction.

[0153] From a clinical perspective, spatial omics applications extend into precision medicine, where the detailed molecular and cellular profiles they provide can be used to customize treatments for individual patients. By correlating spatial molecular patterns and pathology imaging features

with clinical outcomes, the platform enables healthcare providers to make more informed decisions about treatment strategies. This is particularly relevant in oncology, where understanding the spatial distribution of different cell types and their molecular states within a tumor can inform therapeutic approaches. The integration of spatial omics data with clinical information, medical imaging, and AI helps create a more comprehensive view of disease states, enabling more accurate predictions of disease progression and treatment responses.

[0154] In the research context, spatial omics technologies facilitate the creation of comprehensive tissue atlases that capture multiple molecular modalities simultaneously. These atlases may comprise information about gene expression, protein levels, metabolites, and various epigenetic markers, all while maintaining spatial context. Large-scale initiatives (e.g., the MOSAIC project) aim to generate thousands of spatial multi-omics datasets across different cancer types to identify new spatial biomarkers and patient-specific drug targets. This kind of comprehensive molecular mapping, especially when combined with AI-driven analysis enabled by the platform, has the potential to reveal new insights about tissue organization, cell-cell communication, and disease mechanisms that weren't previously observable with traditional methods.

[0155] According to an aspect, the platform is configured to reconstruct three-dimensional tissue architectures from multiple tissue sections, offering a more complete understanding of complex biological structures and their molecular composition. The combination of spatial omics with artificial intelligence enables new possibilities for biomedical research, drug development, and clinical practice, potentially leading to more effective, personalized therapeutic strategies and improved patient outcomes.

[0156] According to an embodiment, the platform can leverage the multi-omics data, particularly spatial omics data, to perform deep visual proteomics analysis to perform molecular profiling. Deep visual proteomics (DVP) represents an integrated approach that combines advanced imaging techniques, artificial intelligence, and mass spectrometry to achieve cell-type-specific molecular profiling while maintaining spatial context within tissue samples. According to an aspect, the DVP workflow begins with formalin-fixed paraffin-embedded (FFPE) tissue sections, which are mounted on specialized membrane slides and subjected to immunofluorescence staining to visualize specific cell types of interest. Following staining, high-resolution microscopy imaging is performed to capture the spatial distribution and morphological features of the marked cells.

[0157] The next phase employs artificial intelligence-driven image analysis, where deep neural networks perform automated cell segmentation and classification. This step creates detailed contour maps of individual cells while maintaining their spatial coordinates and cell-type identity. The AI classification ensures accurate identification of specific cell populations within the complex tissue architecture. Following digital analysis, the identified cells of interest are physically isolated using laser microdissection, guided by the AI-generated contours. This precise extraction maintains the purity of cell-type-specific samples while preserving their molecular integrity.

[0158] The isolated cell populations then undergo specialized sample preparation optimized for small-sample proteomics, followed by ultra-sensitive mass spectrometry analysis. This final step enables comprehensive protein profiling of the specific cell types within their native tissue context. The entire workflow is designed to maintain spatial information while providing deep molecular insights at the single-cell type level. The resulting data combines spatial, morphological, and molecular information, allowing researchers to understand both the location and molecular state of specific cell populations within the tissue microenvironment. This approach is particularly valuable for studying complex tissues where cellular heterogeneity and spatial organization play crucial roles in biological processes or disease states.

[0159] The DVP method distinguishes itself from other spatial omics approaches through its ability to provide deep proteomic coverage while maintaining single-cell type resolution within standard clinical samples. One of its advantages is its compatibility with FFPE tissue samples, making it particularly valuable for analyzing archived clinical specimens and enabling retrospective studies.

The method is adaptable to various tissue types and can be modified to investigate different cell populations of interest through appropriate selection of immunofluorescence markers and AI training parameters.

[0160] An example is provided of the platform using multi-omics data processing to support prediction of a drug response, according to an embodiment. The process may begin with the collection of a plurality of multi-omics data **231** from patient samples. This may comprise whole genome sequencing for genetic variants or obtaining genome sequencing data, using tools such as RNA-seq to obtain gene expression profiles, and mass spectrometry for protein and metabolite levels. The platform may then preprocess and normalize the obtained plurality of multi-omics data. This may comprise providing quality control and filtering of sequencing data, normalization of expression and abundance values, and batch effect correction, if applicable. The platform then integrates the multi-omics data. For example, this may use techniques such as similarity network fusion or multi-omics factor analysis. The platform may build/train a predictive model (e.g., deep neural network) on the integrated data. For instance, such a model may be trained by using drug response data as labels. To generate a prediction, a new patient's multi-omics data is input into the trained predictive model. The model predicts the likelihood of positive drug response. The platform may be configured to interpret the model results. For instance, the platform may identify key features (genes, proteins, metabolites, etc.) driving the prediction. It may provide insights into potential mechanisms of drug action or resistance.

[0161] The platform may be further configured to receive, retrieve, or otherwise obtain a plurality of spatial cell genomics and spatiotemporal imaging data **232**. This combines high-resolution imaging with molecular profiling to map the spatial distribution of gene expression and cellular features within tissues. Processes, mechanisms, components, and subsystems which may be implemented to facilitate the collection of spatial cell genomics and spatiotemporal imaging data may include single-cell RNA sequencing, in situ hybridization techniques (e.g., FISH), high-resolution microscopy (e.g., super-resolution, light-sheet), and image analysis and spatial statistics algorithms. According to an embodiment, spatiotemporal modeling is added which incorporates patient data over time (across multiple treatments and diagnostics). This enables real-time tracking of tumor progression or treatment efficacy, allowing dynamic updates in predictions rather than relying solely on snapshots at the time of biopsy. Additionally, integrating non-image modalities (e.g., molecular data, genetic profiles) further enriches the diagnostic process, improving predictive models for personalized care. For more detailed description of multi-modal data integration, please refer to U.S. patent application Ser. No. 18/801,361 which is incorporated herein by reference. Data integration layer **110** may comprise a multi-modal data integrator component capable of integrating non-imaging modalities into one or more existing prediction models and/or simulation models.

[0162] According to an embodiment, multi-modal data integrator may be incorporated into a federated learning approach to train models across multiple institutions without sharing raw data, preserving privacy while building more robust and generalizable models. Multi-modal data, such as genomics, medical history, and imaging, can be integrated to provide a more comprehensive patient profile. According to an aspect, real-time telematics and sensor data can also be integrated, allowing for continuous patient monitoring and intervention as new data is generated.

[0163] An example is provided of the platform using spatial cell genomics and spatiotemporal imaging data in a drug discovery process to analyze a tumor microenvironment for cancer drug development. The process begins with sample preparation wherein the platform obtains tumor biopsy samples. This may comprise preparing or obtaining prepared tissue sections for imaging and molecular analysis. As a next step, spatial transcriptomics are analyzed. This may comprise performing in situ sequencing or spatial barcoding to capture gene expression data with spatial coordinates. As a next step, multiplexed protein imaging is performed. This may use, for example, cyclic immunofluorescence or CODEX for protein profiling. This can generate a map of multiple protein markers in the same tissue section. Image analysis is then performed. This may comprise

segmenting individual cells in the tissue images and extracting features such as, for example, cell morphology and neighborhood composition. Multi-omics data integration may be performed wherein the platform aligns transcriptomics and proteomic data to the spatial coordinates. This may result in the creation of a multi-layered map of the tumor microenvironment. The platform may then perform spatial pattern analysis to identify spatial patterns of gene expression and cell types. This can allow the platform to characterize tumor heterogeneity and microenvironment composition. Using this information as an input, the platform can identify cell types or spatial regions that could be drug targets as well as assess spatial distribution of existing drug targets. The platform can use spatial patterns to predict likely response to different therapies and/or design combination therapies targeting different spatial regions.

[0164] The platform may be further configured to receive, retrieve, or otherwise obtain a plurality of expert data **233**. Expert opinions and judgment data can be invaluable assets for an AI drug discovery platform, providing unique insights that complement computational models and empirical data. Expert knowledge can be integrated into the platform through various knowledge representation techniques. This might involve creating structured ontologies, decision trees, or rule-based systems that capture expert understanding of drug discovery processes, biological mechanisms, or clinical applications. These knowledge structures can then inform and guide other components of the platform.

[0165] According to an embodiment, the platform can implement a Bayesian framework that incorporates expert opinions as prior probabilities. This approach allows the system to combine expert knowledge with empirical data, updating predictions as new information becomes available. For instance, experts' initial assessments of a compound's potential could be used as priors in models predicting drug efficacy or safety. Expert judgments can be useful in feature selection and weighting for machine learning models. Experts can identify which molecular properties or biological indicators are most likely to be relevant for a particular therapeutic application, helping to focus the models on the most promising areas and potentially improving their predictive power.

[0166] The platform may use expert opinions to validate and refine its predictions. By comparing AI-generated hypotheses or predictions with expert assessments, the system can identify areas of agreement and discrepancy, leading to more robust and trustworthy outputs. In the realm of drug repurposing, expert knowledge about drug mechanisms, off-target effects, and clinical observations can be invaluable. The platform may incorporate this information to guide the exploration of new applications for existing drugs.

[0167] Expert judgment can be useful in designing and interpreting in silico experiments. The platform could use expert input to set up more realistic and relevant virtual screenings or simulations, ensuring that computational experiments align with practical considerations in drug discovery.

[0168] For risk assessment and decision-making, expert opinions can provide context and nuance that might be missing from purely data-driven approaches. The platform may incorporate expert judgments on factors like potential regulatory hurdles, market dynamics, or long-term safety concerns. In the area of target identification and validation, expert knowledge about biological pathways, disease mechanisms, and previous research can help prioritize potential targets and guide further investigation.

[0169] The platform may implement a system for ongoing expert feedback, allowing researchers, providers, payers, patients, regulators or other stakeholders to comment on and rate the platform's various outputs or recommendations. This creates a learning loop where the AI system continuously improves based on expert, layperson, and crowd input. This may also aid in approval and quality and safety assurance in cases where personalized therapeutics are appropriate since system can facility validation and presentation of compliance with specific processes relating to diagnosis, treatment selection, treatment dosing/timing/delivery, sources of remuneration, provider oversight and licensing, patient consent and regulatory approvals where needed via its event

oriented processing approach and auditable databases of such machine and human decision events individually and collectively.

[0170] Expert opinions can be particularly valuable in handling edge cases or rare scenarios where historical data might be limited. The platform can use expert judgments to fill gaps in its knowledge base and make more informed decisions in these situations. For interpreting complex or ambiguous results, the platform can incorporate expert reasoning processes. This may comprise implementing fuzzy logic systems or other AI techniques that can handle the kind of nuanced thinking characteristic of human experts.

[0171] In collaborative drug discovery projects, the platform can employ expert opinions to mediate between different stakeholders, helping to align computational predictions with practical considerations from various domains (e.g., chemistry, biology, clinical practice).

[0172] The platform may be further configured to receive, retrieve, or otherwise obtain a plurality of brain-body interaction data **234**. This data captures the bidirectional communication between the central nervous system and other body systems, including the immune, endocrine, and gastrointestinal systems. This data may be obtained from various sources/processes including (but not limited to) neuroimaging data (fMRI, PET), electrophysiology data (EEG, MEG), immune system markers (cytokines, immune cell populations), endocrine measurements (hormone levels), and gut microbiome profiling.

[0173] An example is provided of the platform leveraging brain-body interaction data in a drug discovery process for developing drugs for neurological disorders with systemic effects. The process begins by collecting a plurality of patient data such as fMRI data to obtain brain activity measurements, blood samples for immune and endocrine markers, and gut microbiome composition profile data. The platform may implement a time series alignment step wherein it synchronizes neuroimaging data with peripheral measurements. This allows for the platform to account for different timescales of various processes. In some implementations, the platform performs network analysis wherein it constructs brain connectivity networks from fMRI data. This may comprise building interaction networks between brain regions and peripheral markers. The platform can identify key interactions. In an embodiment, this comprises using graph theory algorithms to find important nodes and edges in the brain-body network. The platform can detect patterns of brain-body communication associated with disease state. To perform drug target identification, the platform can identify network components that could be targeted to modulate brain-body interactions and predict how modulating these targets might affect the overall system. Simulation computing platform **600** can then simulate drug effects. This may comprise using the brain-body interaction model to simulate potential drug effects in order to predict both central and peripheral effects of candidate drugs. In some embodiments, the platform can design multi-target therapies. For example, the platform may develop drug combinations that target both brain and peripheral systems in particular fashions. This may be optimized for synergistic effects across the brain-body network and rely upon both local cell, cell population, tissue, anatomical or biological system level modeling processes which may be individually or collectively scored to aid in treatment selection or efficacy determination at a point in time or over different finite time horizons of interest. This allows the system to include options for patient, provider, payer or regulator to evaluate competing factors such as quality of life or extension of life or costs or fitness for certain activities (e.g., returning to a sport or taking a trip) against the near-term, long-term prognosis impacts and the practical economic cost considerations. System may also leverage an integrated database of insurance policy language and utilization to determine insurance aware benefit maximization process against one or more of these medical or quality of life factors to aid in treatment sequencing or timing decisions, securing preauthorization, or engaging in protest with insurance providers or public payers. We note that a common exemplary embodiment involves summarizing proposed or completed medical treatment data with justification to insurance providers using LLMs integrated with patient-specific knowledge base and legal obligation

analysis job coordinated by the DCG orchestrated process. We note further that system can not only engage in forward body and health modeling based on express scenario descriptions but can in fact listen to real-time discussions between doctors or doctors and patients to generate proposed scenarios for discussion and evaluation during a consultation, surgery.

[0174] The platform may be configured to receive, retrieve, or otherwise obtain a plurality of data from Internet of Things (IoT) devices **236** to significantly enhance data collection, real-time monitoring, and the overall efficiency of the drug discovery process. The platform can utilize IoT devices to obtain relevant data in various ways. IoT-enabled lab instruments can automatically upload experimental data to the platform in real-time, ensuring immediate data availability for analysis and reducing manual data entry errors. Environmental sensors can track laboratory conditions vital for experimental consistency, while automated cell culture systems can provide continuous monitoring of cell growth and nutrient levels. In clinical trials, IoT wearables can collect real-time physiological data from participants, offering a more comprehensive view of drug effects. Smart pills and drug delivery systems can provide data on patient adherence and physiological responses, valuable for understanding drug efficacy and optimizing dosing regimens.

[0175] According to an embodiment, the platform may also integrate IoT-enabled compound storage and retrieval systems for better sample management, and potentially use implantable or wearable sensors for real-time pharmacokinetic monitoring. Remote patient monitoring through IoT devices can provide more comprehensive data on drug effects in real-world conditions. In the supply chain, IoT sensors can monitor conditions of drug components during transport and storage. Automated synthesis robots and high-throughput screening systems connected to the IoT can provide real-time data on drug synthesis and screening processes. Additionally, IoT-connected bioprinters and 3D cell culture systems can offer data on complex tissue models for drug testing. By leveraging IoT devices, AI drug discovery platform **200** can create a more connected, data-rich environment spanning from the laboratory to clinical trials and beyond. This comprehensive data ecosystem can lead to faster, more informed decision-making, improved experimental design, and ultimately, more efficient and effective drug discovery processes.

[0176] The platform may be configured to receive, retrieve, or otherwise obtain a plurality of integrated medical records **237**. This comprises the collection and analysis of diverse clinical data from electronic health records (EHRs), including demographics, diagnoses, treatments, lab results **235**, and outcomes. The platform may implement one or more of the following techniques, mechanisms, components, or systems/subsystems to support the collection and analysis of integrated medical records: natural language processing (NLP) for unstructured clinical notes, standardized medical ontologies, (e.g., ICD, SNOMED CT, etc.), time series analysis for longitudinal patient data, and privacy-preserving data integration techniques.

[0177] An example is provided of the platform utilizing integrated medical records in a drug discovery process for identifying drug repurposing opportunities. The process begins with a data extraction step. The platform can extract structured data (diagnoses, medications, lab results, etc.) form EHRs. This may comprise the use of NLP to extract relevant information from clinical notes. The platform may further standardize ingested/extracted data. For example, it may map diagnoses to ICD codes and/or normalize drug names and lab test results. The platform can perform patient trajectory modeling by creating temporal sequences of events for each patient and identifying common trajectories and treatment patterns. An outcome definition step may be performed wherein the platform (or platform user) defines positive and negative outcomes based on clinical events and lab results. In some implementations, the platform supports association mining to identify unexpected positive outcomes associated with specific drugs. This may control for confounding factors using, for example, propensity score matching. The platform can perform various network analyses. As an example, a drug-disease network may be constructed based on observed associations. The network analysis can help identify drugs with potential off-label uses. The platform (or platform user) can use the results of the network analysis to generate one or more

hypotheses for drug repurposing. This may comprise prioritizing hypotheses based on supporting evidence and potential impact. As a last step, the platform (or platform user) can design observational studies to further validate repurposing hypotheses and plan for targeted clinical trials to confirm efficacy.

[0178] The platform may be configured to receive, retrieve, or otherwise obtain a plurality of simulated data **238** such as, for example, molecular dynamics simulation data. These are computer simulations of the physical movements of atoms and molecules, allowing for the study of dynamic processes in biological systems. This may comprise the use of force fields (e.g., AMBER, CHARMM) to model atomic interactions, integration algorithms (e.g., Verlet, leap-frog) to solve equations of motion, periodic boundary conditions to simulate bulk systems, and temperature and pressure control algorithms.

[0179] An example is provided of the platform using molecular dynamics simulation data in a drug discovery process for studying drug-protein binding mechanisms. The platform may prepare 3D structures of the target protein and drug molecule. This may comprise solvating the system and adding ions to neutralize the charge. The system then performs energy minimization to remove bad contacts and equilibrate the system under constant temperature and pressure. The platform then performs a series of production simulations. This may comprise running long (microseconds to milliseconds) MD simulations and sampling different binding poses and protein conformations. The platform analyzes the simulation results. For instance, the platform can calculate binding free energies using methods such as molecular mechanics Poisson-Boltzmann surface area (MM-PBSA), analyze protein-drug contacts and binding pocket dynamics, and identify key residues involved in drug binding. As a next step, the platform performs binding pathway characterization using advanced sampling techniques (e.g., metadynamics) to study binding/unbinding pathways. During this process the platform can identify intermediate states and energy barriers. The platform may be configured to support kinetics estimation wherein it estimates k_{on} and k_{off} rates from simulation data and compares those values with experimental binding kinetics data. The platform may then suggest modifications to the drug molecule to improve binding affinity or kinetics and/or perform virtual screening of drug analogues using the MD-derived insights.

[0180] Exemplary databases **220** which may be integrated with platform **200** may comprise, but are not limited to, large chemical databases **221** (e.g., PubChem, ChEMBL, etc.), drug and target database **222** (DrugBank, BindingDB, etc.), structural databases **223** (e.g., Protein Data Bank), biological context databases **224** (e.g., KEGG, UniProt, etc.), virtual screening databases **225** (e.g., ZINC, BindingDB, etc.), and clinical and toxicology databases **226** (e.g., ClinicalTrials.gov, TOXNET, etc.). These types of external databases may have specialized adapters/connectors configured to integrate their data and functionality into AI drug discovery platform **200**.

[0181] As shown, AI-drug discovery platform **200** comprises one or more data storage systems **209** to store, maintain, and manage the large plurality of diverse data types which may be obtained. These may be implemented as a multi-tiered data storage system designed to handle the diverse types of data encountered in drug discovery while ensuring high performance, scalability, and data integrity. In various embodiments this system comprises one or more of the following components: distributed file systems, relational databases, NoSQL databases, document stores, wide-column stores, vector databases, key-value stores, graph databases, time-series databases, object storage, in-memory databases, data warehouses, and/or data lakes. To manage this complex ecosystem of storage systems the DCG orchestrated system may implement one or more of the following strategies: a data catalog system such as Apache Atlas or Alation may be used to maintain metadata about all datasets, their location, and relationships; data virtualization tools such as Denodo or Dremio can be employed to provide a unified view of data across different storages systems; ETL (Extract, Transform, Load) and subordinate data pipeline tools such as Apache NiFi or Airflow may be used to manage subsets of data movement and transformations between different storage systems; a robust backup and disaster recovery system can be implemented to ensure data integrity

and business continuity; and advanced data governance and security measures may be implemented across all storage systems, including encryption at rest and in transit, access controls, and audit logging.

[0182] This multi-tiered approach allows platform **200** to optimize storage and retrieval for different types of data and access patterns. For instance, frequently accessed, performance-critical data might be kept in in-memory databases, while large, infrequently accessed datasets can be stored in object storage or data lakes. The system may be designed to be cloud-agnostic, allowing for deployment across multiple cloud providers or in hybrid cloud-on-premises environments. The entire storage system may be managed by a data orchestration layer that handles data lifecycle management, ensuring that data is stored in the most appropriate system based on its current usage patterns, age, and importance. This orchestration layer may also manage data replication, consistency, and migration between different storage tiers to optimize for performance and cost.

[0183] According to an embodiment, a distributed file system such as, for example, Hadoop distributed file system (HDFS) or Ceph may be implemented as a component of the storage system. This can allow for storage of large volumes of raw data, including sequencing data, high-throughput screening results, and molecular dynamics simulation outputs. The distributed nature helps to ensure high availability and fault tolerance.

[0184] Traditional relational database management systems (RDBMS) like PostgreSQL or MySQL can be used for storing structured data with well-defined schemas and with plugins may also support vectors, graphs or timeseries specialty data within reason. This may comprise experimental metadata, compound libraries, and clinical trial data. These databases can be configured in a clustered setup for high availability and performance.

[0185] To handle semi-structured and unstructured data, NoSQL databases can be employed. For example: document stores like MongoDB or Couchbase for flexible storage of JSON-like data structures, useful for storing diverse experimental results or literature abstracts; wide-column stores like Apache Cassandra for handling time-series data from longitudinal studies or real-time sensor data; and key-value stores like Redis for high-speed caching and temporary data storage to improve system performance.

[0186] Specialized graph databases such as, for example, HugeGraph, GraphAR, Neo4j or Amazon Web Services' Neptune can be used to store and query the knowledge graphs that represent complex relationships between, for example, biological entities, drugs, and diseases. Knowledge graphs serve as a structured representation of biomedical knowledge, capturing entities (e.g., drugs, proteins, diseases, etc.) and their relationships. These graphs can be constructed using information from scientific literature, experimental data, and curated databases. Graph database technologies can be used to store and query these knowledge graphs efficiently. In the context of drug discovery, knowledge graphs can help identify non-obvious connections between biological entities, suggest potential drug repurposing opportunities, and provide context for interpreting experimental results.

[0187] Vector databases such as Pinecone, Faiss, or Milvus may be used for efficient storage and similarity search of high-dimensional vector representations of molecules, proteins, cells, tissues, and other biological entities. Vector databases can be used to efficiently store and query high-dimensional representations of molecular structures, protein sequences, cells, tissues, and other biological entities. These databases enable rapid similarity searches, which are important for tasks like virtual screening and lead optimization. For example, when a researcher identifies a promising molecular scaffold, the vector database can quickly retrieve similar compounds from vast chemical libraries, accelerating the exploration of chemical space.

[0188] For efficiently storing and querying time-series data from experiments or simulations, specialized time-series databases like AWS Timestream, InfluxDB or TimescaleDB may be employed. Cloud-based object storage solutions such as Amazon S3 or Google Cloud Storage may be used for long-term storage of large datasets, raw experimental data, and backups. For ultra-fast processing of frequently accessed data, in-memory databases like Redis or Apache Ignite can be

used, particularly for caching intermediate results or supporting real-time analytics.

[0189] A data warehouse solution like Amazon Redshift or Google BigQuery may be implemented for large-scale analytics and to support business intelligence tools. In some implementations, a data lake architecture using technologies such as Apache Hudi or Delta Lake can be used to store raw and processed data in its native format, enabling flexible schema evolution and supporting diverse analytics workloads.

[0190] A data integration computing system **201** (i.e., data integration layer) is present and configured to serve as the foundation for all subsequent analysis and modeling. The layer is responsible for ingesting, preprocessing, and harmonizing diverse types of data from various sources, creating a unified and coherent data model that can be leveraged by other components of the platform. The complexity of this layer stems from the heterogeneity of data types involved in drug discovery, ranging from molecular-level information to clinical outcomes. Data integration computing platform **201** may create, deploy, and manage various specialized pipelines configured to support various use cases of AI drug discovery platform **200** including, but not limited to, data integration pipelines, drug discovery pipelines, complex analysis pipelines, drug development pipelines, data transformation pipelines, advanced bioinformatics pipelines, comparative genomics and proteomics pipelines, metagenomic pipelines, and sequencing and bioinformatics pipelines.

[0191] An AI and ML core **202** is present and configured to serve as the analytical engine that processes the integrated data and generates insights for drug discovery (and other use cases). This core is composed of several sophisticated subsystems (e.g., modules) that work in concert to tackle complex biological problems using a plurality of specialized machine and deep learning models.

[0192] A simulation computing platform **203** is present and configured for various purposes such as to model and predict complex biological processes across multiple scales. This system integrates various simulation techniques to provide a comprehensive understanding of drug interactions, from molecular dynamics to tissue-level effects. According to an embodiment, simulation computing platform **203** employs a multi-scale simulation framework that seamlessly transitions between different levels of biological organization or structure. This framework may be built on a hierarchical architecture, where simulations at each scale can inform and constrain simulations at other scales, ensuring consistency and biological relevance across the entire system. According to an embodiment, simulation computing platform **203**, which may encompass various types of models (e.g., ODE, PDE, agent-based, metabolic, etc.), utilizes an orchestration component to handle the specifics of simulation management, while interfacing with a higher-level orchestration system that coordinates across the entire AI platform.

[0193] According to an embodiment, AI drug discovery platform **200** comprises an integration and application programming interface (API) manager **204** which serves as a layer that enables seamless communication and data exchange between various systems/subsystems/modules of the platform and external systems. According to an embodiment, this layer is built on a microservices architecture, utilizing containerization technologies like containerd and orchestration tools such as Kubernetes to ensure scalability, resilience, and case of deployment. API manager **204** may be implemented using a combination of RESTful APIs for stateless operations and GraphQL for more complex, data-intensive queries where API intermediation aids in usability. These APIs can be developed using high-performance frameworks such as FastAPI for Python-based services or Express.js for Node.js-based services, allowing for rapid development and efficient execution commonly employing a standard framework or declaration such as OpenAPI specification to enable other languages to easily interface as well with standard libraries. In some implementations, integration and API manager **204** may provide functionality directed to semantic understanding of ingested data and a comprehensive audit log to promote transparency.

[0194] The visualization and user interface component **205** of AI drug discovery platform **200** is a system designed to render complex scientific data into intuitive, interactive visualizations while providing a seamless user experience for researchers and clinicians. According to an embodiment,

this component utilizes a microservices architecture, allowing for modularity and scalability. The backend may be built on a stack that includes high-performance web servers like Nginx for static content delivery and Node.js with Express.js for dynamic API endpoints. For real-time data streaming and updates, the system may employ WebSocket protocols, enabling live updates of visualizations as new data becomes available or simulations progress.

[0195] The frontend of the interface **205** may be developed using modern web technologies, with React.js as a primary framework for building responsive and interactive user interfaces. According to an aspect, to handle the complex state management required for scientific applications, the system utilizes Redux for global state management, coupled with Redux-Saga for managing side effects and asynchronous operations. For 3D molecular visualizations, the platform integrates libraries such as Three.js and specific molecular visualization tools such as NGL Viewer or Mol* Viewer, which provides high-performance rendering of complex molecular structures directly in the browser. These can be augmented with custom WebGL shaders to enhance the visual quality and performance of large-scale molecular scenes.

[0196] Data visualization is an important aspect of user interface **205**, implemented using, for example, a combination of D3.js for custom, interactive visualizations and Plotly.js for more standard scientific plotting needs. For handling large-scale data sets, the system may employ techniques like data streaming and progressive rendering, allowing users to interact with partial results while full computations complete in the background. The interface can also incorporate advanced features like brushing and linking across multiple coordinated views, enabling users to explore relationships between different data representations simultaneously.

[0197] A knowledge graph and reasoning computing platform **207** is a component of AI drug discovery platform **200** designed to capture, represent, and leverage complex biomedical knowledge. A knowledge graph is a large-scale, multi-relational graph database that represents entities (such as drugs, proteins, diseases, and biological processes) as nodes and their relationships as edges. This graph can be constructed using a combination of structured databases (e.g., DrugBank, UniProt, and KEGG), unstructured text from scientific literature processed using advanced natural language processing techniques, and curated expert knowledge. The graph employs a flexible schema that can accommodate diverse types of biomedical information, using ontologies such as Gene Ontology and Disease Ontology to ensure consistent representation of concepts across different data sources.

[0198] The construction of the knowledge graph may comprise several advanced techniques. Entity recognition and relation extraction from scientific literature may be performed using state-of-the-art NLP models, such as BERT-based architectures fine-tuned on biomedical corpora. These models identify relevant entities and their relationships from text, which are then integrated into the graph. According to an embodiment, to handle the inherent uncertainty in extracted information, the graph incorporates probabilistic edges, where the confidence of each relationship is represented as a weight. The graph is continuously updated through an automated pipeline (which may be provided by data integration computing platform **201**) that monitors new publications and databases, ensuring it remains current with the latest biomedical knowledge.

[0199] According to an embodiment, a regulatory compliance and ethics computing platform/module **207** is present and configured to ensure that all operations adhere to legal, ethical, and industry standards throughout the drug development process. This module is built on a robust framework that integrates regulatory guidelines, ethical considerations, and data governance principles into every aspect of the platform's functionality. In some implementations, the module utilizes a rule-based expert system combined with machine learning algorithms to continuously monitor and assess compliance across all activities.

[0200] According to the embodiment, a drug discovery computing platform **208** (also referred to as the drug discovery pipeline) within AI drug discovery platform **200** is a sophisticated, multi-faceted system designed to streamline and accelerate the process of identifying and optimizing potential

drug candidates. This pipeline integrates advanced computational methods with machine learning algorithms to navigate the vast chemical space and identify compounds with promising therapeutic potential.

[0201] FIG. **3** is a high-level architecture diagram of an exemplary personal health database (PHDB) platform, according to an aspect. One or more of the components or functionality described herein with respect to PHDB computing platform **320** may be implemented in various aspects of AI-enhanced cellular modeling and simulation platform **100**. For more detailed information regarding the operation of the PHDB computing platform and variants thereof, please refer to U.S. patent application Ser. No. 18/801,361 which is incorporated herein by reference.

[0202] As shown in FIG. **3**, system **300** offers accessibility to a variety of entities including end users **310**, Internet of Things (IoT) devices **340**, Care Givers **350**, Third-Party Services **330**, and Labs **360** by connecting to various cloud-based **301** platforms (e.g., systems, subsystems, and/or services) via a suitable communication network such as the Internet. End Users **310** have flexibility, choosing to engage in cloud-based processing through either their Personal Computers **315***a-n* which may connect to the cloud-based platforms **301** via a browser-based website or web application, or PHDB-enabled Mobile Devices **310***a-n* (e.g., smart phone, tablet, smart wearable clothing or glasses, headsets etc.). These mobile devices may comprise a PHDB **311***a*, an operating system (OS) **312***a*, and various applications (Apps) **313***a-n*, creating a comprehensive environment for users to manage and interact with their health and preference data. The ability to have authorized disclosure rules and suggestions or delegate sharing and visibility for personal health records or conditions can also vastly simplify medical procedures and improve outcomes for patients and aid in medical decision making and adherence to care intentions, whether informal or through documents like living wills. Current systems force patients into cumbersome manual and often paper disclosure certifications (e.g., outpatient surgery procedure) but could instead be configured to send appropriate status and visibility (even for physical visitation rights in hospital) data to family and friends. This can also better enable post-operative and non-medical facility care by enabling family and friend and personal uploads to the PHDB of photos, interactions, observations, sensor data which can be made available to PHDB processes or to medical staff supporting outcomes.

[0203] A user of the system may collect various personal consumption, environment, activity, and other health-related data from a plurality of sources and store the data in their personal health database. Personal health-related data can include genetic information and medical information associated with the user, as well as other types of biometric, behavioral, and/or physiological information. Personal health-related data may be obtained from various sources including, but not limited to, labs **360**, third-party services **330**, care givers **350**, and IoT devices **340**. For example, genetic information may be obtained from a lab **360** that conducts genetic carrier screening (e.g., autosomal dominant, autosomal recessive, X-linked dominant, X-linked recessive, mitochondrial, etc.) for a user. Ongoing urine data may be fed from Withings new urine sensor kit, body scan data from an at home body scanner/scale, temperature data from thermal cameras or thermometers, sleep data from smart mattress covers, snoring and sleep quality and sleep apnea indicators from wearable microphones along with heart rate and blood oxygen levels, et cetera. Best practices for individuals or couples wishing to improve personal health outcomes or shared goals such as having children now can include genetic indicator monitoring (e.g., for new papers and research) as well as lived experiences and exposures that may enhance or reduce their risk of adverse health outcomes.

[0204] Genetic testing can play a significant role in medical treatment. Some common types of genetic tests that can produce genetic information that can be stored in an individual's PHDB can include diagnostic testing, carrier testing, prenatal testing, newborn screening, pharmacogenetic testing, predictive and presymptomatic testing, forensic testing, and research genetic testing. Diagnostic testing is used to identify or rule out a specific genetic or chromosomal condition. It is done when there is a suspicion based on symptoms or family history. Carrier testing is used to

determine if a person carries a gene for a genetic disorder. This type of testing is often done in people with a family history of genetic disorder or in specific ethnic groups with a higher risk. Prenatal testing is conducted during pregnancy to detect genetic abnormalities in the fetus. Examples include amniocentesis, chorionic villus sampling (CVS), and non-invasive prenatal testing (NIPT). Newborn screening involves a series of tests performed on newborns to detect certain genetic disorders early, allowing for early intervention and treatment. Pharmacogenetic testing analyzes how an individual's genes affect their response to certain medications. This information can help personalize medication dosages and selection. Predictive and presymptomatic testing is used to identify genetic mutations associated with conditions data develop later in life, such as certain types of cancer. Presymptomatic testing is done in individuals who do not yet have symptoms but have a family history of a genetic disorder. Forensic testing is used for identification purposes, such as in criminal investigations or paternity testing. Research genetic testing is conducted as part of research studies to better understand the roles of genetics in health and disease. These tests can provide valuable information for healthcare providers, care givers, individuals, and prospective mates.

[0205] In some implementations, labs **360** may comprise a plurality of types of labs and facilities that could gather genetic, biometric, behavioral, and/or physiological data on a user. Exemplary labs/facilities can include, but are not limited to, research laboratories (e.g., often affiliated with universities or research institutions and conduct studies to gather various types of data), biotechnology companies, healthcare facilities (e.g., hospitals, clinics, and other healthcare facilities may gather data as part of patient care or research studies. This data could include information from medical tests, imaging studies, and patient questionnaires), tech companies (e.g., wearable technology industry), government agencies, and consumer research firms.

[0206] According to the embodiment, caregivers **350** may also provide information to PHDB about the individual which they are providing care for. A caregiver, depending on their role and the context of care, may be responsible for a wide range of medical information. Some common types of medical information that a caregiver might know about or be responsible for include, but are not limited to, patient history (e.g., information about past illnesses, surgeries, medications, allergies, and family medical history), current health status (e.g., information about the patient's current health, including any ongoing medical conditions, symptoms, and vital signs such as blood pressure, heart rate, and temperature), medications (e.g., information about the medications the patient is taking, including dosage, frequency, and any special instructions), treatment plans (e.g., information about the patient's treatment plan, including any medications, therapies, or procedures that have been prescribed), progress notes (e.g., notes on the patient's progress, including any changes in their condition, response to treatment, or other relevant information), diagnostic tests (e.g., information about any diagnostic tests that have been performed, such as blood tests, imaging studies, or biopsies, and the results of those tests), care plan (e.g., information about the overall plan of care for the patient, including goals, interventions, and follow-up care), patient education (e.g., information about legal and ethical issues related to the patient's care such as advance directives, consent for treatment, and confidentiality), and coordination care (e.g., information about coordination of care with other healthcare providers, including referrals, consultations, and care transitions). The specific medical information that a caregiver is responsible for and can provide to the PHDB of their patient will vary depending on the setting and scope of their practice, as well as the needs of the patient.

[0207] According to the embodiment, cloud-based platforms **301** may integrate with various third-party services **330** to obtain information related to a user's genetics, biometrics, behavior, and/or physiological characteristics. For example, platform **301** may obtain an electronic health record (EHR), or a subset thereof, associated with the user for inclusion in the user's PHDB.

[0208] Additionally, a PHDB mobile device **310***a-n* may comprise a plurality of sensors which may be used to monitor and capture various biometric, behavioral, and/or physiological data associated

with the owner (end user) of the PHDB mobile device. Captured sensors data may be stored in PHDB **311***a* either in raw data form, or in a format suitable for storage after one or more data processing operations (e.g., transformation, normalization, etc.) has been performed on the sensor data. In some embodiments, a purpose-built software application **313***a-n* configured to collect, process, and store various sensor data (e.g., biometric, behavioral, physiological, etc.) obtained by sensors embedded into or otherwise integrated with PHDB mobile devices **310***a-n*. Some exemplary sensors that may be embedded/integrated with PHDB mobile device can include, but are not limited to, fingerprint sensor, facial recognition sensor, heart rate sensor, accelerometer, gyroscope, continuous glucose monitor (CGM), Global Positioning System (GPS), microphone, camera, light sensor, electromagnetic sensors, barometer, pedometer/step counter, galvanic skin response (GSR) sensor (e.g., measures skin's electrical conductivity, which can vary with emotional arousal, stress, or excitement), temperature sensor, lidar, and infrared sensor. More advanced sensors might include Raman-based real-time analytics, gas chromatography mass spectrometry, liquid chromatography mass spectrometry, capillary electrophoresis mass spectrometry, which may be of particular use in environmental exposure considerations in health conditions and lived gene expression. These sensors can be used individually or in combination to gather a wide range of data about the user's biometric, behavioral, and physiological characteristics, enabling various applications such as health monitoring, fitness tracking, personalized user experiences, and human genome filtering for compatibility, to name a few. It is important to note that when combined with temporal and graph representations of interactions in the individual's life, this can feed into a much more nuanced biological monitoring, modeling and simulation aid available for personal, family, or medical use. Users who gather such data fastidiously may also be of particular interest to researchers in support of uncertainty reduction and isolation of particular genetic linkages to this litany of more comprehensive lived factors commonly excluded from static genomics analysis.

[0209] In some embodiments, PHDB **311***a* may be stored in the memory of PHDB mobile or wearable device **310***a*. In some embodiments, PHDB **311***a* may be implemented as an encrypted database wherein the plurality of personal health data stored therein is cryptographically encrypted to protect the personal and sensitive data stored therein.

[0210] End users **310** may also engage in edge-based processing referring to computing devices that process data closer to the source of data generation instead of relying solely on a centralized server. Edge devices are situated close to the point where data is generated, such as sensors, cameras, or other Internet of Things devices. The Internet of Things (IoT) **340** devices refer to physical objects embedded with sensors, software, and other technologies that enable them to connect and exchange data over the internet. These devices are part of the broader concept of the Internet of Things, which involves the interconnection of everyday objects to the Internet, allowing them to collect and share data for various purposes. Internet of Things devices find applications in various domains, including smart homes, healthcare, industrial automation, agriculture, transportation, and more. Examples include smart thermostats, wearable health monitors, industrial sensors, and connected vehicles. According to the embodiment, a plurality of IoT devices **340** may be deployed to collect and transmit various types of information related to a user's genetics, biometrics, behavior, and/or physiological characteristics. In some implementations, IoT devices **340** can include a plurality of sensors, devices, systems, and/or the like configured to collect and transmit data to cloud-based platforms **301** for inclusion in the user's PHDB. Some exemplary IoT devices **340** can include fitness trackers, smart scales, smart clothing, smart home devices, genetic testing kits, sleep monitors, health monitoring devices (e.g., devices that measure health parameters such as blood pressure, glucose levels, and oxygen saturation, etc.), and wearable cameras.

[0211] To facilitate proactive filtering across multiple platforms during interactions with prospective mates, the cloud **301** integrates an optional encryption platform **321**, an orchestration computing platform **322**, and a PHDB-related computing platform **320**.

[0212] According to the embodiment, an optional encryption platform **121** may be configured and

deployed to provide strong encryption to protect data from unauthorized access. In addition to using strong encryption algorithms, encryption platform **321** is configured to follow best practices for key management, such as using strong, randomly generated encryption keys, and regularly rotating keys to minimize the risk of unauthorized access. In an embodiment, encryption platform **321** may implement advanced encryption standard (AES) for encrypting the various data stored in PHDB. AES is a symmetric encryption algorithm that is widely used and considered to be very secure. It is often used to encrypt data at rest, such as files stored on PHDB. In an embodiment, encryption platform **321** may utilize RSA which is an asymmetric encryption algorithm commonly used for encrypting data in transit, such as data sent over the Internet. In another embodiment, elliptic curve cryptography (ECC) may be implemented which is an asymmetric encryption algorithm that is known for its efficiency and security. In some embodiments, ECC may be used to encrypt data obtained and transmitted by IoT devices **340** to cloud-based platforms **301**. In some implementations, a combination of encryption schemes may be utilized to provide secure data storage and transmission. For example, personal-health data may be encrypted in the cloud using RSA and then sent to an end user mobile device **310***a* wherein it may be encrypted using AES for storage on PHDB **311***a* of the mobile device.

[0213] In some embodiments, encryption platform **321** may implement homomorphic encryption when processing or otherwise analyzing personal health information. In this way, the system can provide processing of encrypted data without having to decrypt and potentially leak personal information.

[0214] An orchestration platform **322** is present and configured to provide automated management, coordination, and execution of complex tasks or workflows. This can involve deploying and managing software applications, provisioning and managing resources, and coordinating interactions between different components of system **300**. Orchestration platform **322** may automate the deployment and management of virtual machines, containers, and other resources. This can include tasks such as provisioning servers, configuring networking, and scaling resources up or down based on demand. For example, orchestration platform **322** may define and execute a workflow related to the collection, encryption, and distribution (to the appropriate PHDB) of user health-related information. Of particular importance is the ability of the platform to interact with AI/ML systems to aid in explaining, modeling, extracting models, or generating potential items of interest for consideration by medical experts or users. This is further enhanced by the ability for automated planning and modeling simulation services to consider forward scenario analysis of factors (e.g., what if I stopped eating bacon every morning and walked a minimum of 15,000 steps per day instead of my current activity level). This may also help generate financial models to aid users in their personal decision-making and potentially for insurers or medical professionals in theirs. This is becoming more important in the emerging CRISPR/Cas9 and with the sudden emergence of Ozempic and Zapbound era. This is likely to become more challenging for payers, patients and providers if the expected multireceptor agonists such as LY3437943 (a novel triple agonist peptide at the glucagon receptor (GCGR), glucose-dependent insulinotropic polypeptide receptor (GIPR), and glucagon-like peptide-1 receptor (GLP-1R)), emerge and potentially offer large benefits to at risk populations with severe disease and broad-based disease risk factor reductions. Such financial "what if" scenarios will become important when considering the lifetime value of treatment options and potential payment models and is critical to improving patient outcome and better managing continuity of care for healthier and ultimately cheaper patients.

[0215] The PHDB system may further comprise a spatiotemporal modeling subsystem introduces a significant advancement in health data management and analysis through the integration of a spatiotemporal modeling subsystem **323**. This component interfaces with the existing PHDB-related computing platform **320**, expanding the system's capabilities to process and analyze health data across both spatial and temporal dimensions. The spatiotemporal modeling subsystem **323** works in concert with the encryption platform **321** and the orchestration computing platform **322** to

provide a comprehensive, secure, and dynamic approach to personal health data management.

[0216] The spatiotemporal modeling subsystem **323** is designed to create and maintain a four-dimensional representation of an individual's health data. It processes information from various sources, including the PHDB mobile devices **310***a-n*, personal computers **315***a-n*, IoT devices **340**, labs **360**, third-party services **330**, and care givers **350**. This subsystem transforms the traditional static view of health records into a dynamic, evolving model that captures changes in health status over time and across different anatomical locations.

[0217] The spatiotemporal modeling subsystem **323** employs advanced algorithms to construct a time-stabilized three-dimensional mesh of the human body. This mesh serves as a framework onto which various types of health data can be mapped. The subsystem can handle data at different resolution levels, allowing for analysis ranging from cellular-level information to whole-body overviews. By tagging multi-omics data to specific "cells" in the 3D mesh and tracking changes over time, the system provides a spatially and temporally resolved view of biological molecules within tissues or organisms.

[0218] The integration of this subsystem enhances the PHDB system's ability to perform sophisticated analyses. For instance, it enables the study of gene expression patterns in specific regions of the body over time, providing insights into how genetic factors interact with environmental influences to affect health outcomes. This capability is particularly valuable for understanding complex, multifactorial conditions that evolve over time, such as cancer progression or neurodegenerative diseases.

[0219] Furthermore, the spatiotemporal modeling subsystem **323** supports advanced simulation and predictive modeling. By leveraging the comprehensive, four-dimensional health data, it can generate multiple simulation paths based on "seeds" extracted from the PHDB. This feature allows for parametric studies that explore the potential impacts of various factors, including imaging techniques, sampling methods, and environmental exposures. Such simulations can aid in diagnostics, treatment advisory, and treatment calibration, offering a more nuanced and personalized approach to healthcare.

[0220] The concept of "seeds" in the context of the PHDB system refers to specific data points or sets of parameters extracted from a user's personal health database that serve as starting points for simulations or analyses. These seeds are carefully selected snapshots of an individual's health status at a particular point in time, encompassing various types of data such as genomic information, current physiological measurements, lifestyle factors, and environmental exposures.

[0221] The spatiotemporal modeling subsystem **323** can utilize these seeds to initiate multiple simulation paths, allowing for the exploration of various "what-if" scenarios and potential health outcomes. For example, a seed might include a user's current cardiovascular health metrics, genetic predispositions, and lifestyle factors. The system could then generate simulations to predict how changes in diet, exercise, or medication might affect the user's heart health over time. By using seeds from different time points or with varied parameters, the system can conduct parametric studies to investigate the potential impacts of various factors on prospective health outcomes. This may occur through probabilistic reasoning (e.g. evaluating frequency and severity, either positive or negative, of outcome against real outcomes or synthetic data generated by system to approximate privacy preserved or restricted data which cannot be directly shared or synthetic data or simulation data stemming from predictive models) to aid in identifying and communicating a full range of prospective positive, neutral, or negative outcomes. Discretized individual run results may be scored against a quality of life or cost or other user-customized or specific objective function (e.g. accounting for mobility vs longevity vs cost) and such outcomes may be viewed as points or as curves or functions approximating them. Select regions of such scores, i.e. outcome regimes or scenarios, or individual scenarios may be selected by system automatically (e.g. most dangerous, most likely, best case) or by patient, provider or payer for the purpose of discussing potential considerations during decision-making and authorization. This approach enables a more

personalized and predictive form of healthcare, where interventions can be tailored based on simulated outcomes derived from an individual's unique health profile. The use of seeds in this manner significantly enhances the PHDB system's capability to provide nuanced, forward-looking health insights and supports more informed decision-making for both users and healthcare providers.

[0222] The subsystem may also incorporate machine learning and AI processes for classifying individual cells and identifying cellular neighborhoods. These advanced analytical capabilities contribute to the creation of an enhanced 3D (or 4D) mesh that serves as an anchor for all available data. This approach is particularly beneficial for complex modeling techniques such as finite element analysis, fluid modeling, and fluid-structure interaction modeling, which are important for understanding the intricate dynamics of biological systems.

[0223] The spatiotemporal modeling subsystem **323** ingests data from multiple sources within the PHDB ecosystem. It interfaces directly with the PHDB-related computing platform **320** to access the diverse types of data stored in users' personal health databases. This includes spatio-temporal genomic data, microbiome data, phenotype data, biometric data, medical data, activity data, and snapshot data. The subsystem also receives real-time data streams from IoT devices **340** and wearables, which may be part of the PHDB mobile devices **310**a-n. It is possible that these devices stream such data continuously or in highly aperiodic fashions based on available resources, network conditions, battery life, location, user settings and other factors. These varied data streams provide often continuous updates on various physiological parameters, activity levels, and environmental exposures. Additionally, the subsystem can incorporate data from labs **360** and third-party services **330**, which may include detailed medical imaging, test results, and specialized health assessments.

[0224] The data ingestion process is managed by the orchestration computing platform **322**, which ensures that incoming data is properly formatted, validated, and securely transmitted to the spatiotemporal modeling subsystem. The encryption platform **321** plays a role in this process, ensuring that all data remains encrypted during transmission and storage. The spatiotemporal modeling subsystem **323** is designed to work with homomorphically encrypted data, allowing it to perform complex computations and analyses without decrypting sensitive information, thus maintaining user privacy and data security.

[0225] Once the data is ingested, the spatiotemporal modeling subsystem processes it to create and update the 4D model of the user's health. This involves mapping each data point to its appropriate spatial location within the 3D body mesh and associating it with a specific time point. The subsystem employs sophisticated algorithms to interpolate between data points, creating a continuous representation of health parameters across space and time. It also uses machine learning techniques to classify cells, identify patterns, and make predictions based on the accumulated data.

[0226] End users can interact with the spatiotemporal modeling subsystem through various interfaces provided by the PHDB mobile devices **310**a-n and personal computers **315**a-n. The system offers intuitive visualization tools that allow users to explore their health data in a 4D space. Users can navigate through their body model, zooming in on specific organs or tissues, and moving forward or backward in time to observe changes in their health parameters. This interactive visualization can be particularly helpful for understanding the progression of chronic conditions or the effects of treatments over time.

[0227] For more advanced interactions, the system provides query tools that allow users to ask complex questions about their health data. For example, a user might query the system to show all instances where their blood pressure exceeded a certain threshold, with the results displayed as highlighted regions in the 4D model. Users can also set up alerts based on spatiotemporal patterns, such as notifications for rapid changes in a specific health parameter within a particular body region.

[0228] Healthcare providers and researchers, with appropriate permissions, can use more

sophisticated tools to interact with the spatiotemporal modeling subsystem. They can run simulations, perform statistical analyses across populations, and use the system's predictive modeling capabilities to forecast potential health outcomes. The system also supports the creation of custom visualizations and reports, allowing healthcare providers to communicate complex health information to patients in an understandable and visually engaging manner.

[0229] Furthermore, the spatiotemporal modeling subsystem **323** may integrate with augmented and virtual reality systems, enabling immersive interactions with the 4D health model. This can be particularly useful for patient education, surgical planning, or exploring complex physiological processes. Users can literally step inside a virtual representation of their body, gaining a unique perspective on their health data.

[0230] FIG. **4** is a block diagram illustrating an exemplary aspect of an embodiment of the AI-enhanced cellular modeling and simulation platform.

[0231] According to various implementations, AI-enhanced cellular modeling and simulation platform **400** is built on a core architecture combining the distributed computational graph computing platform **401** with a spatiotemporal modeling subsystem **402**. This integration can enable complex workflow orchestration across distributed computing resources while handling complex (e.g., 4D) cellular representations. For instance, when modeling T cell activation in the immune system, the DCG could orchestrate a workflow from data ingestion through single-cell RNA sequencing to simulation of T cell receptor signaling cascades. The spatiotemporal subsystem would allow visualization and analysis of T cell activation progression in different spatial regions of a lymph node over time, providing insights into immune response initiation dynamics.

[0232] According to the embodiment, platform **400** can incorporate a multi-omics data integration computing platform **403** within data integration layer **110**, creating a unified data model to accommodate various types of omics data. This may comprise, for example, implementing data harmonization techniques and developing integrative analysis algorithms. In studying cellular senescence, for example, the platform can integrate genomic data on telomere length, transcriptomic data on senescence-associated secretory phenotype gene expression, proteomic data on p16 and p21 protein levels, and metabolomic data on energy metabolism changes. This comprehensive integration may reveal new biomarkers or therapeutic targets by identifying correlations across different omics layers.

[0233] Curation and marketplace systems **405** may be implemented to manage and share cellular models and datasets. The curation system can be configured to perform data quality checks, standardization processes, and metadata tagging, while the marketplace can provide a secure sharing platform, potentially using blockchain for provenance tracking. For instance, a researcher uploading a new agent-based tumor growth model would have it checked for compliance with standard formats, validated, and tagged with appropriate metadata before being made available to other researchers for use in studies on cancer cell proliferation and metastasis.

[0234] According to an embodiment, the platform may further comprise an AI and ML core system **404** which may comprise one or more predictive analysis models enhanced with LLM computing capabilities. This combination can leverage machine learning models for predicting cellular behavior, augmented by LLM's natural language processing of scientific literature and insight generation. In drug discovery for neurodegenerative diseases, this subsystem may use deep learning to predict small molecule effects on protein aggregation in neurons, while the LLM component can scan recent publications, summarize predicted drug effects, and suggest potential off-target effects based on the drug's structure and known cellular pathways.

[0235] An AI ethics and transparency computing platform **409** may be present in some embodiments of the platform, implementing guidelines for responsible AI use in cellular modeling. This may comprise fairness checks, explainability algorithms, and audit trails for model decisions. When using AI to predict cell fates in developmental biology, for example, this module can check for biases in training data, provide explanations for AI predictions, log all data sources and

algorithmic decisions, and allow researchers to compare AI predictions with known biological mechanisms.

[0236] According to an embodiment, a neurosymbolic AI subsystem can be incorporated to combine data-driven learning with domain knowledge in cellular biology. This may utilize techniques like logic tensor networks or differentiable inductive logic programming. In modeling cell signaling pathways, this AI could learn complex patterns in phosphorylation cascades from experimental data using neural networks, incorporate known rules about protein-protein interactions using symbolic logic, and generate hypotheses about novel signaling interactions that respect both learned patterns and known biological constraints.

[0237] The integration of the distributed computational graph **401** with the spatiotemporal modeling subsystem **402** and the simulation computing platform **407** creates a powerful core architecture for comprehensive complex (e.g., **4**D) cellular representations and multi-scale simulations. This combination allows for the orchestration of complex workflows across distributed computing resources while handling cellular processes at multiple scales and timepoints. The DCG can manage the overall workflow, coordinating data flow and computational tasks, while the spatiotemporal modeling subsystem provides the framework for representing cellular structures and processes in both space and time. Simulation computing platform **407** adds sophisticated simulation capabilities, enabling the modeling of cellular behaviors from molecular interactions to tissue-level effects. For example, in modeling the process of T cell activation in the immune system, this integrated system could orchestrate a workflow that includes: 1) data ingestion from single-cell RNA sequencing, 2) preprocessing and normalization, 3) spatial mapping of cells in a lymph node, 4) temporal modeling of gene expression changes, 5) simulation of T cell receptor signaling cascades, and 6) tissue-level simulation of T cell migration and interaction with antigen-presenting cells. The system could then visualize this process in a 4D representation, showing how T cell activation progresses in different spatial regions of the lymph node over time, providing insights into the dynamics of immune response initiation at multiple biological scales.

[0238] The enhancement of multi-omics data integration capabilities using the data integration computing platform **403** from AI drug discovery platform **130** significantly improves the handling and analysis of diverse biological data types. According to an aspect, this system can implement advanced data harmonization techniques and develop integrative analysis algorithms to create a unified data model that can accommodate various types of omics data, clinical information, and experimental results. It can handle the complexities of integrating data with different formats, scales, and temporal resolutions. For instance, in studying cellular senescence, the platform could integrate genomic data on telomere length, transcriptomic data on senescence-associated secretory phenotype gene expression, proteomic data on p16 and p21 protein levels, metabolomic data on energy metabolism changes, and epigenomic data on chromatin modifications. The data integration computing platform can align and normalize these diverse data types, creating a cohesive multi-omics profile of cellular senescence. This integrated data could then be used to identify novel biomarkers of senescence, understand the temporal progression of the senescence process, and potentially discover interventions to modulate cellular aging. According to an embodiment, the platform can integrate cellular modeling based on tissue neighborhoods, which captures more granular, biologically relevant dynamics at the cellular level. By combining tissue imaging with molecular-level data from 'omics data, this system can simulate interactions within the tumor microenvironment, akin to modeling ecosystems with Generalized Lotka-Volterra (GLV) equations. This can support a deeper understanding of tumor heterogeneity, providing a model for cellular competition and cooperation, useful for treatment strategy development in advanced cancers.

[0239] According to an embodiment, a visualization of a cellular interaction simulation may comprise a dynamic, multi-dimensional representation of the cellular environment. The central feature would be a 3D space representing a tissue section, tumor microenvironment, or other relevant biological context. Within this space, different cell types can be depicted as distinct

entities, possibly color-coded or shape-coded for easy identification-for instance, cancer cells in red, immune cells in blue, and stromal cells in green. These cells would be shown moving within the space, their trajectories potentially indicated by faint trails or in some other manner. When cells come into close proximity, the visualization may display lines or halos connecting them, representing direct cell-cell interactions or paracrine signaling. Internal cellular processes may be illustrated by changing colors or symbols within each cell, indicating gene expression changes or metabolic activity. The background of the visualization might use color gradients or particle systems to represent concentrations of nutrients, growth factors, or drugs diffusing through the environment. To reflect population dynamics based on the Generalized Lotka-Volterra equations, graphs or heat maps can be overlaid, showing real-time changes in population sizes of different cell types. A timeline or clock might be displayed to show the progression of time as the simulation runs. The space between cells can be textured to represent the extracellular matrix, with changes in its composition visualized over time. Specific cellular events like division, death, or phenotype changes can be highlighted with brief visual effects. Finally, the visualization may include user interface elements allowing researchers to zoom in/out, rotate the view, select individual cells for more detailed information, and control simulation parameters. This comprehensive visual representation can provide researchers with an intuitive, information-rich view of the complex cellular interactions and behaviors predicted by the simulation, facilitating deeper insights into cellular processes and potential therapeutic interventions.

[0240] The combination of the curation and marketplace systems **405** with the knowledge graph and reasoning computing platform **408** creates a sophisticated system for managing and sharing cellular models and data. The knowledge graph can represent biological entities (e.g., genes, proteins, metabolites, cellular processes, etc.) as nodes and their relationships as edges, creating a comprehensive representation of cellular biology and may incorporate or build on related knowledge corpora such as atoms, molecules, and bonds not specific to biology. This graph may be continuously updated with curated data from the marketplace and newly generated insights from the platform. Additional examples of distant knowledge corpora which may be updated from time to time may also include corporate data (e.g. in the Financial Industry Business Ontology) and ownership information about specific chemical compounds, processes, patents or licenses. The reasoning component can use advanced algorithms to traverse this multifaceted graph, identifying non-obvious connections and generating hypotheses. For example, in studying cancer cell metabolism, this system could integrate information about metabolic pathways, oncogenes, tumor suppressors, and experimental data on metabolite levels in various cancer types with information about researchers, drugs, ownership and licensing rights. Researchers could query this system to identify potential metabolic vulnerabilities in specific cancer types, discover novel connections between oncogenic signaling and metabolic reprogramming, and find existing drugs that might be repurposed to target cancer metabolism. The marketplace component can allow researchers to share their cellular models, experimental data, and analysis results, fostering collaboration and accelerating discovery in the field of cellular biology. Combining business and scientific data using compatible symbolic representations such as via knowledge graphs with compatibility, either directly or through Connectionist model translation approximations such as via LLM.

[0241] The integration of the AI and ML core **404** with the simulation computing platform **407** creates a powerful analytical engine for cellular modeling and simulation. This combined system incorporates a wide range of machine learning techniques, from traditional statistical methods to advanced deep learning models, capable of handling the complexity and high dimensionality of cellular data. It may comprise specialized architectures like graph neural networks for analyzing cellular interaction networks, recurrent neural networks for modeling temporal dynamics of cellular processes, and generative models for predicting cellular behaviors under novel conditions. For instance, in studying stem cell differentiation, this system could analyze time-series transcriptomic data to predict cell fate trajectories, use reinforcement learning to optimize differentiation

protocols, and employ generative adversarial networks to simulate the effects of various signaling molecules on cell state transitions. The system may also implement transfer learning techniques to apply knowledge gained from one cell type or organism to another, accelerating the modeling of less-studied biological systems.

[0242] According to an embodiment, AI and ML core **404** may further comprise an advanced AI system designed to analyze and interpret gigapixel pathology slides for cancer diagnostics. According to an aspect, the advanced AI system may be implemented as a whole-slide foundation model for digital pathology from real-world data. The whole-slide model operates on real-world data, using gigapixel pathology slides for cancer diagnostics. It has applications in tasks such as cancer subtyping and mutation prediction through large-scale image modeling. The technology leverages advanced techniques like vision transformers and LongNet for long-sequence representation. It utilizes self-supervised learning on unlabeled data to mitigate the demand for annotated data, which is often a major bottleneck in the field of digital pathology. The system has achieved state-of-the-art results across various tasks in digital pathology. It provides a strong foundation for leveraging digital pathology in diagnostic models. According to an embodiment, this technology is further enhanced by integrating it with spatiotemporal modeling and knowledge graph capabilities, which could link together facts and annotate medical records with insights from various data sets.

[0243] The implementation of the regulatory compliance and ethics computing platform **409** ensures responsible AI use in cellular research. This platform can incorporate up-to-date regulatory guidelines, ethical considerations, and data governance principles into every aspect of the platform's functionality. It may use a combination of rule-based systems and machine learning algorithms to continuously monitor and assess compliance across all activities. For example, when researchers are designing in silico experiments on human cellular models, the system could automatically check for compliance with ethical guidelines on human subject research, ensure proper data anonymization for any patient-derived cellular data, and flag any potential issues with the use of certain cell lines or genetic modification techniques. It could also provide guidance on the ethical implications of creating certain types of cellular models, such as human-animal chimeras or synthetic embryo-like structures, ensuring that all research conducted on the platform adheres to current ethical standards and regulations. It may also identify other resources, e.g. companies or researchers or licensees, with relevant experience for reference checks or other commercial feedback or practical experience solicitation.

[0244] The enhancement of the encryption platform and blockchain security system with a integration and API manager **204** improves data protection and secure collaboration in cellular modeling and simulation. This integrated system can provide end-to-end encryption for all data transfers, secure enclaves for sensitive computations, and a blockchain ledger for immutable record-keeping of data access and model usage. The API manager can facilitate secure and efficient communication between different components of the platform and with external systems. For instance, when multiple research groups are collaborating on a large-scale cellular modeling project, this system could provide secure, role-based access to shared cellular models and datasets. It could use homomorphic encryption to allow analysis of sensitive genetic data without decrypting it, record all data access events on a blockchain to ensure transparency and prevent unauthorized use, and use smart contracts to automatically enforce data usage agreements between institutions. The API manager can allow for the secure integration of external tools and databases, such as protein structure prediction services or pathway databases, enhancing the platform's capabilities while maintaining strict security protocols.

[0245] According to an embodiment, platform **400** may further comprise an IoT processing hub for integrating real-time data from cellular experiments and monitoring for incorporating live experimental data into cellular models and simulations. This hub can handle data streams from various lab instruments and cellular monitoring devices, implementing protocols for real-time data

ingestion, quality control, and integration into ongoing simulations or analyses. For instance, in a study of bacterial antibiotic resistance, the IoT hub could collect real-time data from microfluidic devices monitoring bacterial growth, process data from mass spectrometers analyzing metabolite production, and integrate this data into a running simulation of bacterial population dynamics. The system may trigger alerts if unexpected antibiotic resistance emerges, prompting researchers to adjust their experiments in real-time. This real-time data integration allows for the continuous refinement of cellular models based on experimental results, creating a tight feedback loop between in silico predictions and in vitro observations.

[0246] According to an embodiment, platform **400** comprises a real-time adaptive cellular modeling and treatment planning system **700** configured to support real-time data integration into complex cellular modeling and simulation processes.

[0247] This comprehensive integration of advanced components creates a powerful platform for AI-enhanced cellular modeling and simulation **400**, capable of handling the complexity of biological systems across multiple scales and timepoints while ensuring ethical compliance and data security. It provides researchers with sophisticated tools for data analysis, modeling, simulation, and visualization, potentially accelerating discoveries in cellular biology and advancing our understanding of complex biological processes.

[0248] According to an embodiment, platform **400** may support AI-enhanced cellular modeling and simulation by compiling comprehensive cellular data, including genomic, transcriptomic, proteomic, and metabolomic information from both cancer cells and healthy cells. This multi-omics data integration provides a foundation for the subsequent analyses. The AI and simulation components of the platform, trained on datasets of known tumor-associated antigens and cellular interactions, then simulates interactions between potential vaccine candidates and the cellular models. A spatiotemporal modeling subsystem visualizes and analyzes cellular responses to these vaccine candidates across different cellular regions and time points, providing a dynamic view of the cellular behavior. The knowledge graph component links these observed cellular responses to known biological pathways and previous research findings, contextualizing the results within existing scientific knowledge. To account for the inherent uncertainties in biological systems, a stochastic modeling component quantifies the uncertainty in vaccine efficacy predictions. The platform may then employ an optimization module to fine-tune vaccine designs based on multiple factors, including efficacy, cellular stress, and genetic stability. Finally, the simulation computing platform runs multiple in silico experiments, testing various combinations of vaccine components. This comprehensive approach allows for the rapid evaluation and refinement of personalized cancer vaccine candidates, significantly accelerating the drug discovery process.

[0249] FIG. **5** illustrates a distributed embodiment of the system across a plurality of cloud and edge devices. The figure illustrates the distributed architecture of the AI-enhanced cellular modeling and simulation platform, showcasing its scalability and capacity for handling complex computations across a network of interconnected devices. AI-enhanced cellular modeling platform may be implemented as a cloud computing center **500**, which houses high-performance compute clusters **501**, large-scale data storage systems **502**, an AI model training hub **503**, and an orchestration engine **504** (e.g., DCG framework for orchestrating computational tasks). This core infrastructure is connected to various edge devices **510***a-n*, including, for example, lab workstations **510***a*, mobile devices **510***b*, IoT sensors **510***c*, and specialized hardware **510***n* like GPU clusters, through a robust network. Exemplary networks which may be used to facilitate communication between and among central server **500** and the plurality of edge devices **510***a-n* can include, but are not limited to, cellular networks, 5G, fiber optic, and satellite, and/or the like. Small cloud icon **540** with arrows point to the main cloud, suggesting potential for multi-cloud integration.

[0250] The distributed architecture of the platform is designed to handle the immense computational demands of cellular modeling and simulation across a network of interconnected

devices. According to an embodiment, AI-enhanced cellular modeling platform may be implemented as a cloud computing center **500**, which houses several key components. The high-performance compute clusters **501** consist of thousands of interconnected CPUs and GPUs, optimized for parallel processing of complex cellular simulations. These clusters may utilize technologies like CUDA for GPU acceleration and MPI (Message Passing Interface) for distributed computing, enabling them to efficiently run large-scale simulations of cellular eccosystems.

[0251] A large-scale data storage system **502** in the cloud may employ a combination of object storage (e.g., Amazon S3 or Google Cloud Storage) for raw data, and distributed file systems like Hadoop Distributed File System (HDFS) for processed data. This tiered storage approach allows for cost-effective storage of petabytes of cellular imaging data, omics data, and simulation results.

[0252] An AI model training hub **503** in the cloud may leverages distributed machine learning frameworks such as TensorFlow on Kubernetes or PyTorch on Ray. This setup allows for the training of massive neural network models, like transformer-based architectures for processing cellular image sequences or graph neural networks for modeling molecular interactions, across hundreds of GPUs simultaneously.

[0253] An orchestration engine **504** (e.g., DCG-based orchestration), built on technologies like Apache Airflow or Kubernetes, manages the complex workflows of data processing, model training, and simulation execution across the entire distributed system. It dynamically allocates resources, schedules tasks, and ensures fault tolerance.

[0254] According to an embodiment, orchestration engine **504** is implemented as a federated architecture that distributes orchestration responsibilities across multiple semi-autonomous nodes within the network. Rather than relying on a single central control point, the system may employ a mesh of orchestration engines that coordinate through a consensus mechanism, enabling resilient and localized decision-making. Each node may maintain its own orchestration capabilities while participating in a broader orchestration federation, allowing for both independent operation and coordinated actions across the network. This approach enables edge devices and regional clusters to maintain operational autonomy while still participating in larger-scale coordinated computations when needed. According to an aspect, the federated orchestration system dynamically forms orchestration domains based on factors such as geographical proximity, network conditions, and computational requirements. These domains can flexibly merge or separate based on workload demands and system conditions, providing natural load balancing and fault tolerance. The system can employ a distributed ledger to maintain consistency of orchestration state across the federation, while using local policy engines to enforce domain-specific rules and requirements. This architecture particularly benefits scenarios requiring data sovereignty, reduced latency for local operations, and graceful degradation of service during network partitions.

[0255] This infrastructure is connected to various edge devices **510***a-n*, lab workstations **510***a* are equipped with powerful GPUs (e.g., at current time NVIDIA Blackwell or Rubin series) and specialized software for local processing of cellular images and running smaller-scale simulations. These workstations may use containerization technologies Kubernetes and underlying supporting technologies like Docker or containerd to ensure consistency in software environments across different labs.

[0256] Mobile devices **510***b*, such as tablets used by researchers in the lab, run edge-optimized versions of cellular analysis models. These models, compressed using techniques like knowledge distillation or quantization, allow for real-time, on-device analysis of microscopy images.

[0257] IoT sensors **510***c* in lab environments continuously collect data on experimental conditions. These sensors use low-power wide-area network (LPWAN) technologies like LoRaWAN for efficient, long-range data transmission to local edge computing nodes.

[0258] The edge computing nodes **520** and **530**, strategically placed in research institutions, can use technologies like NVIDIA EGX for AI inference at the edge. These nodes run containerized versions of cellular simulation models, allowing for rapid, localized processing of experimental

data without the need to transfer large datasets to the cloud.

[0259] According to an embodiment, the system employs a sophisticated data flow management approach. Raw data from experiments is initially processed at the edge using techniques like federated learning, where edge devices collaboratively train machine learning models without sharing raw data. Processed results and model updates are then securely transmitted to the cloud using, for example, advanced encryption standards (AES) for data in transit.

[0260] The collaborative processing capability is enhanced by the implementation of a distributed ledger technology, such as Hyperledger Fabric, which ensures transparent and tamper-proof recording of data provenance and model updates across the distributed network, according to an embodiment.

[0261] For example, in a multi-institution study on cancer cell behavior, the system might operate as follows: High-resolution time-lapse microscopy data of cancer cell cultures is captured at various research labs. Edge devices in each lab perform initial processing, including cell segmentation and tracking. This processed data is securely transmitted to nearby edge computing nodes, which run more complex analyses, such as cell lineage tracing and morphological feature extraction.

[0262] The cloud infrastructure then aggregates data from all participating institutions, running large-scale simulations of tumor microenvironments using agent-based models and integrating multi-omics data. The central AI models in the cloud identify patterns in cell behavior across different experimental conditions and generate hypotheses about potential drug targets.

[0263] These insights are then disseminated back to the edge devices in each lab, updating their local models and informing the design of new experiments. The entire process is orchestrated by the central engine, which ensures that computational resources are optimally allocated based on the current phase of the research project and the volume of incoming data.

[0264] As another example, consider processing gigapixel pathology slides for cancer diagnostics. In this scenario, high-resolution slide images could be captured and initially processed at edge devices in pathology labs. These edge devices perform preliminary analysis, such as image segmentation and feature extraction, reducing the data volume sent to the cloud. The processed data is then securely transmitted to the cloud infrastructure, where more complex AI models, trained on vast datasets, perform advanced diagnostics and generate detailed reports. The cloud also orchestrates federated learning across multiple institutions, allowing the system to learn from diverse datasets while maintaining data privacy. Results and updated models are then distributed back to the edge devices, enhancing local processing capabilities and enabling real-time, on-site preliminary diagnostics. This distributed approach allows the platform to handle the immense computational demands of analyzing high-resolution pathology images at scale, while also providing rapid insights to pathologists at the point of care.

[0265] This distributed approach allows the AI-enhanced cellular modeling and simulation platform to leverage the collective computational power and data resources of multiple research institutions, enabling unprecedented scale and complexity in cellular behavior studies while maintaining data security and reducing data transfer bottlenecks.

[0266] FIG. **6** is a block diagram illustrating an exemplary embodiment of AI-enhanced cellular modeling and simulation platform configured for federated learning. According to the embodiment, the AI-enhanced cellular modeling and simulation platform implemented as a central cloud hub **600** employs a sophisticated federated learning architecture to harness insights from distributed data sources **622**, **632**, **642** while maintaining the privacy of multiple institutional datasets. This approach is useful in cellular modeling, where sensitive patient information and proprietary research data require stringent protection. The system's architecture centers around a global model **610** housed in the central cloud infrastructure, with local models **624**, **634**, **644** trained on institutional data at each participating research center or hospital (i.e., entities **620**, **630**, **640**). These local models, which could be complex neural networks designed for tasks such as cell type

classification, behavior prediction, or drug response modeling, undergo a carefully orchestrated training process. Initially, each institution prepares its local dataset **622**, **632**, **642**, comprising cellular imaging data, omics data, and clinical information, all of which remain securely within the local environment. The central server then distributes the current global model parameters to all participating institutions.

[0267] The local training process at each institution may comprise fine-tuning the model on its specific dataset, which might include adjusting convolutional neural network layers for cell image analysis, updating recurrent neural network parameters for time-series predictions of cell behavior, or modifying weights in graph neural networks that model cellular interaction networks. Throughout this process, differential privacy techniques may be applied, such as adding calibrated noise to gradients, gradient clipping, and implementing secure multi-party computation protocols, ensuring that individual data points do not unduly influence the model or compromise privacy. After a predetermined number of local training epochs, each institution computes the difference between the updated local model parameters and the original parameters received from the global model.

[0268] The platform may be configured to employ one or more secure aggregation techniques to combine these local model updates. This might involve homomorphic encryption or secure multi-party computation protocols, allowing for computations on encrypted data without revealing individual updates. The central server performs federated averaging on these securely aggregated updates, potentially using weighted averaging based on dataset size or quality, and may incorporate adaptive optimization techniques like FedAdam or FedYogi to improve convergence and handle statistical heterogeneity across institutions. The global model **610** is then updated with these averaged parameters and evaluated on a held-out validation set to assess performance improvements. This process iterates through multiple rounds until the model converges or reaches a predefined number of iterations.

[0269] As an example, consider a scenario where the system is developing a model to predict how cancer cells respond to various drug combinations. The global model might be initialized as a deep neural network that takes as input cellular morphology features, gene expression data, and drug properties. Each participating cancer research center would receive this model and train it on their local dataset of cell lines, drug screening results, and genomic profiles. Local training could involve advanced techniques like curriculum learning, where the model is first trained on simpler tasks such as single-drug responses before progressing to more complex scenarios like drug combination effects. Throughout this process, privacy-preserving techniques ensure that sensitive information about specific cell lines or proprietary drug compounds is not leaked.

[0270] The securely aggregated model updates would capture insights from diverse datasets spanning different cancer types, experimental conditions, and patient populations. The resulting updated global model, benefiting from this diverse learning, can potentially identify novel biomarkers for drug response or suggest unexplored drug combinations for specific cancer subtypes. This federated learning approach allows the AI cellular modeling platform to leverage data from multiple institutions, significantly enhancing its predictive power and generalizability, while maintaining the privacy and security of each institution's valuable data. By enabling collaborative learning without direct data sharing, this system paves the way for more comprehensive and robust cellular models, ultimately accelerating progress in areas such as personalized cancer treatment and drug discovery.

[0271] FIG. **7** is a block diagram illustrating an aspect of the AI-enhanced cellular modeling and simulation platform, a real-time adaptive cellular modeling and treatment planning system.

[0272] The figure illustrates the real-time capabilities of the AI-enhanced cellular modeling and simulation platform. At the left side of the diagram, multiple data input streams converge, representing the diverse sources of real-time information. These streams may comprise, for example, live cell imaging data, which might be high-resolution time-lapse microscopy feeds

capturing cellular dynamics at sub-micron resolution; biosensor readings, potentially including intracellular calcium levels or pH measurements; microfluidic device outputs, which could be monitoring nutrient gradients or drug concentrations; patient vital signs for in vivo studies; and drug response metrics quantifying cellular reactions to therapeutic agents.

[0273] These heterogeneous data streams feed into a real-time data integration hub **710**. This hub employs advanced data processing techniques such as multi-modal data normalization **711** to harmonize inputs from disparate sources, real-time feature extraction **712** using convolutional neural networks for image data and recurrent neural networks for time-series data, and temporal alignment algorithms **713** to synchronize data streams with varying sampling rates and latencies.

[0274] The processed data flows into the heart of the system, represented adaptive AI core **720** This core contains a plurality of interconnected online learning models, each specializing in different aspects of cellular behavior and response. The cell behavior predictor **721** might use a combination of long short-term memory (LSTM) networks and particle filter algorithms to forecast cellular trajectories and state transitions. The drug response analyzer **722** may employ a graph neural network to model the complex interactions between drugs and cellular pathways. The microenvironment modeler **723** can utilize a physics-informed neural network to simulate the dynamic extracellular conditions. The treatment efficacy estimator may be implemented as a reinforcement learning model that optimizes treatment strategies based on observed cellular responses.

[0275] Importantly, these models continuously update their parameters using online learning algorithms such as stochastic gradient descent with adaptive learning rates, allowing them to adapt to changing cellular behaviors and experimental conditions in real-time. The models interact with an anomaly detector **730** which may use techniques like autoencoder-based novelty detection or Gaussian process regression to identify unexpected cellular behaviors or treatment responses.

[0276] When anomalies are detected, the alert system **740** is triggered. This system can use a decision tree algorithm to classify the severity and nature of the anomaly, generating appropriate alerts for a researcher dashboard and/or clinician interface. These alerts are designed to provide actionable insights, such as suggestions for adjusting treatment parameters or flagging potentially significant cellular state transitions.

[0277] The right side of the figure shows exemplary real-time insights **750** output, which includes dynamic cellular model visualizations (possibly using GPU-accelerated rendering for 3D cell simulations), treatment recommendation updates (generated by a multi-armed bandit algorithm for optimal treatment selection), and risk assessment metrics (calculated using Bayesian inference to quantify uncertainties in predictions).

[0278] An element of the system is the continuous feedback and adaptation loop. This loop allows the system to continuously refine its models and predictions based on observed outcomes, using techniques like online gradient boosting to incrementally improve model performance.

[0279] The human-in-the-loop interface **760** emphasizes the collaborative nature of the system. It allows researchers and clinicians to interact with the AI insights, potentially using augmented reality interfaces for immersive data exploration, and provides a means for expert knowledge to be incorporated into the system's decision-making processes.

[0280] As an example, consider monitoring a patient-derived organoid culture for personalized cancer treatment optimization. The system continuously processes microscopy feeds of the organoid, along with real-time measurements of metabolite levels and gene expression data. The cell behavior predictor model might detect subtle changes in cell morphology indicating a shift towards a more invasive phenotype. Simultaneously, the drug response analyzer could identify decreasing effectiveness of the current treatment regimen. The anomaly detector would flag these concerning trends, triggering an alert to the attending oncologist. The treatment efficacy estimator would then generate recommendations for adjusting the treatment strategy, perhaps suggesting a combination therapy approach based on the evolving cellular behavior. The oncologist, through the

human-in-the-loop interface, could review these insights, visualize projections of different treatment scenarios, and make an informed decision on how to adapt the patient's treatment plan in real-time. This continuous, adaptive process enables a level of personalized and responsive treatment planning that was previously unattainable, potentially leading to improved outcomes in complex diseases like cancer.

[0281] All embodiments of the AI-enhanced cellular modeling and simulation platform described herein inherit all functionalities and capabilities of the embodiments described with respect to FIGS. **1-4**, whether explicitly stated or otherwise. These core functionalities and capabilities form the foundation upon which all subsequent embodiments and use cases are built, enhancing and extending the platform's capabilities while retaining its fundamental features and architecture.

[0282] FIG. **8** is a block diagram illustrating an exemplary system architecture for an AI-enhanced cellular modeling and simulation platform **800** comprising a personalized medicine system, according to an embodiment. The personalized medicine system **900** is an advanced computational platform that integrates diverse patient data, including genetic, molecular, and physiological information, to tailor medical treatments to individual patients. The system employs sophisticated data integration techniques, AI-driven cellular modeling, and real-time adaptive algorithms to create and continuously update personalized health profiles. These profiles are used to predict treatment responses, simulate drug interactions, and assess risks, all of which are dynamically adjusted as new patient data becomes available. According to an aspect, the system leverages quantum computing for complex biological simulations and utilizes federated learning to improve its models while maintaining patient privacy. Healthcare providers **152** interact with the system through an intuitive dashboard that presents personalized treatment recommendations, simulation results, and risk assessments. By combining cutting-edge technologies in data analysis, machine learning, and biological modeling, the personalized medicine system aims to optimize treatment strategies, improve patient outcomes, and enhance the overall efficiency of healthcare delivery.

[0283] In some embodiments, personalized medicine system **900** may implement one or more components or functionality of the personalized medicine computing platform as described in U.S. patent application Ser. No. 18/900,608, which is incorporated herein by reference.

[0284] AI-enhanced cellular modeling and simulation platform **800** can be extended to support and enable its capabilities in personalized medicine. The platform can integrate data from wearable devices **810** and medical sensors **820**, providing a continuous stream of real-time patient information. This data, which may include heart rate, oxygen saturation, physical activity levels, and sleep patterns, can be incorporated into the platform's existing data integration framework. The system can then use this information to create a more comprehensive and dynamic patient profile, allowing for real-time monitoring of overall health and treatment effects.

[0285] To process and analyze this continuous data stream, the platform's AI and machine learning core can be enhanced to detect patterns and anomalies that may indicate changes in the patient's condition or response to treatment. For example, the system could be programmed to flag significant changes in heart rate variability or decreased physical activity, which might suggest increased stress or fatigue during treatment. This capability allows for more responsive and adaptive treatment protocols, where the system can recommend adjustments to therapy dosage or timing based on the patient's real-time physiological state.

[0286] The platform's predictive capabilities can be expanded to include AI-powered alerts for potential adverse events. By analyzing patterns in the real-time data from wearables and medical devices, along with the patient's molecular and genetic profile, the system can predict the likelihood of complications such as, for example, chemotherapy-induced cardiotoxicity before they occur. This predictive power enables healthcare providers to take preventive measures, potentially avoiding serious side effects and improving patient outcomes.

[0287] The platform can be adapted to incorporate behavioral and environmental data gathered from wearables and other sources. This information can provide valuable context for treatment

optimization, allowing the system to account for factors like sleep quality, exercise levels, and environmental exposures when making treatment recommendations. For instance, the system could suggest adjustments to medication schedules based on a patient's sleep patterns or recommend lifestyle changes that could enhance treatment efficacy.

[0288] The platform's existing visualization and user interface components can be expanded to support telehealth and remote monitoring capabilities. By integrating with telemedicine platforms and home-based medical devices, the system can enable continuous remote patient monitoring. This feature allows healthcare providers to track symptoms, side effects, and physiological responses without requiring in-person clinic visits, potentially reducing the burden on healthcare systems while improving patient care.

[0289] Lastly, the platform's machine learning capabilities can be enhanced to create a continuous learning system. As the platform collects and processes more real-time patient data, it can continuously refine its predictive models and treatment recommendations. This ongoing learning process ensures that the system becomes increasingly accurate and personalized over time, adapting to new medical knowledge and individual patient responses. By incorporating these additional features, the AI-enhanced cellular modeling and simulation platform can provide a more comprehensive, responsive, and personalized approach to patient care, fully realizing the potential of real-time data integration in personalized medicine.

[0290] FIG. **9** is a block diagram illustrating an aspect of the AI-enhanced cellular modeling and simulation platform, a personalized medicine system. According to the aspect, the personalized medicine system **900** is an advanced computational platform designed to tailor medical treatments to individual patients based on their unique genetic, molecular, and physiological profiles. This system integrates various components to create a comprehensive approach to personalized healthcare.

[0291] The personalized medicine system implements a robust data integration and processing framework. This framework begins by collecting diverse patient data from multiple sources, including, but not limited to, electronic health records, genetic tests, and real-time monitoring devices. A patient-specific data parser **901**, a specialized module within this framework, extracts and standardizes this information, ensuring that all data is in a compatible format for further analysis. This standardized data is then fed into the existing multi-omics data integration platform, which combines genomic, transcriptomic, proteomic, etc. information to create a holistic view of the patient's biological state.

[0292] Once the patient data is integrated, the system employs advanced modeling techniques to create and store a personalized cellular model **902**. This process leverages the AI and ML core system in conjunction with the simulation computing platform. A genetic variation interpreter **903** plays a role in this stage by translating the patient's genetic mutations and variations into parameters that can be used in the cellular model. This personalized model serves as a digital representation of the patient's physiology at the cellular level, allowing for highly specific simulations and predictions.

[0293] The treatment response prediction component **904** of the system utilizes this personalized cellular model to forecast how the patient might respond to various treatment options. This component combines the capabilities of the AI and ML core system with the knowledge graph and reasoning computing platform. By analyzing the patient's cellular model in the context of known biological pathways and previous treatment outcomes, the system can generate informed predictions about the efficacy of different therapies. The integrated treatment response simulator enhances this process by running detailed simulations of how specific treatments might interact with the patient's unique cellular environment.

[0294] According to an embodiment, personalized medicine system **900** is configured to dynamically adjust treatment recommendations based on ongoing patient data. The real-time adaptive cellular modeling and treatment planning system, augmented with a new treatment

efficacy feedback loop **905**, continuously monitors the patient's response to treatment. As new data becomes available, whether from regular check-ups, continuous monitoring devices, or new diagnostic tests, the system updates its models and predictions accordingly. This dynamic approach ensures that treatment plans evolve in response to changes in the patient's condition, such as the development of drug resistance in cancer treatments.

[0295] To further refine treatment selections, the system incorporates advanced drug interaction simulations. Building upon the existing simulation computing platform and AI drug discovery platform, a new patient-specific drug response predictor **906** has been developed. This predictor combines the patient's cellular model with detailed drug interaction simulations to forecast how an individual patient might respond to specific medications or combination therapies. This capability is particularly valuable in complex cases where patients may be taking multiple medications or have comorbidities that could affect treatment efficacy.

[0296] Recognizing the inherent uncertainties in medical predictions, personalized medicine system **900** comprises robust uncertainty quantification and risk assessment capabilities. The existing method for uncertainty quantification can be adapted and enhanced with a new personalized risk assessment module **907**. This module translates statistical uncertainties into patient-specific risk profiles for different treatment options, providing healthcare providers with a clear understanding of the potential outcomes and their likelihoods for each patient.

[0297] To make this complex information accessible and actionable, the system features an advanced visualization and reporting interface. Building upon the existing visualization and user interface system, a new personalized treatment dashboard **908** has been developed. This dashboard presents personalized treatment recommendations, simulation results, and risk assessments in an intuitive format. Healthcare providers can interact with this dashboard to explore different treatment scenarios, while patients can use a simplified version to better understand their treatment options and expected outcomes.

[0298] The personalized medicine system can also leverage cutting-edge quantum computing technologies to enhance its predictive capabilities. A quantum-classical hybrid computing module **909** has been integrated into the system, allowing for advanced simulations of genetic variations and their impacts on disease progression and treatment response. This module works in concert with classical computing resources to provide deeper insights into complex biological processes that are challenging to model with traditional computing methods alone.

[0299] According to an implementation, to continuously improve its predictive models while maintaining patient privacy, the system employs a federated learning approach. The existing federated learning architecture can be adapted specifically for personalized medicine applications, with the addition of a personalized medicine federated learning coordinator **910**. This allows the system to learn from distributed patient data across multiple healthcare institutions without centralizing sensitive information, thereby enhancing the model's accuracy and generalizability while adhering to strict privacy standards.

[0300] According to some implementations, personalized medicine system **900** comprises a sophisticated combination therapy simulator to address complex cases where single-drug treatments may prove insufficient. This feature leverages the system's advanced cellular modeling and AI-driven predictive algorithms to simulate the effects of various drug combinations on a patient's unique molecular profile. The process begins by utilizing the patient's personalized cellular model, which is constructed from their comprehensive multi-omics data. This model serves as a virtual representation of the patient's biological state at the cellular level.

[0301] The system can employ the AI and ML core, in conjunction with the drug interaction simulation module, to iteratively test different drug combinations in this virtual environment. For each potential combination, the system simulates how the drugs might interact with each other and with the patient's cellular mechanisms. This may comprise modeling potential synergistic effects, where drugs work together to enhance overall efficacy, as well as possible antagonistic interactions

that could reduce treatment effectiveness or increase side effects. The simulation takes into account factors such as drug absorption, distribution, metabolism, and excretion, all tailored to the patient's specific genetic and physiological characteristics.

[0302] As the system runs through numerous potential combinations, it continuously evaluates and ranks them based on predicted efficacy, side effect profiles, and overall patient outcomes. The AI leverages its knowledge graph and reasoning capabilities to interpret these results in the context of known biological pathways and previous clinical outcomes. This process allows the system to identify promising drug combinations that may not be immediately obvious to human clinicians, potentially uncovering novel treatment strategies tailored to the individual patient.

[0303] Throughout the simulation process, the system's uncertainty quantification module assesses the confidence levels of its predictions, providing clinicians with a clear understanding of the risks and potential outcomes associated with each combination. The real-time adaptive component of the system allows for continuous refinement of these predictions as new patient data becomes available during treatment, enabling dynamic adjustments to the combination therapy as needed.

[0304] The results of these simulations can be presented to healthcare providers through the personalized treatment dashboard, offering an intuitive visualization of the most promising drug combinations, their predicted effects, and associated confidence levels. This approach to combination therapy simulation empowers clinicians to make more informed decisions about complex treatment strategies, potentially improving patient outcomes in cases where standard single-drug approaches may fall short.

[0305] According to an embodiment, personalized medicine system **900** comprises capabilities for predictive diagnostics and biomarker discovery, leveraging its sophisticated AI and machine learning algorithms to identify and monitor personalized biomarkers that indicate treatment effectiveness. This process begins with a comprehensive analysis of the patient's multi-omics data, including genomics, transcriptomics, proteomics, and metabolomics information. The system's AI core, in conjunction with its knowledge graph and reasoning platform, analyzes this data to identify potential biomarkers that are uniquely relevant to the individual patient's condition and treatment plan.

[0306] These biomarkers may include specific gene expression patterns, protein levels, metabolites, or other molecular indicators that are predicted to correlate with treatment response. The system utilizes its cellular modeling capabilities to simulate how these biomarkers might change in response to various treatments, creating a personalized set of indicators for each patient. As treatment progresses, the system continuously tracks these biomarkers through periodic testing, such as blood samples or other minimally invasive procedures. The real-time adaptive component of the system processes this ongoing data, comparing actual biomarker levels and trends to the predicted patterns.

[0307] If discrepancies are detected between the observed and predicted biomarker behaviors, the system can quickly flag these issues and suggest potential adjustments to the treatment plan. For instance, if a biomarker indicating drug resistance begins to rise unexpectedly, the system might recommend altering the drug dosage or switching to an alternative therapy. The uncertainty quantification module provides confidence levels for these predictions and recommendations, ensuring that healthcare providers have a clear understanding of the reliability of the biomarker data.

[0308] Furthermore, the system's federated learning capabilities allow it to continuously refine its biomarker discovery algorithms by learning from anonymized data across multiple patients and institutions. This approach enables the system to identify novel biomarkers that may not have been previously associated with specific conditions or treatments, potentially leading to breakthroughs in personalized diagnostics.

[0309] The personalized treatment dashboard presents the biomarker data and its implications in an easily interpretable format, allowing healthcare providers to monitor treatment efficacy in real-time

and make data-driven decisions about adjusting therapies. This predictive diagnostics and biomarker discovery capability enhances the system's ability to provide truly personalized medicine, enabling rapid adaptation of treatment strategies based on each patient's unique molecular response patterns.

[0310] In operation, these components work together to provide a comprehensive personalized medicine solution. An example process begins when a patient's data is input into the system. The data integration framework processes this information, creating a standardized profile that is used to generate a personalized cellular model. This model is then analyzed by the treatment response prediction component, which generates initial treatment recommendations. These recommendations are refined through drug interaction simulations and risk assessments, with all results presented via the personalized treatment dashboard.

[0311] As treatment progresses, the system continuously updates its models and predictions based on new patient data. The real-time adaptive component ensures that any changes in the patient's condition are quickly reflected in updated treatment recommendations. Throughout this process, the system leverages its quantum computing capabilities for complex simulations and uses federated learning to improve its models based on outcomes from similar cases across its network.

[0312] This integrated approach allows the personalized medicine system to provide highly tailored treatment strategies that adapt to each patient's unique and evolving medical needs. By combining advanced AI and machine learning techniques with comprehensive biological modeling and real-time data analysis, the system represents a significant advancement in the field of personalized medicine, offering the potential for improved patient outcomes and more efficient healthcare delivery.

[0313] FIG. **10** is a block diagram illustrating an exemplary system architecture for an AI-enhanced cellular modeling and simulation platform **1000** comprising a drug discovery system, according to an embodiment. According to the embodiment, drug discovery system **1100** is an advanced computational platform that integrates artificial intelligence, cellular modeling, and comprehensive impact analysis to accelerate the identification and development of new therapeutic compounds, with a particular focus on personalized cancer vaccines. The system utilizes a sophisticated drug-cell interaction simulator to model how potential drug compounds interact with cellular structures at a molecular level. It then employs a drug candidate prioritization engine to rank potential candidates based on efficacy, safety, and other critical factors. A cancer vaccine design module inverts the traditional drug discovery process to create personalized vaccines based on patient-specific cancer cell characteristics. The system also incorporates multi-dataset analysis capabilities, treatment scenario modeling, and holistic impact assessment, considering factors such as long-term quality of life, economic implications, and healthcare accessibility. By combining these advanced components, drug discovery system **1100** not only accelerates the drug development process but also ensures that new treatments are optimized for real-world implementation and patient benefit, representing a significant advancement in the field of pharmaceutical research and personalized medicine.

[0314] FIG. **11** is a block diagram illustrating an aspect of an AI-enhanced cellular modeling and simulation platform, a drug discovery system. According to the embodiment, drug discovery system **1100** is implemented as an advanced computational platform designed to accelerate the process of identifying and developing new therapeutic compounds, with a particular focus on personalized cancer vaccines. This system integrates various components to create a comprehensive approach to drug discovery, leveraging artificial intelligence and cellular modeling techniques.

[0315] According to the embodiment, drug discovery system **1100** comprises an advanced drug-cell interaction simulator **1101**, which builds upon the existing simulation computing platform and AI/ML core system. This simulator creates detailed models of how potential drug compounds interact with cellular structures at a molecular level. It takes into account factors such as binding

affinities, metabolic processes, and potential off-target effects. The simulator can process large libraries of chemical compounds, rapidly assessing their potential efficacy and safety profiles in a virtual environment.

[0316] Working in tandem with the simulator is a drug candidate prioritization engine **1102**. This component analyzes the results from the drug-cell interaction simulations and ranks potential drug candidates based on a complex set of criteria. These criteria may include, for example, predicted efficacy, safety profiles, case of synthesis, and potential for personalization. The engine leverages machine learning algorithms trained on historical drug development data to make these assessments, continuously improving its predictive capabilities as it processes more data.

[0317] The system may further comprise a cancer vaccine design module **1103**. This component inverts the traditional drug discovery process by starting with the specific characteristics of a patient's cancer cells and working backwards to design a personalized vaccine. It integrates patient-specific multi-omics data, analyzing the unique genetic and molecular features of the individual's cancer. Using this information, it identifies potential tumor-specific antigens that could be targeted by a personalized vaccine. The module then simulates how different vaccine designs might interact with these targets, optimizing for both efficacy and safety.

[0318] To handle the complexity of modern drug discovery, which often involves analyzing multiple large datasets, the system includes a variable analysis technique coordinator **1104**. This component orchestrates the application of various analytical methods across diverse datasets, which may include, but is not limited to, genomic data, proteomic profiles, clinical trial results, and published literature. By coordinating these analyses, the system can identify patterns and potential drug candidates that might be missed by more traditional, siloed approaches to data analysis.

[0319] A comprehensive treatment impact analyzer **1105** is present and extends the system's capabilities beyond mere drug discovery. This module can simulate various treatment scenarios, taking into account not just the immediate health outcomes but also long-term quality of life considerations. It models how different treatment options might affect a patient's daily life, potential side effects, and overall well-being. This holistic approach ensures that the drug discovery process is aligned with real-world patient needs and preferences.

[0320] Complementing this is the holistic impact assessment engine **1106**, which adds an economic and lifestyle dimension to the analysis. This component calculates the total cost of different treatment options, including factors such as ongoing medication needs, potential lifestyle changes, and long-term care requirements. It can model these impacts over the expected lifetime of a patient, providing a comprehensive view of the true cost and impact of a particular treatment approach.

[0321] Recognizing the importance of treatment accessibility, the system also incorporates a healthcare accessibility predictor **1107**. This forward-looking component forecasts the availability of proposed treatments based on factors such as geographic location, projected changes in healthcare infrastructure, and potential supply chain issues. This ensures that the drug discovery process is grounded in practical considerations of treatment delivery and long-term viability.

[0322] All these components work together in a seamless workflow. The process typically begins with the input of a target disease profile or patient-specific cancer data. The system then leverages its drug-cell interaction simulator to assess potential compounds or design personalized vaccines. The results are prioritized and analyzed for their comprehensive impact, including health outcomes, quality of life, and economic factors. Throughout this process, the system continuously learns and refines its models based on new data and outcomes.

[0323] The entire system is tied together through a user-friendly interface (e.g., visualization and user interface **115**) that allows researchers and clinicians to input parameters, view results, and interact with the drug discovery process. This interface provides visualizations of molecular interactions, treatment impact projections, and economic analyses, making complex data accessible and actionable.

[0324] By combining advanced AI techniques with comprehensive biological modeling and real-

world impact assessment, drug discovery system **1100** represents a significant advancement in the field. It has the potential to dramatically accelerate the development of new drugs and personalized treatments, particularly in complex areas like cancer therapy, while ensuring that these new treatments are optimized for real-world implementation and patient benefit.

[0325] FIG. **12** is a block diagram illustrating an exemplary system architecture for an AI-enhanced cellular modeling and simulation platform **1200** comprising a cellular engineering system, according to an embodiment. According to the embodiment, cellular engineering system **1300** is an advanced computational platform designed to model, analyze, and manipulate cellular structures with a specific focus on fascia and its interactions with surrounding tissues. Fascia, often referred to as the "most neglected part of our body," is now starting to receive attention for its critical role in various physiological functions. Fascia is a connective tissue that encases muscles, organs, and other structures in the body. Serving as an integral component in maintaining structural integrity, supporting tissue, and facilitating communication between cells and tissues. To fully understand cellular and tissue dynamics, especially in disease modeling and therapeutic interventions, it is essential to incorporate fascia into advanced simulation and modeling systems.

[0326] The system utilizes a fascia-specific simulation module that creates detailed models of fascia structure and function across multiple biological scales. It comprises specialized components such as the fascia-tissue interaction analyzer, fascia communication simulator, and tumor-fascia interaction predictor to provide comprehensive insights into fascia's role in health and disease. The system also features a synthetic fascia designer for creating artificial fascia structures, a fascia pain and adhesion simulator for modeling chronic pain conditions, and a fascia treatment optimization engine for generating personalized treatment plans. By leveraging advanced AI and machine learning techniques, multi-scale modeling, and a user-friendly interface, this system enables researchers **151** and clinicians **152** to gain deep insights into fascial biology, design novel therapeutic approaches, and develop personalized treatments for a wide range of fascia-related conditions, from chronic pain to cancer.

[0327] FIG. **13** is a block diagram illustrating an aspect of an AI-enhanced cellular modeling and simulation platform, a cellular engineering system **1300**. The cellular engineering system is implemented as an advanced computational platform designed to model, analyze, and manipulate cellular structures with a particular focus on fascia and its interactions with surrounding tissues. This system integrates various components to create a comprehensive approach to cellular engineering, leveraging artificial intelligence and multi-scale modeling techniques.

[0328] According to the embodiment, cellular engineering system **1300** is the fascia-specific simulation module **1301**, which builds upon the simulation computing platform and AI/ML core system. This module creates detailed models of fascia structure and function, taking into account its unique properties such as its role in structural support, biomechanical communication, and involvement in disease progression. The module simulates fascia at multiple scales, from the molecular level to tissue-wide interactions, providing a holistic view of fascia behavior in various physiological and pathological conditions.

[0329] Working in tandem with the simulation module is a fascia-tissue interaction analyzer **1302**. This component models how fascia interacts with surrounding tissues, organs, and cellular structures. It integrates data from various biological scales, leveraging the multi-omics data integration platform to create a comprehensive picture of the complex relationships between fascia and other bodily systems. This analyzer is useful for understanding how changes in fascia can affect overall tissue function and health.

[0330] A fascia communication simulator **1303** is present in this embodiment of the system, designed to model the complex biochemical and biomechanical signaling pathways that occur through fascia. This component simulates how mechanical forces and biochemical signals are transmitted through the fascial network, providing insights into how these communications influence cellular behavior, tissue function, and even systemic health. The simulator leverages

machine learning algorithms trained on extensive datasets of cellular signaling to predict how various stimuli might propagate through the fascial network.

[0331] For oncological applications, the system incorporates a tumor-fascia interaction predictor **1304**. This specialized module simulates how tumors interact with and invade fascia, providing insights for cancer research and treatment planning. It can model the mechanical properties of both fascia and tumor tissues, predicting how tumors might grow, spread, and respond to various treatment strategies. This component is particularly valuable for designing targeted therapies and predicting treatment outcomes in cancers that involve fascial invasion.

[0332] A synthetic fascia designer **1305** is an innovative component that enables the design and optimization of artificial fascia for various applications. This module uses advanced AI algorithms to create synthetic fascia structures that can be used for tumor containment, post-surgical support, or to enhance other body functions. It takes into account factors such as material properties, biocompatibility, and desired mechanical characteristics to generate optimal designs for specific clinical needs.

[0333] To address pain management and mobility issues, the system includes a fascia pain and adhesion simulator **1306**. This module models the formation of fascial adhesions and simulates their impact on pain perception and movement restriction. By integrating data on tissue mechanics, nerve signaling, and patient-reported outcomes, this simulator provides a comprehensive view of how fascial issues contribute to chronic pain conditions.

[0334] According to the embodiment, a fascia treatment optimization engine **1307** ties all these components together to generate personalized treatment plans. This engine analyzes the outputs from the various simulation and prediction modules to design tailored interventions for individual patients. It can suggest, for example, optimal approaches for fascia manipulation in physical therapy, guide the design of surgical interventions, or propose targeted drug therapies based on the patient's unique fascial characteristics.

[0335] All these components work together in a seamless workflow. An exemplary process typically begins with the input of patient-specific data, which is used to generate detailed fascia models. These models are then analyzed by the various simulation and prediction modules to generate insights into the patient's condition and potential treatment approaches. The system can simulate various intervention scenarios, predicting outcomes and potential side effects. Throughout this process, the system continuously learns and refines its models based on new data and outcomes.

[0336] The entire system is tied together through a user-friendly interface that allows researchers and clinicians to interact with the fascia models, design synthetic fascia structures, and plan personalized treatments. This interface provides visualizations of fascial structures, simulations of cellular interactions, and projections of treatment outcomes, making complex data accessible and actionable for healthcare providers.

[0337] Various advanced AI and machine learning algorithms may be used in simulating the behavior of engineered cells within the cellular engineering system. These algorithms can capture the complex, dynamic nature of cellular processes and predict outcomes of various modifications. Deep Neural Networks, particularly recurrent neural networks and Long Short-Term Memory networks, are valuable for modeling the temporal dynamics of cellular processes, capturing complex time-dependent behaviors in engineered cells. Graph Neural Networks excel at modeling cellular interaction networks, protein-protein interactions, and signaling pathways, providing insights into how modifications to one component might affect the entire system. Generative Adversarial Networks can generate synthetic data for rare cellular events or predict potential cellular states under various conditions, which is particularly useful when experimental data is limited.

[0338] Reinforcement Learning (RL) algorithms can be employed to optimize cellular engineering strategies, treating the cellular environment as the "environment" in the RL framework to find

optimal sets of genetic modifications. Gaussian Process Regression may be used for modeling uncertainty in cellular behavior predictions, important when dealing with the inherent stochasticity of biological systems. Variational Autoencoders can perform dimensionality reduction and feature extraction from high-dimensional cellular data, helping to identify the most important factors influencing engineered cell behavior. Adapted versions of Transformer models, typically used in natural language processing, could analyze sequences in biological data, such as protein sequences or time-series gene expression data.

[0339] Physics-informed Neural Networks (PINNs) integrate physical laws into the learning process and are particularly useful for modeling cellular mechanics or reaction-diffusion processes in engineered tissues. Ensemble methods like random forests or gradient boosting machines can combine multiple models, potentially capturing different aspects of cellular behavior for more robust predictions. Evolutionary algorithms could be used to evolve optimal cellular designs in silico, mimicking the process of directed evolution in the lab but at a much faster rate. The choice of algorithm depends on the specific aspect of cellular behavior being modeled, the type and amount of available data, and the particular engineering objectives. Often, a combination of these techniques might be used to capture the full complexity of engineered cellular systems, providing a comprehensive and nuanced understanding of cellular behavior under various conditions and modifications.

[0340] By combining advanced AI techniques with comprehensive biological modeling and a specific focus on fascia, cellular engineering system **1300** represents a significant advancement in the field. It has the potential to dramatically improve our understanding of fascia's role in health and disease, accelerate the development of novel therapies, and enable truly personalized treatment approaches for a wide range of conditions involving fascia.

[0341] FIG. **14** is a block diagram illustrating an exemplary system architecture for an AI-enhanced cellular modeling and simulation platform **1400** comprising a synthetic biology system, according to an embodiment. According to the embodiment, the synthetic biology system **1500** is an advanced computational platform designed to model, simulate, and control microbots and biobots for medical applications. The system utilizes a microbot environment simulator that creates detailed models of physiological microenvironments, coupled with a microbot design optimizer that leverages AI to create tailored microbot designs. It incorporates a swarm intelligence controller for managing collective behaviors, a drug release simulator for optimizing therapeutic delivery, and a magnetic field simulator for precise navigation control. For biobots, a morphogenesis predictor simulates their self-assembly and development. Real-time operations are managed through a telemetry analyzer, allowing dynamic adjustments based on live feedback which may be across multiple patients or subjects. The system also includes an operating room environment simulator to model clinical deployment and use scenarios. By integrating these components with advanced AI, multi-scale simulation modeling, and a user-friendly interface, the synthetic biology system enables researchers and clinicians to design, test, and deploy sophisticated microbot and biobot systems for a wide range of medical interventions, from targeted drug delivery to tissue repair, improving minimally invasive treatments and reducing risk in unavoidably invasive processes.

[0342] FIG. **15** is a block diagram illustrating an aspect of an AI-enhance cellular modeling and simulation platform, a synthetic biology system. According to the embodiment, synthetic biology system **1500** is implemented as an advanced computational platform designed to model, simulate, and control microbots and biobots for various medical applications. This system integrates multiple components to create a comprehensive approach to synthetic biology, leveraging artificial intelligence, multi-scale modeling techniques, and real-time control mechanisms.

[0343] According to the embodiment, synthetic biology system **1500** is the microbot environment simulator **1501**, which builds upon the simulation computing platform and spatiotemporal modeling subsystem. This module creates detailed models of the microenvironment where microbots will operate, taking into account factors such as fluid dynamics, tissue interactions, and

physiological barriers. The simulator provides a virtual testing ground for microbot designs and operations, allowing researchers to predict and optimize microbot behavior in various biological contexts.

[0344] Working in tandem with the environment simulator is a microbot design optimizer **1502**. This component leverages AI algorithms to design and refine microbot structures based on specific medical applications and environmental constraints. It considers factors such as size, shape, propulsion mechanism, and payload capacity to create optimized microbot designs tailored to particular tasks, such as targeted drug delivery or tissue repair.

[0345] A swarm intelligence controller **1503** is a key innovation in this system, designed to manage and optimize the collective behavior of microbot swarms. This component simulates how multiple microbots interact with each other and their environment, developing strategies for coordinated movement and task execution. It employs advanced algorithms to ensure efficient swarm behavior while minimizing the computational load on individual microbots.

[0346] For drug delivery applications, the system comprises a microbot drug release simulator **1504**. This specialized module models how drugs are released from microbots and interact with target tissues. It takes into account factors such as drug pharmacokinetics, local tissue properties, and microbot positioning to predict the efficacy of drug delivery and optimize release patterns in space, time, and condition.

[0347] A magnetic field simulator **1505** is important for microbots that rely on external magnetic fields for navigation and control. This module models the magnetic environment, simulating how microbots will respond to applied fields and identifying potential sources of interference. It helps in designing optimal control strategies and planning for necessary shielding or environmental modifications in clinical settings.

[0348] For biobots and biohybrid robots, the biobot morphogenesis predictor **1506** simulates the self-assembly and development of these living machines from cellular components. This module models complex biological processes such as cell differentiation, tissue formation, and emergent behaviors, allowing researchers to design biobots with specific functionalities without direct genetic manipulation.

[0349] The real-time operation of microbots is managed by the microbot telemetry analyzer **1507**, which processes data from microbot sensors and integrates it into the overall system. This component enables dynamic adjustments to microbot behavior based on real-time feedback, ensuring that operations can be fine-tuned in response to changing physiological conditions or unexpected obstacles.

[0350] According to an aspect, an operating room environment simulator **1508** models the broader surgical environment, considering factors such as electromagnetic interference, sterility requirements, and the integration of microbot control systems with existing medical equipment. This module helps in planning safe and effective microbot deployments in clinical settings.

[0351] All these components work together in a seamless workflow. An exemplary process typically begins with the design of microbots or biobots using the design optimizer, followed by virtual testing in the environment simulator. The swarm intelligence controller then develops strategies for coordinated operation, which are refined through iterative simulations. For drug delivery applications, the drug release simulator predicts therapeutic outcomes, while the magnetic field simulator ensures precise navigation. Throughout an operation, the telemetry analyzer provides real-time feedback, allowing for dynamic adjustments to the swarm's behavior.

[0352] The entire system is tied together through a user-friendly interface that allows researchers and clinicians to design microbot systems, simulate their operation in virtual physiological environments, and control their deployment in real-world settings. This interface provides visualizations of microbot behavior, simulations of drug delivery or tissue interactions, and real-time monitoring of microbot operations.

[0353] The synthetic biology system leverages a diverse array of AI and ML algorithms to model,

simulate, and optimize microbot and biobot designs and operations. Deep neural networks, such as RNNs and LSTM networks, can be employed to model the temporal dynamics of microbot behavior in complex biological environments. These networks are adept at capturing the time-dependent interactions between microbots and their surroundings. Reinforcement learning algorithms, such as Deep Q-Networks (DQN) or Proximal Policy Optimization (PPO), can be utilized to optimize swarm control strategies, allowing microbots to learn and adapt their collective behavior in response to changing environmental conditions. For designing the structure and functionality of individual microbots, GANs or VAEs may be employed to explore novel designs that meet specified criteria.

[0354] PINNs may be implemented for simulating the complex fluid dynamics and electromagnetic interactions that govern microbot movement and control. These networks incorporate physical laws into their architecture, ensuring that predictions adhere to fundamental principles of physics. For modeling drug release and diffusion, graph neural networks can be used to represent the molecular interactions between drugs, microbots, and target tissues. Evolutionary algorithms, such as genetic algorithms or differential evolution, can be applied to optimize microbot designs and swarm behaviors over multiple generations of simulations. Machine learning techniques like Gaussian process regression or Monte Carlo Markov chain based sampling can be employed for uncertainty quantification, providing confidence intervals for predictions of microbot behavior and drug efficacy.

[0355] For real-time control and adaptation, online learning algorithms such as online gradient descent or follow-the-regularized-leader can be used to update microbot control strategies based on incoming telemetry data. Natural language processing techniques, including transformer models, can be adapted to analyze and interpret complex sequences of microbot actions and physiological responses. Additionally, advanced simulation techniques like agent-based modeling, coupled with machine learning, can be used to create detailed, multi-scale models of microbot-tissue interactions. These diverse AI and ML approaches, when integrated within the synthetic biology system, enable the creation of sophisticated, adaptive, and highly optimized microbot and biobot systems for a wide range of medical applications.

[0356] By combining advanced AI techniques with comprehensive biological and physical modeling, the synthetic biology system represents a significant advancement in the field of medical microbots and biobots. It has the potential to accelerate the development of these technologies, enable more precise and effective medical interventions, and open new avenues for minimally invasive treatments across a wide range of medical conditions.

[0357] FIG. **16** is a block diagram illustrating an exemplary system architecture for an AI-enhanced cellular modeling and simulation platform **1600** comprising a microbiome simulation and monitoring system, according to an embodiment. According to the embodiment, microbiome simulation and monitoring system **1700** is an advanced computational platform designed to analyze, model, and predict complex interactions between microbiomes and host organisms-including at various system or spatial segments across whole organism(s), organ specific (e.g. brain or stomach), or system (e.g. digestive system). It utilizes a microbiome sequence analyzer for processing genomic and proteomic data, coupled with a temporal dynamics tracker for monitoring microbiome changes over time. The system incorporates a multi-site microbiome integrator to model interactions between different body sites, and a sophisticated microbiome-host interaction Simulator to model the interplay between microbes and host physiology. It features a disease risk predictor and a drug interaction predictor for health outcome forecasting and personalized medicine applications. The microbiome intervention optimizer generates tailored strategies for microbiome modulation, while a gene-edited microbe simulator explores cutting-edge therapeutic possibilities. By integrating these components with advanced AI, multi-omics analysis, and a user-friendly interface, the system enables researchers and clinicians to gain deep insights into microbiome dynamics, predict health outcomes, and design personalized interventions. This comprehensive

approach positions the microbiome simulation and monitoring system as a powerful tool for advancing microbiome research and its applications in personalized healthcare.

[0358] FIG. **17** is a block diagram illustrating an aspect of an AI-enhanced cellular modeling and simulation platform, a microbiome simulation and monitoring system. According to the embodiment, microbiome simulation and monitoring system **1700** is implemented as an advanced computational platform designed to analyze, model, and predict the complex interactions between microbiomes and host organisms. This system integrates various components to create a comprehensive approach to microbiome research and personalized medicine, leveraging artificial intelligence, multi-omics data analysis, and sophisticated simulation techniques.

[0359] According to the embodiment, microbiome simulation and monitoring system **1700** comprises a microbiome sequence analyzer **1701**, which builds upon the data integration and multi-omics platforms. This module processes and analyzes genomic and proteomic data from microbiome samples, identifying and characterizing the diverse microbial species present in different body sites. It employs advanced bioinformatics algorithms to interpret sequencing data, providing a detailed profile of the microbiome composition.

[0360] Working in concert with sequence analyzer **1701** is a microbiome temporal dynamics tracker **1702**. This component leverages the system's data storage and spatiotemporal modeling capabilities to track changes in microbiome composition over time. It allows researchers to observe how microbiome populations evolve in response to various factors such as diet, medication, or environmental changes, providing insights into the dynamic nature of host-microbiome relationships.

[0361] A multi-site microbiome integrator **1703** is a key innovation in this system, designed to model and analyze interactions between microbiomes in different body sites. This component simulates how changes in one microbial community (e.g., the gut microbiome) might influence others (e.g., the oral or skin microbiome), providing a holistic view of the body's microbial ecosystem. It can use advanced machine learning algorithms to identify patterns and correlations across different microbiome sites, enhancing our understanding of systemic microbial influences on health.

[0362] Central to the system's predictive capabilities is the microbiome-host interaction simulator **1704**. This module models the complex interplay between microbiomes and host physiological systems. It simulates how microbial metabolites, immune system interactions, and other microbiome-derived factors influence various aspects of host health, from digestion to neurological function. The simulator integrates data from multiple biological scales, from molecular interactions to organ-level effects, providing a comprehensive view of microbiome-host dynamics.

[0363] A microbiome-disease risk predictor **1705** leverages the system's AI and knowledge graph capabilities to forecast potential health outcomes based on microbiome profiles. This module analyzes patterns in microbiome composition and relates them to known disease associations, helping to identify individuals at higher risk for certain conditions. It continuously updates its predictive models as new research and clinical data become available, improving its accuracy over time.

[0364] For therapeutic applications, the microbiome-drug interaction predictor **1706** simulates how an individual's microbiome might influence drug metabolism and efficacy. This component is useful for personalized medicine approaches, as it helps clinicians anticipate how a patient's unique microbial profile might affect their response to various treatments. It can predict potential side effects or reduced efficacy due to microbiome-drug interactions, allowing for more tailored and effective treatment strategies.

[0365] A microbiome intervention optimizer **1707** takes the insights generated by other components and translates them into actionable interventions. This module designs personalized strategies to modulate microbiome composition for health benefits, such as dietary recommendations, probiotic supplementation, or targeted antimicrobial therapies. It uses

optimization algorithms to balance multiple health objectives and constraints, providing clinicians with evidence-based intervention plans.

[0366] For cutting-edge research applications, a gene-edited microbe simulator **1708** models the behavior and effects of genetically modified microbes within the microbiome. This component allows researchers to explore potential therapeutic applications of engineered microbes, simulating their interactions with native microbiome populations and predicting their impact on host health.

[0367] All these components work together in a seamless workflow. An exemplary process typically begins with the analysis of microbiome sequencing data, which is then integrated with host physiological data and tracked over time. The system simulates microbiome-host interactions, predicts health outcomes and drug responses, and generates personalized intervention strategies. Throughout this process, the system continuously learns and refines its models based on new data and research findings.

[0368] The entire system is unified through a user-friendly interface that allows researchers and clinicians to explore microbiome data, run simulations, and design interventions. This interface provides visualizations of microbiome compositions, interactive models of host-microbiome interactions, and detailed reports on predicted health outcomes and recommended interventions.

[0369] Microbiome simulation and monitoring system **1700** employs a diverse array of AI and ML algorithms to analyze, model, and predict microbiome-host interactions. Deep learning techniques, such as convolutional neural networks (CNNs) and RNNs, can be used to process and analyze complex microbiome sequencing data, identifying patterns and features that might be missed by traditional bioinformatics approaches. Transformer models, originally developed for natural language processing, can be adapted to analyze long sequences of genomic data, capturing long-range dependencies in microbial genomes. For temporal modeling of microbiome dynamics, LSTM networks or Temporal Convolutional Networks (TCNs) can be employed to capture time-dependent changes in microbial populations. Unsupervised learning techniques, such as autoencoders or VAEs, can be used for dimensionality reduction and feature extraction from high-dimensional microbiome data, helping to identify key microbial signatures associated with health or disease states.

[0370] Graph neural networks are particularly valuable for modeling complex interactions within microbial communities and between microbes and host systems, representing these relationships as nodes and edges in a graph structure. Reinforcement learning algorithms, such as Deep Q-Networks (DQN) or Proximal Policy Optimization (PPO), can be utilized to optimize intervention strategies, learning from simulated outcomes to design effective microbiome modulation approaches. For predicting disease risks and health outcomes, ensemble methods like random forests or gradient boosting machines can be employed, combining multiple models to improve prediction accuracy and robustness. Bayesian networks can be used to model causal relationships between microbiome composition, host factors, and health outcomes, providing interpretable insights into the mechanisms underlying microbiome-host interactions.

[0371] Advanced simulation techniques, such as numerical simulation via tools like finite element analysis, computational fluid dynamics, fluid-structure interactions and other physics based models may be combined with broader system dynamics models such as via agent-based modeling coupled with machine learning, can be used to create detailed, multi-scale models of microbiome ecosystems. These models can simulate the behavior of individual microbial species and their interactions within the community. Generative models, including GANs or VAEs, can be employed to generate synthetic microbiome data, helping to augment limited datasets or explore potential microbiome states. For analyzing the effects of interventions or perturbations on the microbiome, causal inference models like Structural Equation Modeling (SEM) or Bayesian causal networks can be utilized. Natural language processing techniques can be adapted to analyze and integrate information from scientific literature, enhancing the system's knowledge base. Furthermore, PINNs can be used to incorporate known biological principles into machine learning models, ensuring that

predictions and simulations adhere to established microbiological and physiological laws. This diverse toolkit of AI and ML algorithms enables the microbiome simulation and monitoring system to tackle the complex, multifaceted challenges of microbiome research and its applications in personalized medicine.

[0372] By combining advanced AI techniques with comprehensive biological modeling and clinical insights, the microbiome simulation and monitoring system represents a significant advancement in microbiome research and personalized medicine across humans, animals and crops or plants. It has the potential to revolutionize our understanding of how microbiomes influence health, enable more precise and effective medical interventions, and open new avenues for microbiome-based therapies across a wide range of health conditions and may prove especially valuable in enhancing preventative and wellness focused medicine to reduce acute medical crises.

[0373] FIG. **18** is a block diagram illustrating an exemplary system architecture for an AI-enhanced cellular modeling and simulation platform **1800** comprising a phage dynamics analysis system, according to an embodiment. According to the embodiment, phage dynamics analysis system **1900** is an advanced computational platform designed to model, analyze, and optimize phage-based therapies for medical applications. It utilizes a nonlinear gene expression simulator for modeling complex protein production mechanisms, coupled with an automated cryo-EM analysis module for rapid structural analysis of phages and bacteria. The system incorporates a phage-bacteria dynamics simulator to model intricate interactions between phages and their bacterial hosts, while a cross-resistance predictor forecasts potential resistance development. For therapeutic applications, it features a recursive protein design optimizer and a phage-tissue interaction modeler to ensure efficacy and safety. The societal impact simulator assesses population-level effects of phage therapy, while the phage therapy protocol optimizer integrates all components to design personalized treatment plans. By leveraging advanced AI, multi-scale modeling, and a user-friendly interface, this system enables researchers and clinicians to develop highly targeted phage therapies, predict outcomes, and address the growing challenge of antibiotic-resistant infections. This comprehensive approach positions the phage dynamics analysis system as a powerful tool for advancing phage therapy research and its applications in personalized medicine.

[0374] FIG. **19** is a block diagram illustrating an aspect of an AI-enhanced cellular modeling and simulation platform, a phage dynamics analysis system. According to an embodiment, phage dynamics analysis system **1900** is implemented as an advanced computational platform designed to model, analyze, and optimize phage-based therapies for medical applications. This system integrates various components to create a comprehensive approach to phage therapy research and development, leveraging artificial intelligence, multi-scale modeling techniques, and sophisticated simulation capabilities.

[0375] According to an embodiment, phage dynamics analysis system **1900** comprises a nonlinear gene expression simulator **1901**, which builds upon the AI and ML core system and simulation computing platform. This module creates detailed models of complex protein production mechanisms, including, for example, rolling circle reverse transcription, enabling the simulation of nonlinear gene expressions observed in phage-bacteria interactions. It provides a foundation for understanding and manipulating these unique biological processes for therapeutic purposes.

[0376] Working in tandem with the gene expression simulator is an automated cryo-EM analysis module **1902**. This component processes and analyzes cryo-electron microscopy (Cryo-EM) data, providing high-resolution structural information about phages, bacteria, and their interactions. By automating this process, the system can rapidly generate and interpret structural data, feeding this information back into other modules for more accurate modeling and prediction.

[0377] Central to the system's predictive capabilities is the phage-bacteria dynamics simulator **1903**. This module models the complex interactions between phages and bacteria, including bacterial defense mechanisms and phage infection processes. It can simulate how different phages might interact with various bacterial strains, providing insights for designing effective phage

therapies.

[0378] A cross-resistance predictor **1904** is another innovation in this system, designed to forecast potential resistance development, including cross-resistance between antivirals and antibiotics. This component analyzes patterns in bacterial responses to different therapeutic agents, helping to identify strategies that minimize the risk of resistance development and ensure the long-term efficacy of phage therapies.

[0379] For therapeutic applications, a recursive protein design optimizer **1905** may be configured to use cryo-EM data and AI algorithms to iteratively design and optimize proteins for phage therapy. This module can create custom phage proteins or modify existing ones to enhance their therapeutic efficacy, stability, or specificity for target bacteria.

[0380] According to an embodiment, a phage-tissue interaction modeler **1906** simulates how phage therapy affects engineered tissues and organ models. This component is useful for predicting the broader physiological impacts of phage therapy, ensuring that treatments are not only effective against target bacteria but also safe for host tissues.

[0381] To address broader public health concerns, a societal impact simulator **1907** models the population-level effects of phage therapy and potential resistance development. This module helps researchers and policymakers understand the long-term implications of widespread phage therapy use, informing decisions about treatment protocols and public health strategies.

[0382] Tying all these components together is the phage therapy protocol optimizer **1908**. This module designs and optimizes personalized phage therapy protocols based on patient-specific data and predicted outcomes from the other system components. It considers factors such as the patient's specific bacterial infection, potential resistance issues, and predicted tissue-level effects to create tailored treatment plans.

[0383] An exemplary process typically begins with the analysis of a patient's bacterial infection using the cryo-EM module and gene expression simulator. The phage-bacteria dynamics simulator then models potential phage therapies, while the cross-resistance predictor assesses risks. The protein design optimizer may be employed to create or modify phages for optimal effectiveness. The tissue interaction modeler and societal impact simulator provide broader context for the proposed therapy. Finally, the protocol optimizer integrates all this information to generate a personalized treatment plan.

[0384] Throughout this process, the system continuously learns and refines its models based on new data and outcomes. The AI and ML core system supports this adaptive learning, constantly improving the accuracy and predictive power of each component.

[0385] The entire system **1900** is unified through a user-friendly interface that allows researchers and clinicians to explore phage-bacteria interactions, design phage therapies, and predict treatment outcomes. This interface provides visualizations of molecular structures, simulations of phage-bacteria dynamics, and detailed reports on predicted therapy efficacy and potential risks.

[0386] Phage dynamics analysis system **1900** employs a diverse array of AI and ML algorithms to model, simulate, and optimize phage-based therapies. Deep learning techniques such as RNNs and LSTM networks, can be used to model the temporal dynamics of phage-bacteria interactions and predict infection outcomes over time. Convolutional Neural Networks may be used for processing and analyzing cryo-EM images, automating the identification of structural features in phages and bacteria. For modeling complex, nonlinear gene expression mechanisms like rolling circle reverse transcription, PINNs can be employed to incorporate known biological principles into the simulations. GNNs may be implemented for representing and analyzing the complex interaction networks between phages, bacteria, and host cells, cell populations, capturing the multi-scale nature of these biological systems.

[0387] Cell population modeling, beyond individual cell types, is critical for many applications of the system. For example spatial models can be critical for predicting the behavior and ultimate disposition of cell populations and often involve compartmentalized ordinary differential equations,

stochastic differential equations of motion, partial differential equations and various computational approaches that have been derived from cellular automata. The system is capable of advancing analysis well beyond current state of the art by enabling deconvolution of cell population dynamics from single cell data and identification of heterogeneous cell populations where single cell measurements at every time point exist inside the population (e.g., flow cytometric analysis) but single-cell time series data is not available because of specific cell discardment after each population sample measurement.

[0388] One of the additional advantages of the system is that its database of models and parameter ranges and sets, including error measurements and distributions from model to empirical observations at patient and population level, enables more effective and trustworthy analysis. Using parameters obtained in different studies and modeling runs for patients can be useful to approximate the lower and upper bounds of potential parameter values, but alignment to the biological system being modeled requires careful consideration. In one embodiment, biologically realistic parameter sets are proposed for evaluation by a hyperparameter optimization process in the system which allows for models to rapidly assess fitness for purpose with express model invalidation techniques and model structure determinations. This capability is critical since model parameter selection is just as important as model design and structure in many cases.

[0389] For protein design and optimization, the system can utilize generative models such as VAEs or GANs to explore novel phage protein structures. These may be combined with reinforcement learning algorithms, like Deep Q-Networks or PPO, to optimize phage proteins for specific therapeutic goals. Ensemble methods, such as random forests or gradient boosting machines, can be employed for predicting resistance development and cross-resistance, integrating multiple predictive models for more robust forecasts.

[0390] The system can leverage NLP techniques, including transformer models, to analyze and integrate information from scientific literature, enhancing its knowledge base on phage-bacteria interactions. According to an aspect, for simulating population-level impacts of phage therapy, agent-based modeling coupled with machine learning can be used to create detailed, multi-scale models of microbial ecosystems and their responses to phage interventions. Bayesian optimization techniques can be applied to efficiently search the vast parameter space of potential phage therapy protocols, balancing exploration and exploitation to find optimal treatment strategies.

[0391] To handle the uncertainty inherent in biological systems, the phage dynamics analysis system can employ probabilistic programming techniques, such as Markov Chain Monte Carlo (MCMC) methods or variational inference, to quantify uncertainties in its predictions and provide confidence intervals for therapeutic outcomes. Evolutionary algorithms, including genetic algorithms and evolutionary strategies, may be used to evolve and optimize phage cocktails for maximum effectiveness against target bacteria. According to an aspect, unsupervised learning techniques like t-SNE or UMAP can be applied for dimensionality reduction and visualization of high-dimensional phage-bacteria interaction data, aiding in the discovery of patterns and relationships that might not be immediately apparent. This diverse toolkit of AI and ML algorithms enables phage dynamics analysis system **1900** to tackle the complex, multifaceted challenges of phage therapy development and optimization.

[0392] By combining advanced AI techniques with comprehensive biological modeling and clinical insights, the phage dynamics analysis system represents a significant advancement in phage therapy research and personalized medicine. It has the potential to revolutionize our approach to treating bacterial infections, especially those resistant to traditional antibiotics, by enabling the development of highly targeted and effective phage-based therapies.

[0393] FIG. **20** is a block diagram illustrating an exemplary system architecture for an AI-enhanced cellular modeling and simulation platform **2000** comprising an epidemiological analysis system, according to an embodiment. According to the embodiment, epidemiological analysis system **2100** is an advanced computational platform designed to model, analyze, and predict the spread of

infectious diseases across multiple scales, from cellular to global levels. It comprises a multi-scale epidemiological simulator for comprehensive disease modeling, coupled with an epidemiological data aggregator that integrates diverse real-time health and environmental data. The system features an epidemic risk predictor for assessing outbreak risks, a public health intervention optimizer for evaluating response strategies, and a personal epidemic risk advisor for individual-level guidance. It incorporates a unique neuro-immune response simulator to model how physiological responses to infection influence disease dynamics, and an epidemiological scenario generator for long-term planning. By leveraging advanced AI and machine learning techniques, real-time data analysis, and sophisticated simulation capabilities, this system enables public health officials, researchers, and individuals to make informed decisions during outbreaks. It provides a powerful tool for proactive disease surveillance, optimized intervention strategies, and personalized risk assessment, potentially revolutionizing our approach to managing public health crises and mitigating the impact of infectious diseases on society.

[0394] FIG. **21** is a block diagram illustrating an aspect of an AI-enhanced cellular modeling and simulation platform, an epidemiological analysis system. According to the embodiment, epidemiological analysis system **2100** is implemented as an advanced computational platform designed to model, analyze, and predict the spread and impact of infectious diseases across multiple scales, from cellular interactions to global population dynamics. This system integrates various components to create a comprehensive approach to epidemiological research and public health decision-making, leveraging artificial intelligence, real-time data analysis, and sophisticated simulation techniques.

[0395] According to the embodiment, a multi-scale epidemiological simulator **2101** is present and builds upon the simulation computing platform and spatiotemporal modeling subsystem. This module creates detailed models of disease spread at various levels, from cellular interactions within an infected individual to population-level transmission dynamics. It provides a foundation for understanding how microscopic events, such as viral replication within cells, translate into macroscopic phenomena like disease outbreaks in communities.

[0396] Working in tandem with the simulator is the epidemiological data aggregator **2102**. This component collects and processes diverse real-time health indicators and environmental data from numerous sources, including public health systems, clinical diagnostics, social media, and environmental sensors. It integrates this data into the system, providing up-to-date information on disease prevalence, population movement, and environmental factors that may influence disease spread.

[0397] Supporting the system's predictive capabilities is an epidemic risk predictor **2103**. This module analyzes patterns in the integrated data to forecast potential disease outbreaks and assess risks at multiple scales. It considers factors such as population density, travel patterns, and environmental conditions to generate risk maps and alert public health officials to emerging threats.

[0398] A public health intervention optimizer **2104** is designed to simulate and evaluate various intervention strategies. This component models the potential impacts of different public health measures, such as vaccination campaigns, social distancing policies, or travel restrictions. By running multiple simulations with different parameters, it helps policymakers identify the most effective strategies for containing outbreaks and minimizing societal disruption.

[0399] For individual-level guidance, a personal epidemic risk advisor **2105** provides personalized risk assessments and health recommendations during disease outbreaks. This module considers an individual's health status, location, and behavior patterns to offer tailored advice on risk mitigation, such as suggesting when to wear masks or avoid crowded areas.

[0400] The neuro-immune response simulator **2106** adds a unique dimension to the system by modeling how neural detection of infection influences individual and population-level disease dynamics. This component simulates how the body's early response to infection, including sickness behaviors like fatigue and social withdrawal, affects disease spread within communities.

[0401] Tying all these components together is a epidemiological scenario generator **2107**. This module creates and analyzes various disease outbreak scenarios for policy planning and preparedness. It can simulate the emergence of new pathogens, the reemergence of known diseases in new regions, or the impact of evolving viral strains, providing a platform for "what-if" analyses useful for long-term public health planning.

[0402] An exemplary workflow of system **2100** typically begins with the continuous ingestion of real-time data by the epidemiological data aggregator. This data feeds into the multi-scale epidemiological simulator, which generates current and projected disease spread models. The epidemic risk predictor then assesses these models to identify potential outbreak risks. Based on these risks, the public health intervention optimizer simulates various response strategies, while the personal epidemic risk advisor generates individual-level recommendations.

[0403] Throughout this process, the neuro-immune response simulator adds nuance to the models by accounting for how individual physiological responses to infection influence broader disease dynamics. The epidemiological scenario generator uses all this information to create comprehensive future scenarios, allowing for proactive planning and policy development.

[0404] The system's AI and ML core plays a role in this workflow, continuously learning from new data and outcomes to refine its predictive models and improve the accuracy of its simulations. This adaptive learning capability ensures that the system becomes increasingly effective over time, particularly in response to novel or evolving health threats.

[0405] The entire system is unified through a user-friendly interface that allows public health officials, researchers, and individuals to interact with the epidemiological models, run simulations, and access personalized risk assessments. This interface provides visualizations of disease spread, interactive models of intervention impacts, and detailed reports on predicted outcomes under various scenarios.

[0406] Epidemiological analysis system **2100** employs a diverse array of AI and ML algorithms to model, predict, and analyze disease spread and public health interventions. Deep learning techniques, such as RNNs and LSTM networks, can be used to model the temporal dynamics of disease spread and predict future outbreak patterns based on historical data. Convolutional Neural Networks can be applied to analyze spatial patterns in disease spread, particularly useful when working with geographical health data. Graph Neural Networks may be implemented for modeling complex social networks and how they influence disease transmission, capturing the intricate relationships between individuals and communities. For integrating diverse data sources, transformer models can be employed to process and contextualize heterogeneous input data, including textual health reports, numerical statistics, and time-series data from various sensors and monitoring systems.

[0407] Reinforcement learning algorithms, such as Deep Q-Networks or PPO, can be utilized to optimize intervention strategies, learning from simulated outcomes to design effective public health policies. Bayesian networks and probabilistic graphical models are useful for capturing uncertainty in disease spread and intervention effectiveness, providing probabilistic forecasts and risk assessments. Ensemble methods like random forests or gradient boosting machines can be employed for robust prediction of outbreak risks, combining multiple models to improve accuracy and reliability. For scenario analysis and long-term planning, generative models such as VAEs or GANs can be used to generate plausible future outbreak scenarios.

[0408] The system can leverage natural language processing techniques to analyze and integrate information from scientific literature and public health reports, enhancing its knowledge base on disease characteristics and intervention efficacy. For modeling complex, multi-scale interactions between individual physiology and population-level disease dynamics, agent-based modeling coupled with machine learning can create detailed simulations of how individual behaviors and immune responses affect overall epidemic trajectories. Evolutionary algorithms can be employed to simulate the evolution of pathogens and the development of drug resistance. Dimensionality

reduction techniques like t-SNE or UMAP may be applied to visualize high-dimensional epidemiological data, aiding in the discovery of patterns and relationships in complex datasets.

[0409] Furthermore, physics-informed neural networks can be used to incorporate known epidemiological principles into machine learning models, ensuring that predictions adhere to established biological and physical laws governing disease spread.

[0410] By combining advanced AI techniques with comprehensive biological modeling, real-time data integration, and multi-scale analysis, the epidemiological analysis system represents a significant advancement in public health informatics. It has the potential to revolutionize how we approach disease surveillance, outbreak response, and long-term health policy planning. This system enables more proactive and precise public health interventions, from individual behavioral changes to global policy decisions, potentially saving lives and reducing the societal impact of infectious diseases.

[0411] FIG. **22** is a block diagram illustrating an exemplary system architecture for an AI-enhanced cellular modeling and simulation platform **2200** configured for ecosystem-level analysis, according to an embodiment. According to an embodiment, an ecosystem-level analysis system **2300** is an advanced computational platform designed to model, analyze, and predict the complex dynamics of disease ecosystems, with a primary focus on cancer and endometriosis use cases to highlight various system functionalities and capabilities. According to an aspect, it utilizes a disease ecosystem data integrator for processing multi-omics data, coupled with a generalized Lotka-Volterra (GLV) simulator for modeling disease ecosystems using ecological principles. The system features a cellular neighborhood analyzer for simulating interactions between different cell populations, an ecosystem-based therapy response predictor for forecasting treatment outcomes, and an immune-disease ecosystem interaction simulator for modeling immune system dynamics within the disease environment. It may incorporate a quantum-enhanced medical image analyzer for advanced imaging analysis and an ecosystem-based personalized treatment optimizer for tailoring therapeutic strategies. By leveraging artificial intelligence, multi-scale modeling, and quantum computing techniques, this system enables clinicians **152** and researchers **151** to gain deep insights into disease ecosystems, predict treatment responses, and design personalized therapeutic approaches. This comprehensive platform has the potential to enhance the understanding and treatment of complex diseases by considering their full ecological complexity, potentially leading to more effective, targeted therapies and improved patient outcomes.

[0412] FIG. **23** is a block diagram illustrating an aspect of an AI-enhanced cellular modeling and simulation platform, an ecosystem-level analysis system. According to the embodiment, ecosystem-level analysis system **2300** is implemented as an advanced computational platform designed to model, analyze, and predict the complex dynamics of disease ecosystems, with a particular focus on exemplary cancer and endometriosis use cases. This system integrates various components to create a comprehensive approach to understanding and treating these conditions as complex adaptive systems, leveraging artificial intelligence, multi-omics data analysis, and sophisticated simulation techniques.

[0413] According to the embodiment, ecosystem-level analysis system **2300** comprises a disease ecosystem data integrator **2301**, which builds upon the data integration and multi-omics platforms of AI-enhanced cellular modeling and simulation platform **2200** and variants thereof. This module collects and processes diverse cellular and molecular data, including genomics, transcriptomics, proteomics, and metabolomics information from diseased tissues. It creates a holistic view of the disease ecosystem, capturing the heterogeneity and interactions between different cell populations within tumors or endometriotic lesions.

[0414] Working in concert with the data integrator is the generalized Lotka-Volterra (GLV) simulator **2302**. This module models disease ecosystems using GLV equations, which are typically used in ecological modeling. It simulates the complex interactions, competition, and cooperation between different cell populations within the disease environment. This approach allows for a

deeper understanding of how diverse cell types within a tumor or lesion interact and evolve over time, providing insights into disease progression and potential treatment targets.

[0415] A cellular neighborhood analyzer **2303** is present in this embodiment of system **2300**, designed to simulate and analyze interactions between different cell populations within the disease ecosystem. This component models how various cell types, including, for example, cancer cells, immune cells, and stromal cells, interact within their local microenvironment. It provides insights into how these interactions contribute to disease pathology, resistance to treatments, and potential vulnerabilities that can be exploited therapeutically.

[0416] Central to the system's predictive capabilities is an ecosystem-based therapy response predictor **2304**. This module simulates how different therapeutic interventions might affect the dynamics of the disease ecosystem. By modeling the impact of various treatments on different cell populations and their interactions, it helps clinicians anticipate treatment outcomes and design more effective therapeutic strategies. This component may be utilized for predicting the emergence of treatment resistance and identifying combination therapies that might be more effective than single-agent approaches.

[0417] An immune-disease ecosystem interaction simulator **2305** adds another layer of complexity to the analysis. This module specifically models how the immune system interacts with the disease ecosystem. It simulates processes such as immune cell infiltration, activation, and suppression within the tumor or lesion environment. This capability is useful for understanding immune evasion mechanisms and designing effective immunotherapies.

[0418] For advanced imaging analysis, the system may comprise a quantum-enhanced medical image analyzer **2306**. This component leverages quantum computing algorithms and/or hardware to process and analyze medical images with great detail and efficiency. For example, it can enhance the resolution and interpretation of imaging data, improving the detection and characterization of disease features that might be missed by conventional imaging techniques.

[0419] Tying all these components together is an ecosystem-based personalized treatment optimizer **2307**. This module integrates the insights gained from all other components to design tailored treatment strategies for individual patients. It may receive one or more outputs from other system components and process this data accordingly. It considers the unique characteristics of each patient's disease ecosystem, including cellular composition, molecular profiles, and predicted responses to various therapies. By simulating multiple treatment scenarios, it can identify the most promising therapeutic approaches for each patient, potentially improving treatment outcomes and reducing side effects.

[0420] An exemplary process typically begins with the integration of patient-specific data by the disease ecosystem data integrator. This data feeds into the GLV simulator and cellular neighborhood analyzer to generate a comprehensive model of the patient's disease ecosystem. The immune-disease ecosystem interaction simulator then adds immune system dynamics to this model. The ecosystem-based therapy response predictor uses these models to simulate various treatment scenarios, while the quantum-enhanced medical image analyzer provides additional insights from imaging data. Finally, the personalized treatment optimizer integrates all this information to generate tailored treatment recommendations.

[0421] Throughout this process, the system's AI and ML core continuously learns from new data and outcomes to refine its predictive models and improve the accuracy of its simulations. This adaptive learning capability ensures that the system becomes increasingly effective over time, particularly in response to new research findings and treatment modalities.

[0422] The entire system may be unified through a user-friendly interface that allows clinicians and researchers to interact with the disease ecosystem models, run simulations, and access personalized treatment recommendations. This interface may provide visualizations of cellular interactions, simulations of treatment effects, and detailed reports on predicted outcomes under various therapeutic scenarios.

[0423] Ecosystem-level analysis system employs a diverse array of AI and ML algorithms to model, predict, and analyze complex disease ecosystems. Deep learning techniques such as graph neural networks, can be used to model the intricate interactions between different cell types within the tumor or lesion microenvironment, capturing the spatial and functional relationships in cellular neighborhoods. Recurrent neural networks and LSTM networks can model the temporal dynamics of disease progression and treatment responses. Generative adversarial networks might be employed to simulate and generate synthetic data representing various disease states or treatment scenarios, enhancing the system's predictive capabilities. For integrating multi-omics data, autoencoders and VAEs can be used for dimensionality reduction and feature extraction, helping to identify key molecular signatures in the disease ecosystem.

[0424] Reinforcement learning algorithms, such as DQN or PPO, may be utilized to optimize treatment strategies, learning from simulated outcomes to design effective therapeutic regimens. Evolutionary algorithms can be employed to simulate the evolution of cell populations within the disease ecosystem, modeling how different cell types adapt and compete over time. For predictive modeling, ensemble methods like random forests or gradient boosting machines can be used to forecast treatment responses based on the complex interplay of various factors within the disease ecosystem. Natural language processing techniques can be applied to analyze and integrate information from medical literature and clinical notes, enhancing the system's knowledge base.

[0425] In some embodiments, the system can leverage quantum machine learning algorithms, such as quantum support vector machines or quantum neural networks, to process high-dimensional data and solve complex optimization problems more efficiently than classical algorithms. These quantum algorithms can be particularly useful in analyzing the vast combinatorial space of potential cellular interactions and treatment combinations. Agent-based modeling, coupled with machine learning, can create detailed simulations of how individual cells and cell populations behave within the disease ecosystem. Bayesian networks and probabilistic graphical models can be used to capture uncertainty in disease progression and treatment outcomes, providing probabilistic forecasts that account for the stochastic nature of biological systems. Furthermore, physics-informed neural networks may be implemented which can incorporate known biological principles into machine learning models, ensuring that predictions adhere to established laws governing cellular behavior and interactions. This exemplary (non-limiting) set of AI and ML algorithms enables the ecosystem-level analysis system to address the complex, multifaceted challenges of modeling and treating diseases as dynamic, adaptive ecosystems.

[0426] By combining advanced AI techniques with comprehensive biological modeling, multi-omics data integration, and quantum-enhanced analysis, the ecosystem-level analysis system represents a significant advancement in the approach to understanding and treating complex diseases like cancer and endometriosis. It has the potential to revolutionize personalized medicine by enabling more precise, ecosystem-based treatment strategies that consider the full complexity of disease biology. This system could lead to more effective therapies, reduced treatment resistance, and improved patient outcomes in the management of these challenging conditions.

[0427] FIG. **24** is a block diagram illustrating an exemplary system architecture for an AI-enhanced cellular modeling and simulation platform **2400** configured for AI-enhanced image analysis in histology and pathology, according to an embodiment. According to the embodiment, an AI image analysis system **2500** is an advanced computational platform designed to improve histopathology and molecular diagnostics by integrating high-resolution image analysis with spatially resolved multi-omics data. According to some embodiments, it utilizes a spatial-omics data integrator to combine diverse data types, including histology images and molecular profiles, while preserving spatial context. The system features a sophisticated histopathology image analyzer that employs deep learning techniques to identify and classify cellular structures and abnormalities. A tumor microenvironment simulator models complex cellular interactions, while a space-time stabilized modeling engine enables longitudinal analysis of tissue changes. The platform includes a multi-

scale disease progression predictor for forecasting disease trajectories and a spatial-omics based treatment optimizer for personalized therapy design.

[0428] According to an embodiment, the system is configured to implement a holistic approach, incorporating environmental and lifestyle data through a holistic patient modeler, and its practical application in clinical settings via an AI-assisted diagnostic support system. By leveraging artificial intelligence and machine learning, the system continuously learns and improves its performance, offering pathologists and researchers powerful tools for more accurate diagnoses, in-depth understanding of disease mechanisms, and personalized treatment planning. This platform has the potential to significantly enhance the field of pathology, enabling more precise, data-driven approaches to disease diagnosis, prognosis, and treatment optimization.

[0429] FIG. **25** is a block diagram illustrating an aspect of an AI-enhanced cellular modeling and simulation platform, an AI image analysis system. According to the embodiment, AI image analysis system **2500** is implemented as an advanced computational platform designed to integrate, analyze, and interpret complex histopathological images alongside spatially resolved multi-omics data. This system leverages cutting-edge artificial intelligence and machine learning techniques to provide deep insights into cellular ecosystems, disease progression, and personalized treatment strategies in the field of pathology.

[0430] According to various embodiments, AI image analysis system **2500** comprises a spatial-omics data integrator **2501**, which builds upon the existing data integration and multi-omics platforms. This module collects and processes diverse data types, including high-resolution histology images, spatially resolved genomics, transcriptomics, and proteomics data. It creates a unified data representation that preserves the spatial context of molecular information within tissue samples, providing a foundation for subsequent analysis and modeling.

[0431] The system may further comprise a histopathology image analyzer **2502**. This module employs deep learning algorithms, such as convolutional neural networks and vision transformers, to analyze histology and pathology images at multiple scales. It can identify and classify different cell types, detect structural abnormalities, and quantify various tissue features. The analyzer is capable of processing both digitized whole-slide images and images captured from conventional microscopes, making it versatile for different clinical settings.

[0432] A tumor microenvironment simulator **2503** is designed to model and simulate the complex interactions within the tumor ecosystem. This component integrates the spatial-omics data with the image analysis results to create detailed, spatially-aware models of tumor microenvironments. It simulates how different cell types, including, for example, cancer cells, immune cells, and stromal cells, interact within their local context, providing insights into tumor behavior, progression, and potential treatment responses.

[0433] Supporting the system's longitudinal analysis capabilities is a space-time stabilized modeling engine **2504**. This module creates and/or analyzes patient-specific models that account for changes in tissue structure and cellular composition over time. It can employ advanced registration and normalization techniques to align data from multiple imaging sessions, enabling the tracking of disease progression or treatment response at the cellular level over extended periods.

[0434] A multi-scale disease progression predictor **2505** builds upon these models to forecast how diseases might evolve over time. It integrates information from cellular, tissue, and organ-level analyses to provide comprehensive predictions of disease trajectories. This component is particularly valuable for understanding complex, heterogeneous diseases like cancer, where different regions of a tumor may evolve differently.

[0435] For translating these insights into clinical action, a spatial-omics based treatment optimizer **2506** uses the integrated data and predictive models to design personalized treatment strategies. It simulates how different therapeutic interventions might affect the disease ecosystem, considering factors like drug penetration, target engagement, and potential resistance mechanisms within the

spatial context of the tissue.

[0436] A holistic patient modeler **2507** may be present to add another dimension to the analysis by incorporating environmental and lifestyle data. This module integrates information on factors like diet, exercise, environmental exposures, and stress levels with the spatial-omics and imaging data. This comprehensive approach allows for a more nuanced understanding of disease risk, progression, and treatment response in the context of a patient's overall health and lifestyle.

[0437] Tying all these components together is the AI-assisted diagnostic support system **2508**. This module synthesizes insights from all other components to provide pathologists with AI-driven recommendations and visualizations. It can highlight regions of interest in images, suggest potential diagnoses, and provide quantitative assessments of disease characteristics. Importantly, it's designed to augment rather than replace the pathologist's expertise, offering a powerful tool to enhance diagnostic accuracy and efficiency.

[0438] An exemplary process typically begins with the integration of histopathology images and spatial-omics data by the spatial-omics data integrator. This data is then analyzed by the Histopathology Image Analyzer and fed into the tumor microenvironment simulator for detailed modeling. The space-time stabilized modeling engine and multi-scale disease progression predictor use these inputs to create longitudinal models and predictions. The spatial-omics based treatment optimizer then leverages these models to suggest personalized treatment strategies. Throughout this process, the holistic patient modeler incorporates broader health and lifestyle factors, while the ai-assisted diagnostic support system provides user-friendly interfaces for pathologists to interact with the system's insights.

[0439] The AI and ML core can support this workflow, continuously learning from new data and outcomes to refine its models and improve the accuracy of its analyses and predictions. This adaptive learning capability ensures that the system becomes increasingly effective over time, particularly as it's exposed to more diverse cases and receives feedback from pathologists.

[0440] The entire system may be unified through a user-friendly interface that allows pathologists and researchers to interact with the AI-driven analyses, explore spatial-omics data, and access diagnostic support. This interface provides intuitive visualizations of complex data, including overlays of molecular information on histology images, 3D reconstructions of tumor microenvironments, and interactive tools for exploring predictive models.

[0441] The AI image analysis system employs a diverse array of advanced AI and ML algorithms to process, analyze, and interpret complex histopathological images and spatial-omics data. Deep learning architectures, particularly convolutional neural networks such as ResNet, Inception, or EfficientNet, form the backbone of the histopathology image analyzer, enabling detailed feature extraction and classification of cellular structures. These can be augmented with attention mechanisms or transformer architectures like Vision Transformer (ViT) to capture long-range dependencies in whole-slide images. For integrating spatial-omics data, graph neural networks can be utilized to model the complex relationships between different cellular components within their spatial context. Unsupervised learning techniques, such as autoencoders or variational autoencoders, can be employed for dimensionality reduction and feature extraction from high-dimensional spatial-omics data, helping to identify key molecular signatures in the tissue microenvironment.

[0442] The tumor microenvironment simulator can leverage agent-based modeling techniques combined with reinforcement learning algorithms to simulate the dynamic interactions between different cell types within the tumor ecosystem. For longitudinal analysis, recurrent neural networks or Long Short-Term Memory networks can be employed in the space-time stabilized modeling engine to capture temporal dynamics of tissue changes. The multi-scale disease progression predictor might utilize ensemble methods like random forests or gradient boosting machines, or more advanced techniques like neural ODEs for modeling complex disease trajectories. For treatment optimization, reinforcement learning algorithms such as Deep Q-

Networks or PPO can be used to navigate the vast space of potential treatment combinations. Natural language processing techniques, including transformer models like BERT, can be applied to analyze and integrate information from pathology reports and medical literature. The system can also employ Bayesian deep learning techniques to quantify uncertainties in its predictions, providing confidence intervals that are useful for clinical decision-making. Generative models, such as generative adversarial networks or diffusion models, could be used for data augmentation or to generate synthetic examples of rare pathologies. Furthermore, federated learning techniques can be implemented to enable collaborative learning across multiple institutions while preserving data privacy, important for building robust models from diverse patient populations.

[0443] By combining advanced AI techniques with comprehensive spatial-omics integration and sophisticated modeling capabilities, the AI image analysis system represents a significant advancement in digital pathology. It has the potential to improve how pathologists diagnose and monitor diseases, how researchers understand complex cellular ecosystems, and how clinicians design personalized treatment strategies. This system could lead to more accurate diagnoses, more effective treatments, and a deeper understanding of disease mechanisms at the cellular and molecular level.

[0444] FIG. **26** is a block diagram illustrating an exemplary system architecture for an AI-enhanced cellular modeling and simulation platform **2600** configured for quantum computing in advanced applications of cellular modeling, according to an embodiment. According to an embodiment, a quantum computing cellular modeling system **2700** is an advanced computational platform that integrates cutting-edge quantum computing technologies with traditional AI and machine learning approaches to revolutionize cellular modeling and simulation. It utilizes a quantum simulation engine for complex cellular process modeling, a quantum image processing module for enhanced cellular imaging, and a quantum drug-target interaction simulator for advanced drug discovery. The system also features a quantum biomarker detection system for early disease diagnosis, a quantum-enhanced 3D cellular modeler for comprehensive spatial-temporal analysis, and a quantum sensor interface for integrating highly sensitive cellular measurements.

[0445] What sets this system apart is its quantum-AI hybrid learning module, which seamlessly integrates quantum and classical computing paradigms, enabling the platform to leverage the unique strengths of both. By harnessing quantum phenomena such as superposition and entanglement, the system can simultaneously explore multiple cellular states and interactions, potentially uncovering insights that are computationally intractable with classical methods alone. This comprehensive approach allows for unprecedented precision in simulating cellular processes, analyzing complex biological data, and optimizing drug discovery pipelines. The quantum computing cellular modeling system represents a significant leap forward in biomedical research, offering the potential to accelerate drug development, enable earlier disease detection, and deepen our understanding of fundamental cellular biology.

[0446] FIG. **27** is a block diagram illustrating an aspect of an AI-enhanced cellular modeling and simulation platform, a quantum computing cellular modeling system. According to the embodiment, quantum computing cellular modeling system **2700** is implemented as an advanced computational platform that integrates cutting-edge quantum computing technologies with traditional AI and machine learning approaches to revolutionize cellular modeling and simulation. This system leverages the unique properties of quantum mechanics, such as superposition and entanglement, to enhance various aspects of cellular research, drug discovery, and diagnostics.

[0447] According to some embodiments, a quantum simulation engine **2701**, which builds upon the existing simulation computing platform and AI/ML core. This engine implements quantum algorithms specifically designed for cellular simulations, focusing on complex processes like protein folding and intricate cellular interactions. It may utilize quantum superposition to simultaneously model multiple cellular states, allowing for a more comprehensive exploration of cellular behavior. The engine employs techniques such as the quantum approximate optimization

algorithm (QAOA) to optimize these simulations, potentially uncovering cellular dynamics that are computationally intractable with classical methods.

[0448] Working in concert with quantum simulation engine **2701** is a quantum image processing module **2702**. This component enhances the platform's ability to process and analyze cellular images with unprecedented detail. By leveraging quantum algorithms for image processing, it can significantly reduce noise and improve resolution in cellular imaging data. This module integrates with the existing visualization and user interface system, providing researchers with crystal-clear, high-resolution visualizations of cellular structures and processes.

[0449] A quantum drug-target interaction simulator **2703** is present in this embodiment system's drug discovery capabilities. Building on the capabilities of the AI drug discovery platform, this module uses quantum algorithms to simulate drug-target interactions at the molecular level with extreme precision. It can model complex quantum mechanical effects in molecular binding, potentially identifying novel drug candidates that might be overlooked by classical simulation methods. This component works closely with the quantum-classical hybrid optimizer **2705**, which combines quantum and classical optimization techniques to efficiently navigate the vast space of potential drug formulations and predict their efficacy and potential side effects.

[0450] For advanced diagnostics, the system incorporates a quantum biomarker detection system **2704**. This module employs quantum algorithms to analyze biological samples for subtle biomarkers that might indicate the early stages of disease. It has the potential to detect molecular signatures that are too faint or complex for classical analysis methods, possibly enabling much earlier disease detection and intervention. This system integrates with the existing data integration platform to correlate these biomarker findings with other patient data, providing a comprehensive health assessment.

[0451] A quantum sensor interface **2706** is a component that integrates data from quantum sensors capable of detecting minute changes in cellular environments. These quantum sensors, which might utilize technologies like nitrogen-vacancy centers in diamonds, can provide unprecedented sensitivity in measuring cellular properties such as magnetic fields, pH levels, or molecular concentrations. The interface module ensures that this highly precise data is seamlessly incorporated into the platform's cellular models and simulations.

[0452] To create comprehensive 3D models of cellular activities, the system employs a quantum-enhanced 3D cellular modeler **2707**. This module leverages quantum computing to integrate multi-modal imaging data and generate highly detailed, dynamic 3D models of cells and cellular processes. It works in tandem with the spatiotemporal modeling subsystem to create 4D models that capture both spatial and temporal aspects of cellular behavior with quantum-enhanced precision.

[0453] Tying all these quantum components together with the classical AI systems is the quantum-AI hybrid learning module **2708**. This component facilitates the integration of quantum computing capabilities with existing AI and machine learning models. It enables the development of quantum-enhanced machine learning algorithms that can process and learn from the complex, high-dimensional data generated by quantum simulations and sensors. This hybrid approach allows the system to leverage the strengths of both quantum and classical computing paradigms, potentially leading to breakthroughs in pattern recognition, predictive modeling, and data analysis in cellular biology.

[0454] The entire system operates through a unified workflow that begins with data input, which could be molecular structures for drug discovery, cellular images for analysis, or patient samples for diagnostics. This data is processed through the relevant quantum-enhanced modules, with the quantum-AI hybrid learning module coordinating the integration of quantum and classical computing resources as needed. The results are then synthesized and presented through the user interface, providing researchers with unprecedented insights into cellular processes, potential drug candidates, or diagnostic findings.

[0455] Throughout its operation, the system continuously learns and adapts. The AI core, enhanced by quantum machine learning techniques, refines its models based on new data and outcomes. This adaptive capability ensures that the quantum computing cellular modeling system becomes increasingly accurate and effective over time, pushing the boundaries of what's possible in cellular modeling and analysis.

[0456] Quantum computing cellular modeling system **2700** employs a diverse array of AI, ML, and quantum algorithms to enhance cellular modeling and analysis. Quantum-enhanced neural networks, such as Quantum Convolutional Neural Networks (QCNN) and Quantum Recurrent Neural Networks (QRNN), can be used for complex pattern recognition in cellular images and time-series data, potentially identifying subtle features that classical networks might miss. Variational Quantum Algorithms (VQAs), including the Quantum Approximate Optimization Algorithm (QAOA) and Variational Quantum Eigensolver (VQE), can be applied to optimize cellular process simulations and drug-target interactions. Quantum support vector machines (QSVM) might be employed for classification tasks in diagnostics, potentially offering improved performance for high-dimensional biomarker data. For molecular simulations, quantum algorithms like Quantum Phase Estimation (QPE) can be used to calculate molecular energies more efficiently than classical methods.

[0457] The system can also leverage quantum-enhanced versions of classical ML algorithms, such as Quantum Principal Component Analysis (QPCA) for dimensionality reduction of complex cellular data, and Quantum K-Means for clustering analysis of cell populations. Quantum annealing algorithms, implemented on specialized hardware, could be used for optimization problems in drug discovery and cellular pathway analysis. For integrating classical and quantum approaches, hybrid algorithms like Quantum-Classical Neural Networks can be employed, where certain layers of the network are implemented on quantum hardware for enhanced feature extraction. Quantum Generative Adversarial Networks (qGANs) might be used for generating synthetic cellular data or for modeling rare cellular states. Additionally, quantum-inspired algorithms like Tensor Networks can be used for efficient representation and manipulation of high-dimensional cellular data, even on classical hardware. These quantum and quantum-inspired algorithms, when integrated with classical AI and ML techniques, provide the Quantum Computing Cellular Modeling System with a powerful toolkit for pushing the boundaries of cellular modeling and analysis.

[0458] By combining the power of quantum computing with advanced AI techniques and comprehensive cellular modeling capabilities, this system represents a significant leap forward in biomedical research and healthcare technology. It has the potential to accelerate drug discovery, enable earlier and more accurate disease detection, and provide deeper insights into the fundamental processes of life at the cellular level. This could lead to breakthrough treatments for complex diseases, more personalized medical approaches, and a profound advancement in our understanding of cellular biology.

[0459] FIG. **28** is a block diagram illustrating an exemplary system architecture for an AI-enhanced cellular modeling and simulation platform **2800** configured for quantum computing in advanced applications of cellular modeling, according to an embodiment. According to an embodiment, an AI predictive oncology system **2900** is an advanced computational platform designed to support cancer prognosis and treatment through the integration of cutting-edge artificial intelligence, multi-omics data analysis, and personalized medicine approaches. According to an aspect, it utilizes a multi-token cancer progression model that simultaneously forecasts multiple aspects of cancer evolution, an oncology treatment optimizer for personalized therapy recommendations, and a clinical-genomic data harmonizer for integrating diverse patient data. The system features an oncology patient digital twin for comprehensive patient modeling, a cancer treatment response simulator for predicting therapy outcomes, and an oncology AI Explainer to ensure interpretability of AI-driven insights.

[0460] A feature of this system is its ability to create a holistic, dynamic representation of each

patient's cancer profile and potential disease trajectories. By leveraging multi-token prediction approaches and integrating vast amounts of clinical, genomic, and research data, the system can provide oncologists with unprecedented insights into cancer progression and treatment efficacy. The AI predictive oncology system offers a powerful tool for personalizing cancer care, potentially improving treatment outcomes by identifying optimal therapeutic strategies tailored to each patient's unique cancer profile. This comprehensive approach allows for more precise, effective, and adaptive cancer management, representing a significant advancement in the field of oncology and personalized medicine.

[0461] FIG. **29** is a block diagram illustrating an aspect of an AI-enhanced cellular modeling and simulation platform, a quantum computing cellular modeling system. According to an embodiment, AI predictive oncology system **2900** is implemented as an advanced computational platform designed to support cancer prognosis and treatment through the integration of cutting-edge artificial intelligence, multi-omics data analysis, and personalized medicine approaches. This system leverages the power of multi-token prediction models, comprehensive patient profiling, and sophisticated treatment response simulations to provide oncologists with unprecedented insights into cancer progression and optimal treatment strategies.

[0462] According to some embodiments, AI predictive oncology system **2900** comprises a multi-token cancer progression model **2901**, which builds upon the AI and ML core system and simulation computing platform. This module implements a multi-token prediction approach, similar to advanced language models, to simultaneously forecast multiple aspects of cancer progression. By treating various cancer markers, genetic mutations, and physiological changes as "tokens," the system can model the complex, interdependent nature of cancer evolution. This approach allows for a more nuanced and comprehensive prediction of disease trajectories, capturing subtle interactions that might be missed by traditional prognostic methods.

[0463] Working in concert with the progression model is an oncology treatment optimizer **2902**. This component leverages the existing AI drug discovery platform and knowledge graph to generate and refine personalized cancer treatment plans. It takes into account the predicted disease progression, the patient's unique genetic profile, and a vast database of treatment outcomes to suggest optimal therapeutic strategies. The optimizer can evaluate complex combination therapies and adjust recommendations based on simulated treatment responses, potentially identifying effective interventions that might not be immediately apparent to human oncologists.

[0464] A clinical-genomic data harmonizer **2903** plays a role in integrating diverse data sources, including electronic health records (EHR) and genomic databases. This module builds upon the existing data integration platforms to create a unified, consistent representation of each patient's medical history, genetic predispositions, and current health status. It may employ advanced data harmonization techniques to reconcile disparate data formats and nomenclatures, ensuring that all relevant information is accurately incorporated into the patient's profile.

[0465] Central to the system's personalized approach is a oncology patient digital twin **2904**. This module creates a comprehensive digital representation of each cancer patient, integrating data from the clinical-genomic data harmonizer with simulated cellular models and predicted disease trajectories. The digital twin serves as a virtual testbed for exploring treatment options and their potential outcomes, allowing oncologists to gain insights into how different interventions might affect the patient's specific cancer and overall health.

[0466] A cancer treatment response simulator **2905** is a component in evaluating potential treatment strategies. Building on the existing simulation capabilities and cellular neighborhood analysis, this module creates detailed models of how different cancer types and individual patients might respond to various treatments. It simulates the effects of therapies at multiple scales, from molecular interactions to tissue-level responses, providing a holistic view of treatment efficacy and potential side effects.

[0467] To ensure that the AI's decision-making process is transparent and trustworthy, the system

may incorporates an oncology ai explainer **2906**. This module translates the complex computations and predictions of the AI models into clear, interpretable explanations for oncologists. It provides visualizations, confidence intervals, and rationales for its recommendations, useful for integrating AI insights into clinical decision-making processes.

[0468] These components work together in a seamless workflow, starting with the integration of a patient's clinical and genomic data. The harmonized data is used to create the patient's digital twin, which then serves as input for the multi-token progression model. As the model generates predictions about the cancer's potential trajectories, the treatment optimizer begins evaluating possible interventions. The treatment response simulator then models how these interventions might affect the patient's cancer, with results feeding back into the optimizer for refinement.

[0469] Throughout this process, the AI explainer provides ongoing insights, helping oncologists understand the system's reasoning and predictions. The digital twin is continuously updated with new data and simulation results, creating a dynamic representation of the patient's evolving condition and treatment response.

[0470] The entire system may be unified through a user-friendly interface that allows oncologists to explore predictions, simulate treatment scenarios, and access AI-generated insights. This interface provides intuitive visualizations of cancer progression trajectories, treatment efficacy comparisons, and patient-specific risk assessments.

[0471] The AI predictive oncology system employs a diverse array of advanced AI and ML algorithms to model, predict, and optimize cancer progression and treatment. According to an aspect, for the multi-token cancer progression model, transformer-based architectures similar to GPT (Generative Pre-trained Transformer) models may be adapted for multi-token prediction of cancer progression, capturing complex temporal dependencies in disease evolution. Recurrent Neural Networks, particularly Long Short-Term Memory networks, might be used to model the temporal dynamics of cancer biomarkers and treatment responses over time. For integrating multi-omics data, deep learning techniques such as multi-modal deep Boltzmann machines or cross-modal autoencoders could be employed to fuse information from various data sources like genomics, transcriptomics, and clinical data.

[0472] The oncology treatment optimizer might leverage reinforcement learning algorithms, such as DQN or PPO, to navigate the complex space of treatment options and optimize therapy selections. Ensemble methods like random forests or gradient boosting machines could be used for robust prediction of treatment outcomes, while Bayesian Networks might model the causal relationships between genetic factors, treatments, and outcomes. For the cancer treatment response simulator, physics-informed neural networks could be employed to incorporate known biological principles into the simulation of drug responses. The system might also use GANs to synthesize realistic patient data for training and simulation purposes, especially useful for rare cancer types with limited data.

[0473] Natural Language Processing techniques, including named entity recognition and relationship extraction models, may be applied to extract relevant information from clinical notes and research literature. For the oncology ai explainer, techniques like SHAP (SHapley Additive explanations) values or LIME (Local Interpretable Model-agnostic Explanations) could be used to provide interpretable insights into the AI's decision-making process. Additionally, graph neural networks might be employed in the knowledge graph component to model complex relationships between genes, proteins, drugs, and diseases. Dimensionality reduction techniques like t-SNE or UMAP could be used for visualizing high-dimensional patient data. Finally, federated learning approaches might be implemented to allow collaborative model training across multiple healthcare institutions while preserving patient privacy. This diverse set of exemplary AI and ML algorithms enables the AI predictive oncology system to tackle the complex, multifaceted challenges of cancer prediction, progression modeling, and personalized treatment optimization.

[0474] By combining advanced AI techniques with comprehensive biological modeling and clinical

data integration, the AI predictive oncology system represents a significant leap forward in personalized cancer care. It has the potential to dramatically improve treatment outcomes by providing oncologists with deeper insights into each patient's unique cancer profile and helping to identify the most effective treatment strategies. This system can lead to more precise, effective, and personalized cancer treatments, potentially improving patient outcomes and quality of life while optimizing the use of healthcare resources.

[0475] FIG. **30** is a block diagram illustrating an exemplary system architecture for an AI-enhanced cellular modeling and simulation platform **3000** configured for simulating basal cognition with oncology and regenerative medicine applications, according to an embodiment. According to the embodiment, oncology simulation and regenerative medicine system **3100** is an advanced computational platform that integrates principles of basal cognition with cutting-edge AI and cellular modeling techniques to enhance the understanding of cancer progression, tissue regeneration, and complex cellular behaviors. According to various aspects, it utilizes a basal cognition simulator to model non-neuronal cellular "intelligence," a bioelectric communication modeler to simulate signaling processes, and a cellular cooperation breakdown simulator to model cancer development. For regenerative medicine, it features an emergent tissue formation simulator and a tissue growth optimization controller, enabling detailed modeling and real-time optimization of tissue engineering processes.

[0476] This system implements a holistic approach to modeling cellular behaviors and interactions, inspired by the concept that simple cells can exhibit complex, collective problem-solving abilities. By incorporating a collective intelligence ai framework, the system not only simulates biological processes but also translates these insights into novel AI architectures. A basal cognition-based disease evolution simulator extends these capabilities to model disease progression from a new perspective. This approach allows for insights into cancer development, tissue regeneration, and the emergent properties of cellular collectives, potentially leading to breakthroughs in cancer treatment, regenerative medicine, and biologically-inspired AI design.

[0477] FIG. **31** is a block diagram illustrating an aspect of an AI-enhanced cellular modeling and simulation platform, a quantum computing cellular modeling system. According to the aspect, oncology simulation and regenerative medicine system **3100** is implemented as an advanced computational platform that integrates principles of basal cognition with AI and cellular modeling techniques to improve the understanding of cancer progression, tissue regeneration, and complex cellular behaviors. This system leverages the concept that non-neuronal cells exhibit forms of intelligence and problem-solving abilities, applying this insight to simulate and analyze cellular interactions in both healthy and diseased states.

[0478] According to the aspect, a basal cognition simulator **3101** is present, which builds upon the simulation computing platform and AI/ML core. This module models the "intelligence" exhibited by non-neuronal cells, simulating how cellular collectives communicate, make decisions, and solve problems without a centralized nervous system. It captures the emergent behaviors arising from simple cellular interactions, providing a foundation for understanding complex tissue-level phenomena.

[0479] Working in concert with basal cognition simulator **3101** is a bioelectric communication modeler **3102**. This component simulates the role of bioelectric signaling in cellular coordination and tissue formation. It can model how electrical signals propagate through cellular networks, influencing gene expression, cell behavior, and overall tissue organization. This module is particularly useful for understanding the self-organizing principles underlying tissue regeneration and cancer development.

[0480] A cellular cooperation breakdown simulator **3103** may be configured for modeling cancer progression. Building on the tumor microenvironment simulator, this module focuses on how cancer cells deviate from normal cellular coordination. It simulates the processes by which cells "go rogue," losing their group identity and breaking away from the body's regulatory systems. This

component may be used for understanding the early stages of cancer development and for identifying potential interventions to restore normal cellular behavior.

[0481] For regenerative medicine applications, the system incorporates an emergent tissue formation simulator **3104**. This module models how simple cellular interactions lead to the formation of complex tissue structures. It simulates the collective decision-making processes that enable cells to organize into functional organs and tissues, providing insights that can be applied to tissue engineering and regenerative therapies.

[0482] A collective intelligence AI framework **3105** represents an innovative approach to AI system design inspired by basal cognition principles. This module develops and simulates multi-agent AI systems that mimic the collective problem-solving abilities observed in cellular systems. By emulating the distributed intelligence seen in biological tissues, this framework can help create more robust and adaptable AI systems for various applications.

[0483] To support real-time applications in tissue engineering, the system includes a tissue growth optimization controller **3106**. This module continuously monitors simulated tissue growth, adjusting conditions based on basal cognition principles to ensure optimal development. It may simulate the fine-tuning of factors such as, for example, nutrient gradients, mechanical stresses, and bioelectric signals to guide tissue formation towards desired outcomes.

[0484] A basal cognition-based disease evolution simulator **3107** extends the system's capabilities in modeling disease progression. This module simulates how changes in cellular collective behaviors contribute to the evolution of diseases like cancer. It may be configured to model the breakdown of normal tissue homeostasis, the emergence of drug resistance, and the progression of metastasis, all through the lens of basal cognition principles.

[0485] An example workflow executed by system **3100** may proceed as follows: starting with the simulation of basic cellular behaviors by the basal cognition simulator. The bioelectric communication modeler then simulates the signaling processes that coordinate these behaviors across cellular populations. In cancer simulations, the cellular cooperation breakdown simulator models how these coordinated behaviors begin to fail, leading to tumor formation and progression.

[0486] For regenerative medicine applications, the emergent tissue formation simulator takes the coordinated cellular behaviors and models how they lead to the development of complex tissues and organs. The tissue growth optimization controller then fine-tunes these simulations in real-time, mimicking the adaptive processes seen in natural tissue development.

[0487] Throughout these processes, the collective intelligence AI framework analyzes the emergent behaviors and decision-making processes, translating biological insights into novel AI architectures. Meanwhile, the disease evolution simulator continuously models how changes in cellular behavior and communication might lead to pathological states, providing a dynamic view of disease progression.

[0488] The entire system may be unified through a user-friendly interface that allows researchers to explore simulations, adjust parameters, and visualize complex cellular behaviors and tissue-level phenomena. This interface provides intuitive representations of bioelectric fields, cellular decision-making processes, and emergent tissue structures.

[0489] Oncology simulation and regenerative medicine system **3100** employs a diverse array of AI and ML algorithms to model complex cellular behaviors and interactions. Some exemplary (non-limiting) AI and ML algorithms which may be implemented in one or more embodiments are described herein. For simulating basal cognition, cellular automata models enhanced with reinforcement learning algorithms can be used to capture emergent behaviors in cell populations. GNNs may be implemented for modeling intercellular communication and bioelectric signaling, representing cells as nodes and their interactions as edges. Deep reinforcement learning algorithms, such as PPO or Soft Actor-Critic (SAC), can be employed in the tissue growth optimization controller to fine-tune growth conditions in real-time.

[0490] For modeling cancer progression, evolutionary algorithms combined with agent-based

modeling can simulate the breakdown of cellular cooperation and the emergence of rogue cancer cells. GANs might be used to generate synthetic data for rare cancer types or to model potential tissue structures in regenerative applications. RNNs, particularly LSTM networks, can model the temporal aspects of disease evolution and tissue regeneration. For analyzing complex patterns in bioelectric fields, CNNs adapted for spatiotemporal data can be employed.

[0491] The collective intelligence AI framework might utilize multi-agent reinforcement learning techniques, such as Multi-Agent Deep Deterministic Policy Gradients (MADDPG), to develop AI systems inspired by cellular collective behaviors. For integrating and analyzing multi-modal data from various simulations, transformer-based architectures like BERT or GPT, adapted for scientific data, could be used. Unsupervised learning techniques such as VAEs or Self-Organizing Maps (SOMs) might be employed for discovering latent patterns in cellular behavior data. Additionally, PINNs can be used to incorporate known biophysical principles into the simulations, ensuring that AI predictions align with established scientific knowledge.

[0492] By combining advanced AI techniques with the principles of basal cognition and comprehensive cellular modeling, oncology simulation and regenerative medicine system **3100** represents a significant leap forward in the ability to understand and manipulate complex biological systems. It has the potential to improve cancer research by providing new insights into tumor formation and progression, enhance regenerative medicine by optimizing tissue engineering processes, and inspire new approaches to AI design based on biological principles of collective intelligence. This system could lead to more effective cancer therapies, advanced tissue engineering techniques, and novel AI systems capable of solving complex, distributed problems in ways inspired by nature's own problem-solving mechanisms.

[0493] FIG. **32** is a block diagram illustrating an exemplary system architecture for an AI-enhanced cellular modeling and simulation platform **3200** configured for advanced image analysis and simulation, according to an embodiment. According to the embodiment, advanced image analysis and simulation system **3300** is a computational platform that improves medical diagnostics and treatment planning by integrating multi-modal imaging, AI-driven analysis, and comprehensive physiological modeling. This system goes beyond traditional image analysis by creating dynamic, spatiotemporal models of patient health, enabling predictive simulations and personalized treatment optimization. It ingests and analyzes data from various imaging modalities, integrates this information with other health data, and creates a rich, multi-dimensional representation of the patient's health over time.

[0494] What sets this system apart is its ability to generate comprehensive spatiotemporal models of patient physiology and anatomy, simulate disease progression, and optimize treatment strategies in real-time. It can incorporate data from wearable devices and medical equipment, ensuring that patient models remain up-to-date. The system also uniquely combines classical numerical simulations with AI/ML models, allowing for more accurate modeling of complex physiological processes. By synthesizing insights across multiple medical disciplines and providing intuitive visualizations, this platform offers clinicians a powerful tool for personalized patient care. This comprehensive approach has the potential to improve diagnostic accuracy, enable earlier interventions, and optimize treatment strategies across various medical fields, particularly in oncology, leading to better patient outcomes and more efficient healthcare delivery.

[0495] In some implementations, image analysis and simulation system **3300** may integrate with and/or other comprise components and/or functionality associated with AI image analysis system **2500**.

[0496] FIG. **33** is a block diagram illustrating an aspect of an AI-enhanced cellular modeling and simulation platform, an advanced image analysis and simulation system. According to the aspect, advanced image analysis and simulation system **3300** is a cutting-edge computational platform designed to revolutionize medical diagnostics and treatment planning through the integration of multi-modal imaging, AI-driven analysis, and comprehensive physiological modeling. This system

goes beyond traditional image analysis by creating dynamic, spatiotemporal models of patient health, enabling predictive simulations and personalized treatment optimization.

[0497] According to various aspects, multi-modal image integration module **3301**, which builds upon the existing AI and ML core system and visualization interface. This component ingests and analyzes data from various imaging modalities, including, but not limited to, mammograms, CT scans, MRIs, and ultrasounds. It employs advanced machine learning algorithms, such as convolutional neural networks and transformer models, to extract relevant features and detect anomalies across different imaging types. This module not only enhances the accuracy of diagnoses but also provides a more comprehensive view of the patient's condition by correlating information from multiple sources.

[0498] Working in concert with the image integration module is the spatiotemporal health data annotator **3302**. This component takes the analyzed imaging data and integrates it with other health information, such as electronic health records, genetic profiles, and laboratory results. It annotates this diverse data within a spatiotemporal context, creating a rich, multi-dimensional representation of the patient's health over time. This annotated data serves as the foundation for subsequent modeling and analysis tasks and aids in specific individualization of models based on adjustments to parameters (e.g., via hyperparameter optimization processes for error minimization between empirical observations and simulation models or machine learning models) or through techniques such as model weight adjustments, latent space modeling or synthetic data generation or analysis.

[0499] A space-time stabilized patient model generator **3303** may be present in various aspects. It utilizes the annotated health data to create and continuously update a comprehensive spatiotemporal model of the patient's physiology and anatomy. This model goes beyond static representations, capturing the dynamic nature of biological processes and allowing for the simulation of how a patient's condition might evolve over time. The generator can employ physics-informed neural networks and differential equation solvers to ensure that the models adhere to known biological principles while incorporating patient-specific data.

[0500] For oncology applications, an early-stage disease evolution simulator **3304** is leveraged. This module takes the patient model and simulates potential progression paths of early-stage diseases, particularly cancers. It considers factors such as tumor growth rates, angiogenesis, and potential metastatic behavior, providing clinicians with a range of possible scenarios to inform early intervention strategies.

[0501] A personalized treatment response simulator **3305** builds upon these disease models to optimize treatment strategies. It simulates how different interventions might affect the patient's condition, taking into account factors such as drug efficacy, radiation therapy outcomes, and surgical options. This module may employ reinforcement learning algorithms to continuously refine and optimize treatment plans based on both simulated outcomes, broader synthetic data sets, and real patient data both attributed and anonymized.

[0502] To ensure that the system remains up-to-date with the patient's current condition, the real-time patient data integrator **3306** continuously incorporates data from wearable devices, imaging, recreational equipment, health and wellness sensors (e.g., scales, blood pressure monitors, blood oxygen sensors, environmental particulate and radon and air quality sensors, urine sensors, implanted medical devices) and medical equipment. This module can use stream processing techniques and online learning algorithms (e.g., with stream or microbatching over finite time horizon context windows and periodic model retraining on broader data sets for individual or populations) to update the patient model in real-time, allowing for dynamic adjustments to simulations and treatment recommendations as new data becomes available.

[0503] A hybrid simulation orchestrator **3307** represents a significant advancement in medical modeling. It coordinates and integrates classical numerical simulations, such as computational fluid dynamics for blood flow analysis, fluid structure interactions for arteries and veins, with AI/ML models. This hybrid approach allows for more accurate and comprehensive simulations of complex

physiological processes, bridging the gap between traditional physics-based modeling and data-driven AI approaches. It also supports system-led exploration of different types of models, not just limited to AI/ML vs numerical modeling approaches but also specific subsets of such techniques like interface modeling approaches. For example Finite Difference Method (FDM) versus Finite Element Method (FEM) or numerical techniques using grids versus meshless methods of analysis for fluids, fluid structure or structure modeling. We note that several variability conditions in interface problems make differing approximation methods an effective requirement across different fluid-solid interaction, fluid-fluid interaction, solid-solid interaction problems to include specialized thermodynamic analysis where heat transfer considerations are also present. Within the set of representative Interface Finite Element Modeling techniques which are known to the system, comparisons between or selection of techniques such as Elliptic Interface Problem, Immersed Boundary Method, Matched Interface and Boundary Method (including Galerkin variants such as Finite Element Galerkin Immersed Methods, Partially Penalized Galerkin Immersed Finite Element Methods, or Interior Penalty Discontinuous Galerkin Schemes), Reproducing Kernel Particle Method, or Algorithm Focused on Solid Surface.

[0504] Tying all these components together is the multi-disciplinary insight synthesizer **3308**. This module aggregates insights from various medical disciplines, considering the outputs from all other system components. It may employ knowledge graph technologies and natural language processing to generate comprehensive, easy-to-understand reports that provide clinicians with a holistic view of the patient's condition and treatment options.

[0505] As an example workflow of system **3300**, consider starting with the ingestion and analysis of multi-modal imaging data. The analyzed data is then annotated and integrated into the spatiotemporal health database, which feeds into the patient model generator. This model serves as the basis for disease progression simulations and treatment optimizations. Throughout this process, real-time data is continuously integrated, and hybrid simulations are run to provide the most accurate and up-to-date insights.

[0506] The entire system may be unified through a user-friendly interface that allows clinicians to explore patient models, run simulations, and access multi-disciplinary insights. This interface provides intuitive visualizations of complex data, including 3D renderings of anatomical structures, time-lapse simulations of disease progression, and interactive treatment planning tools.

[0507] Advanced image analysis and simulation system employs a diverse array of AI and ML algorithms to process, analyze, and simulate complex medical data. Some exemplary (non-limiting) AI and ML algorithms which may be implemented in one or more embodiments are described herein. For image analysis, convolutional neural networks such as U-Net or Mask R-CNN may be utilized for segmentation and anomaly detection across various imaging modalities. Transformer models like Vision Transformer (ViT) or DETR (Detection Transformer) can be applied for more sophisticated image understanding tasks. For integrating multi-modal data, cross-modal attention mechanisms and fusion networks may be employed to correlate information from different imaging sources. The system can leverage recurrent neural networks, particularly LSTM networks or Gated Recurrent Units (GRUs), for modeling temporal aspects of patient health data and disease progression.

[0508] In creating spatiotemporal patient models, the system can utilize physics-informed neural networks to ensure that AI predictions adhere to known physiological principles. For simulating disease progression and treatment responses, reinforcement learning algorithms such as PPO or SAC can be employed to optimize treatment strategies. Generative models, including VAEs or Generative Adversarial Networks GANs, might be used to synthesize potential disease progression scenarios or to generate synthetic medical images for training purposes. The system also incorporates graph neural networks for modeling complex relationships in physiological systems and for knowledge representation in the multi-disciplinary insight synthesis. For real-time data integration and online learning, algorithms like online gradient descent or follow-the-regularized-

leader may be utilized. Additionally, ensemble methods such as random forests or gradient boosting machines can be employed for robust prediction tasks. The system also leverages natural language processing techniques, including BERT or GPT models adapted for medical text, to process clinical notes and generate comprehensive reports.

[0509] By combining advanced AI techniques with comprehensive physiological modeling and real-time data integration, the Advanced Image Analysis and Simulation System represents a significant leap forward in personalized medicine. It has the potential to dramatically improve diagnostic accuracy, enable earlier interventions, and optimize treatment strategies across various medical fields, particularly in oncology. This system could lead to more effective, personalized patient care, potentially improving outcomes and quality of life while reducing healthcare costs through more targeted and efficient interventions.

[0510] According to various aspects, AI-enhanced cellular modeling and simulation platform may comprise systems, methods, and components directed to cellular machinery assembly. These embodiments can enable improved intracellular modeling and the understanding of how viral, bacterial, phage, and obelisk impacts manifest. A cellular machinery assembly system may be present and implemented as an advanced computational platform designed to model, simulate, and analyze the complex processes involved in the assembly of cellular structures, with a particular focus on critical components such as kinetochores. This system integrates various specialized modules to create a comprehensive approach to understanding cellular machinery assembly, leveraging artificial intelligence and multi-scale modeling techniques.

[0511] According to the aspect, the system may comprise a protein clustering simulator, which models the concentration-dependent aggregation of proteins crucial for cellular structure formation. This module simulates how proteins like CENP-T cluster together when present in high concentrations, a process fundamental to the formation of complex cellular structures. The simulator uses advanced algorithms to model the dynamic interactions between individual proteins, accounting for factors such as local concentration gradients, molecular affinities, and spatial constraints within the cellular environment.

[0512] Working together with the clustering simulator is a recursive protein complex designer. This AI-driven component iteratively designs and optimizes protein complexes based on desired assembly properties. It employs machine learning algorithms, trained on vast datasets of known protein interactions and structures, to predict how different protein combinations might assemble and function. The designer can generate novel protein configurations, simulate their assembly process, and refine these designs based on performance metrics related to stability, functionality, and efficiency of assembly.

[0513] The system may further comprise a kinetochore assembly predictor, which specifically models the formation of these critical cellular structures. This predictor integrates data from the protein clustering simulator and the recursive protein complex designer to forecast how kinetochores form under various cellular conditions. It considers factors such as the availability of key proteins, the dynamics of their clustering, and the sequential assembly of different kinetochore components. This module is particularly valuable for understanding how errors in kinetochore assembly might lead to chromosome segregation issues during cell division.

[0514] A cellular machinery defect analyzer works closely with the kinetochore assembly predictor to identify potential flaws in the assembly process. This module uses pattern recognition algorithms and comparative analysis against known healthy assembly processes to flag anomalies that could indicate defective machinery formation. It can simulate various types of defects, such as protein misfolding, improper clustering, or mistimed assembly steps, and predict their potential impacts on cellular function.

[0515] Tying these components together is a multi-scale assembly impact evaluator. This sophisticated module assesses how molecular-level assembly processes influence higher-level biological functions across different scales. It creates a bridge between the microscopic world of

protein interactions and the macroscopic realm of cellular, tissue, and organism-level effects. The evaluator uses hierarchical modeling techniques to simulate how small changes in protein assembly can propagate through biological systems, potentially leading to significant impacts on health and disease states.

[0516] The platform's data integration layer plays a role in harmonizing diverse data types, including proteomic data, high-resolution imaging results, and experimental findings on protein interactions. This layer employs advanced data processing algorithms to normalize and integrate data from various sources, ensuring that all components of the system work with consistent, high-quality information.

[0517] The AI and machine learning core of the system continually learns from new data and simulations, refining its predictive models and improving the accuracy of its analyses. This adaptive learning capability allows the system to evolve its understanding of cellular machinery assembly processes over time, incorporating new scientific discoveries and experimental results into its models.

[0518] For real-time analysis and adaptation, the system includes a component that can interface with laboratory equipment, allowing for the integration of live experimental data. This feature enables researchers to validate model predictions against actual biological observations, creating a feedback loop that continually improves the system's accuracy and relevance.

[0519] The visualization and user interface component of the cellular machinery assembly system provides researchers with intuitive ways to interact with the complex data and models. It offers dynamic, 3D visualizations of protein clustering and complex assembly processes, allowing researchers to observe simulated assembly events in real-time and at multiple scales.

[0520] In operation, these components work together to provide a comprehensive analysis of cellular machinery assembly. For instance, in studying kinetochore formation, the protein clustering simulator might first model the aggregation of CENP-T proteins. The recursive protein complex designer would then predict how these clusters interact with other kinetochore components. The kinetochore assembly predictor would use this information to forecast the formation of complete kinetochores, while the cellular machinery defect analyzer would identify any potential issues in the assembly process. The multi-scale assembly impact evaluator would then assess how variations in this assembly process might affect chromosome segregation and overall cell division.

[0521] Throughout this process, the system continuously refines its models based on new data and observed outcomes, ensuring that its predictions and analyses remain at the cutting edge of cellular biology research. By providing this deep, multi-scale understanding of cellular machinery assembly, the system offers unprecedented insights into fundamental biological processes, with far-reaching implications for our understanding of cellular health, disease progression, and potential therapeutic interventions.

[0522] According to various aspects, AI-enhanced cellular modeling and simulation platform may comprise systems, methods, and components directed to obelisk lifeform modeling and simulation. An obelisk modeling system may be present and implemented as an advanced computational platform designed to simulate, analyze, and predict the behavior and potential applications of the newly discovered obelisk RNA structures within human biological systems. This cutting-edge system integrates various specialized modules to create a comprehensive approach to understanding obelisk-cell interactions, their impact on cellular processes, and their potential therapeutic applications.

[0523] The system may comprise an obelisk structure simulator, which models the unique rod-shaped structure of obelisks and their molecular properties. This module utilizes advanced molecular dynamics simulations to represent the three-dimensional structure of obelisks, their stability in various cellular environments, and their potential conformational changes. The simulator considers factors such as RNA sequence, secondary structure formation, and interactions with cellular components to provide a detailed representation of obelisk behavior at the molecular

level.

[0524] Working together with the structure simulator is a cellular instruction decoder. This component simulates how cells interpret and respond to the genetic instructions delivered by obelisks. It employs machine learning algorithms trained on vast datasets of RNA-cell interactions to predict how different obelisk sequences might be translated into cellular responses. The decoder can simulate various cellular processes, including gene expression changes, protein synthesis, and metabolic shifts, providing insights into how obelisks might be used to modulate cellular behavior for therapeutic purposes.

[0525] An obelisk-microbiome interaction analyzer may be used to study and predict how obelisks interact with and influence the human microbiome. This module integrates data from microbiome sequencing, metabolomics, and host-microbe interaction studies to create a comprehensive model of how obelisks might affect microbial populations and, consequently, human health. It can simulate scenarios such as how introduced therapeutic obelisks might alter microbial community structures or how naturally occurring obelisks contribute to microbiome homeostasis.

[0526] Assisting the system's therapeutic applications is an RNA-based therapeutic optimizer. This AI-driven component designs and optimizes obelisk-like RNA structures for specific therapeutic applications. It uses advanced algorithms to generate potential obelisk sequences, simulates their behavior using an obelisk structure simulator and cellular instruction decoder, and iteratively refines designs based on predicted efficacy and safety profiles. This optimizer can generate candidates for various applications, from immune system modulation to targeted drug delivery.

[0527] An obelisk evolution predictor component is a tool that forecasts how obelisk structures might evolve within the body over time. It may consider factors like the microbiome composition, immune responses, and cellular uptake rates to model the dynamic changes in obelisk populations and structures. This predictor is useful for understanding the long-term effects of obelisk-based therapies and for designing interventions that remain effective over extended periods.

[0528] These specialized components interact with the existing modules of the AI-enhanced cellular modeling and simulation platform. For instance, the immune response modulation modeling component, an extension of the immune-disease ecosystem interaction simulator, can integrate data from the obelisk-microbiome interaction analyzer and the cellular instruction decoder to predict how obelisk-based therapies might enhance or modulate immune responses. This integration allows for the simulation of complex scenarios, such as using obelisks to boost immune recognition of cancer cells or to dampen autoimmune responses.

[0529] The platform's data integration layer plays a role in harmonizing diverse data types, including RNA sequencing data, microbiome profiles, and experimental findings on obelisk-cell interactions. This layer employs advanced data processing algorithms to normalize and integrate data from various sources, ensuring that all components of the system work with consistent, high-quality information.

[0530] A real-time therapeutic adjustment component, built upon the real-time adaptive cellular modeling system, incorporates obelisk-specific feedback mechanisms. This allows the system to process real-time data on the effects of obelisk-based therapies and adjust treatment plans accordingly. For example, it might recommend changes in obelisk dosage or structure based on observed changes in a patient's immune response or microbiome composition.

[0531] A global RNA discovery integration module extends the platform's knowledge graph and reasoning capabilities to connect with and analyze global RNA databases. This component enables the system to continuously learn from new discoveries in the field of RNA biology, potentially identifying novel obelisk-like structures and predicting their functions and therapeutic potential.

[0532] The multi-scale obelisk impact modeling component assesses how obelisk-mediated therapies affect cellular, tissue, and organism-level health outcomes. It may integrate data and predictions from various system components to provide a holistic view of obelisk impacts across different biological scales. This capability is important for predicting both the efficacy and potential

side effects of obelisk-based interventions.

[0533] A visualization of obelisk interactions component provides researchers with intuitive ways to interact with the complex data and models generated by the system. It can offer dynamic, 3D visualizations of obelisk structures, their interactions with cells and microbiomes, and their impacts on cellular processes. These visualizations can be scaled from molecular-level interactions to organism-wide effects, providing a comprehensive view of obelisk behavior and impacts.

[0534] In operation, these components work together to provide a comprehensive analysis of obelisk structures and their potential applications. For instance, in developing a new obelisk-based therapy for a specific disease, the RNA-based therapeutic optimizer might generate potential obelisk designs. These designs would then be simulated using the obelisk structure simulator and cellular instruction decoder to predict their cellular effects. The obelisk-microbiome interaction analyzer would assess potential impacts on the microbiome, while the immune response modulation modeling component would predict effects on the immune system. The obelisk evolution predictor would forecast the long-term behavior of the therapy, and the multi-scale obelisk impact modeling component would assess overall health impacts.

[0535] Throughout this process, the system continuously refines its models based on new data and observed outcomes, ensuring that its predictions and analyses remain at the cutting edge of RNA biology and therapeutic development. The real-time therapeutic adjustment component allows for dynamic optimization of treatments based on patient responses, while the global RNA discovery integration module ensures the system stays updated with the latest findings in the field.

[0536] By providing this deep, multi-scale understanding of obelisk structures and their interactions with biological systems, the obelisk modeling system offers unprecedented insights into these novel RNA entities. This comprehensive approach has far-reaching implications for our understanding of cellular biology, the human microbiome, and the development of innovative RNA-based therapies that could revolutionize treatment strategies for a wide range of diseases.

[0537] FIG. **54** is a block diagram illustrating an exemplary system architecture for an AI-enhanced cellular modeling and simulation platform **5400** configured for enhanced patient communication, according to an embodiment. According to the embodiment, patient communication system **5500** is an advanced platform designed to enhance how medical information is conveyed to patients. By leveraging artificial intelligence, data visualization, and personalized modeling, the system creates interactive, easy-to-understand explanations of complex medical concepts. It generates dynamic animations that illustrate cellular and tissue-level processes, overlays diagnostic information onto these visuals, and provides personalized scenarios to help patients understand potential outcomes of various treatment options.

[0538] The system aims to empower patients with knowledge, enabling them to make informed decisions about their health. It can adapt its communication style to each patient's emotional and cognitive needs, offering empathetic explanations and answering questions in natural language. The system also considers the impact of treatments on a patient's quality of life, simulating how different choices might affect daily activities and long-term well-being. By continuously updating its predictions based on real-time data and allowing patients to explore different scenarios, the system serves as a comprehensive tool for patient education, decision support, and improved communication with healthcare providers and family members. This holistic approach to patient communication has the potential to significantly enhance patient engagement, understanding, and ultimately, health outcomes.

[0539] FIG. **55** is a block diagram illustrating an aspect of an AI-enhanced cellular modeling and simulation platform, a patient communication system. According to various aspects, patient communication system **5500** is implemented as an advanced computational platform designed to bridge the gap between complex medical information and patient understanding. This system leverages cutting-edge AI technologies, data visualization techniques, and personalized modeling to create comprehensive, interactive, and empathetic communication packages tailored to individual

patients' needs. By integrating various specialized modules, the system offers a holistic approach to patient education and decision support, enhancing the overall healthcare experience.

[0540] According to the aspect, the system comprises a dynamic cellular animation engine **5501**, which builds upon the existing visualization and user interface system. This engine creates personalized, interactive animations of cellular and tissue phenomena, allowing patients to visualize their conditions at a microscopic level. The animations are not static; they dynamically adapt based on patient-specific data and can seamlessly transition between different scales, from molecular interactions to whole-body systems. This multi-scale visualization capability helps patients understand how cellular processes relate to their overall health and symptoms.

[0541] Working together with the animation engine is a diagnostic data visualization module **5502**. This component overlays relevant diagnostic information onto the cellular animations, providing context and meaning to the visualizations. For example, it might highlight areas of abnormal cell growth in a cancer patient's scan or illustrate how cholesterol buildup affects blood flow in a patient with heart disease. This integration of diagnostic data with visual representations helps patients grasp the implications of their test results in a more intuitive manner.

[0542] A patient-specific scenario generator **5503** is a component that leverages the multi-scale disease progression predictor. This module creates personalized scenario variations based on probability-aware models, allowing patients to explore potential outcomes of different treatment options or lifestyle changes. By inputting various parameters, such as treatment adherence or lifestyle modifications, patients can see how their choices might affect their health trajectory over time. This feature is particularly valuable for patients dealing with chronic conditions or facing complex treatment decisions.

[0543] Central to the system's communication capabilities is the natural language generation module **5504** for patient communication. This AI-driven component generates clear, empathetic explanations of diagnoses and treatment options, tailored to each patient's level of understanding and emotional state. It can produce written summaries, spoken explanations, or even conversational responses to patient queries. The module employs advanced natural language processing techniques to ensure that medical jargon is translated into easily understandable terms without losing the essential meaning.

[0544] A continuous prediction update module **5505** ensures that the system remains responsive to changes in the patient's condition or new medical information. By integrating real-time data from various sources, including wearable devices and electronic health records, this module continuously refines predictions and updates visualizations. This dynamic approach allows for a more accurate and up-to-date representation of the patient's health status, ensuring that communication remains relevant and timely.

[0545] To support informed decision-making, the system may further comprise an interactive decision support tool with a patient preference input module **5506**. This tool allows patients to express their priorities, concerns, and preferences regarding treatment options. The system then processes these inputs alongside medical data to provide personalized recommendations and visualizations of potential outcomes. For instance, a patient prioritizing quality of life over aggressive treatment can see how different approaches might affect their daily activities and long-term well-being.

[0546] A quality of life impact simulator is a unique component that predicts and visualizes how different treatment options might affect a patient's daily life and long-term well-being. This module considers factors such as potential side effects, recovery time, and lifestyle changes associated with various treatments. By providing tangible representations of how treatments might impact day-to-day activities, patients can make more informed decisions that align with their personal goals and values.

[0547] For broader health communications, the system incorporates a public health communication module **5507**. This component adapts the scenario generator to create visualizations and

explanations suitable for group-level health communications. It can be used by healthcare organizations, employers, or public health agencies to illustrate the impact of health initiatives, explain the importance of preventive measures, or demonstrate the collective benefits of actions like vaccination programs.

[0548] A stakeholder communication package creator may be present and designed to generate shareable, easy-to-understand summaries of a patient's condition and treatment plan. This tool recognizes that healthcare decisions often involve family members, caregivers, and other stakeholders. It creates tailored communication packages that help patients effectively convey their health situation and decisions to their support network, fostering better understanding and support.

[0549] Integrating these components may be an empathetic AI dialogue system, which serves as an overarching interface for patient interactions. This system is trained to generate empathetic, informative conversations tailored to individual patients' emotional and cognitive needs. It can engage in natural language conversations, answering questions, providing explanations, and offering emotional support throughout the patient's healthcare journey.

[0550] An external visualization tool connector **5508** allows the system to interface with sophisticated 3D modeling software like Blender, enabling the creation of high-fidelity visualizations when needed. This capability is particularly useful for creating detailed anatomical models or complex molecular visualizations that go beyond the capabilities of the built-in animation engine.

[0551] In operation, these components work together to provide a comprehensive communication experience. For example, when a patient receives a new diagnosis, the system first generates a personalized animation illustrating the condition at a cellular level. The diagnostic data visualization module overlays relevant test results onto this animation. The natural language generation module then provides a clear, empathetic explanation of the diagnosis, while the scenario generator shows potential progression paths. The patient can use the interactive decision support tool to explore treatment options, with the quality of life impact simulator showing how each option might affect their daily life. Throughout this process, the empathetic AI dialogue system engages with the patient, answering questions and providing emotional support. The system continuously updates its predictions and visualizations as new data becomes available, ensuring that the patient always has the most current information.

[0552] This integrated approach allows the patient communication system to address the diverse needs of patients throughout their healthcare journey. By providing clear, personalized, and interactive information, the system empowers patients to better understand their conditions, actively participate in their care decisions, and effectively communicate with their healthcare providers and support network. The result is a more informed, engaged, and confident patient, potentially leading to better healthcare outcomes and improved patient satisfaction.

DETAILED DESCRIPTION OF EXEMPLARY ASPECTS

[0553] The methods and processes described herein are illustrative examples and should not be construed as limiting the scope or applicability of the AI-enhanced cellular modeling and simulation platform. These exemplary implementations serve to demonstrate the versatility and adaptability of the platform. It is important to note that the described methods may be executed with varying numbers of steps, potentially including additional steps not explicitly outlined or omitting certain described steps, while still maintaining core functionality. The modular and flexible nature of the AI-enhanced cellular modeling and simulation platform allows for numerous alternative implementations and variations tailored to specific use cases or technological environments. As the field evolves, it is anticipated that novel methods and applications will emerge, leveraging the fundamental principles and components of the platform in innovative ways. Therefore, the examples provided should be viewed as a foundation upon which further innovations can be built, rather than an exhaustive representation of the platform's capabilities.

[0554] FIG. **34** is a flow diagram illustrating an exemplary method **3400** for designing personalized

cancer vaccines, according to an embodiment. According to the embodiment, the process for designing personalized cancer vaccines begins at step **3401** with the compilation of comprehensive cellular data from the patient's cancer cells and healthy cells. This data may comprise genomic, transcriptomic, proteomic, and metabolomic information, providing a multi-omics profile of the patient's cellular landscape. Using this data, at step **3402** the system generates detailed cellular models that accurately represent the patient's unique cancer cell characteristics. These models serve as the foundation for subsequent analyses and simulations. The system then employs advanced AI algorithms to simulate interactions between potential vaccine candidates and the generated cellular models at step **3403**. These simulations may be based on extensive datasets of known tumor-associated antigens and cellular interactions, allowing for precise predictions of vaccine efficacy.

[0555] Throughout the process, the system visualizes and analyzes cellular responses to vaccine candidates across different cellular regions and time points at step **3404**, providing a dynamic, spatiotemporal understanding of potential vaccine effects. These observed cellular responses can be linked to existing knowledge such as known biological pathways and previous research findings at step **3405**, contextualizing the results within the broader scope of cancer biology. To account for the inherent uncertainties in biological systems, the method incorporates stochastic modeling at step **3406** to quantify the uncertainty in vaccine efficacy predictions. This information is useful for assessing the reliability of the results and guiding further refinement of the vaccine design.

[0556] At step **3407** the system then enters an iterative optimization phase, fine-tuning the vaccine design based on multiple factors comprising, but not limited to, efficacy, cellular stress, and genetic stability. This optimization process leverages the insights gained from the simulations and analyses to create a vaccine candidate tailored to the patient's specific cancer profile. To validate and further refine the design, the system runs multiple in silico experiments at step **3408**, testing various combinations of vaccine components. These virtual experiments allow for rapid evaluation of numerous vaccine formulations without the need for physical samples. At step **3409**, the system outputs a final personalized cancer vaccine design, along with comprehensive data on its predicted efficacy and potential effects. This method, by leveraging advanced AI and computational techniques, enables the rapid development of highly personalized cancer vaccines, potentially revolutionizing cancer treatment approaches.

[0557] In some implementations, the method may further comprise generating a comparative analysis of the personalized vaccine design against alternative treatment options, considering predicted health outcomes, quality of life considerations, and economic factors. In such an implementation, the system can aggregate data on the personalized vaccine design and alternative treatment options, including standard chemotherapy regimens, targeted therapies, and immunotherapies. It then utilizes predictive modeling algorithms, such as ensemble machine learning methods or Bayesian networks, to forecast health outcomes for each treatment option. These predictions are based on the patient's specific cancer profile, treatment histories of similar patients, and the latest clinical trial data.

[0558] To assess quality of life considerations, the system can incorporate patient-reported outcome measures (PROMs) and health-related quality of life (HRQOL) data from previous studies. It uses natural language processing to analyze qualitative data from patient testimonials and case studies, extracting insights on side effects, treatment burden, and overall patient experience for each treatment option. The system can employ multi-criteria decision analysis (MCDA) techniques to weigh these factors against the predicted health outcomes.

[0559] For economic factors, the system conducts a comprehensive cost-effectiveness analysis. This may comprise calculating quality-adjusted life years (QALYs) for each treatment option and estimating both direct medical costs (e.g., drug costs, administration, follow-up care) and indirect costs (e.g., lost productivity, caregiver burden). The system can use Markov models or discrete event simulation to project long-term costs and outcomes, accounting for factors like potential relapses or secondary health effects.

[0560] The comparative analysis then integrates these health outcome predictions, quality of life assessments, and economic evaluations using a sophisticated multi-dimensional scoring system. This system employs techniques like the analytic hierarchy process (AHP) or PROMETHEE method to balance these diverse factors and generate an overall comparative score for each treatment option.

[0561] Furthermore, the system can generate a detailed report visualizing the comparative analysis results. This may comprise interactive dashboards showing side-by-side comparisons of treatment options across various metrics, sensitivity analyses to account for uncertainties in the predictions, and personalized risk-benefit profiles. The report may also highlight key differentiators of the personalized vaccine approach, such as its potential for reduced side effects or improved long-term outcomes.

[0562] This comprehensive comparative analysis provides patients, healthcare providers, and payers with a nuanced, data-driven assessment of the personalized vaccine design in the context of available treatment alternatives. It enables informed decision-making by considering not just clinical efficacy, but also quality of life impact and economic implications, thus supporting a holistic approach to personalized cancer care.

[0563] FIG. **35** is a flow diagram illustrating an exemplary federated learning process **3500** for training a cellular model across one or more separate institutions, according to an embodiment. The federated learning method implemented in the AI-enhanced cellular modeling and simulation platform enables collaborative learning across multiple institutions while preserving data privacy.

[0564] According to the embodiment, the process begins at step **3501** with the initialization of a global model, typically (but not always) a deep neural network architecture suitable for cellular analysis tasks, such as a combination of convolutional and recurrent layers for processing spatial and temporal cellular data. At step **3502** the global model is securely distributed to participating institutions using encrypted channels and digital signatures to ensure authenticity. Each institution then trains this model on its own curated local dataset at step **3503**, which may include, but is not limited to, multi-omics data, cellular imaging data, and clinical outcomes. At step **3504** the local training process employs techniques such as differential privacy, where noise is added to gradients, and gradient clipping to prevent overfitting to local data peculiarities. The model may then be trained on the prepared and secure local data at step **3505**.

[0565] After a predetermined number of local epochs, each institution computes model updates at step **3506**, represented as the difference between the updated and initial model parameters. These updates are then securely aggregated **3507** using, for example, cryptographic techniques like homomorphic encryption or secure multi-party computation, allowing computations on encrypted data without exposing individual contributions. A central server (e.g., AI-enhanced cellular modeling and simulation platform) performs federated averaging at step **3508** on these encrypted updates, potentially using at step **3509** adaptive optimization techniques like FedAdam to handle statistical heterogeneity across institutions. At step **3510** the global model is then updated with the averaged parameters and re-distributed to the institutions for the next round of training at step **3511**. At step **3512** the updated global model is evaluated on a held-out validation set to assess performance improvements. This process repeats for multiple rounds until the model converges or a predefined number of rounds is reached or some other training and/or performance criteria is satisfied. At step **3513** a final test is conducted on the updated global model before it may be deployed.

[0566] Throughout this process, the system may implement several advanced techniques to enhance learning and security. These can include adaptive learning rates based on the Fisher information matrix to optimize convergence, periodic model pruning to reduce communication overhead, and differential privacy guarantees at both local and global levels to prevent reconstruction of individual patient data. According to an aspect, the method further comprises a mechanism for detecting and mitigating potential adversarial attacks, such as model poisoning

attempts, by employing robust aggregation techniques and anomaly detection on model updates.

[0567] For example, in the context of predicting cancer cell responses to various treatment modalities, the federated learning system and method could operate as follows: The global model, initially trained on publicly available cancer cell line databases, is distributed to cancer research centers worldwide. Each center then fine-tunes this model on its proprietary patient-derived xenograft data, capturing unique aspects of tumor heterogeneity and microenvironment influences on treatment response. The secure aggregation of these local learnings allows the global model to capture a diverse range of cancer cell behaviors and drug responses, significantly enhancing its predictive power across different cancer types and patient populations. This collaborative approach enables the development of a more robust and generalizable model for predicting treatment outcomes, while ensuring that sensitive patient data and proprietary research information never leave the local institutions, thereby addressing critical data privacy and intellectual property concerns in cancer research.

[0568] FIG. **36** is a flow diagram illustrating an exemplary method **3600** for real-time adaptive modeling, according to an embodiment. The real-time adaptive modeling method in the AI-enhanced cellular modeling and simulation platform is designed to continuously process and analyze streaming data from various sources, adapting its models and predictions in real-time. This method leverages a combination of online learning algorithms, streaming data processing techniques, and adaptive neural network architectures to maintain up-to-date and accurate cellular models. According to the embodiment, the process begins at step **3601** by initializing a base model trained on historical data, which could be a hybrid architecture combining convolutional neural networks for spatial feature extraction from cellular images, recurrent neural networks for temporal dynamics, and graph neural networks for modeling intercellular interactions. As new data streams in from sources such as live-cell imaging systems, microfluidic devices, and biosensors, it is first preprocessed using adaptive normalization techniques to handle concept drift and ensure compatibility with the model's input format at step **3602**.

[0569] An aspect of the method is an ensemble of online learning models, each specializing in different aspects of cellular behavior. These models may employ techniques such as incremental learning with elastic weight consolidation to incorporate new information without catastrophic forgetting of previously learned patterns. At step **3603** the preprocessed streaming data is fed through the ensemble of online learning models. The system can use a dynamic weighted voting scheme to generate and combine predictions from these specialized models at step **3604**, with weights adjusted based on recent performance metrics (e.g., prediction accuracy, etc.) at step **3605**. The process may comprise applying incremental learning with elastic weight consolidation. To handle sudden changes in cellular behavior, the method incorporates a change point detection algorithm at step **3606** based on martingale theory, triggering rapid model updates at step **3608** when significant shifts are detected. Additionally, the system maintains a sliding window of recent data for periodic batch updates, using techniques like experience replay to reinforce learning of important but infrequent events. An optional step **3609** may be performed wherein the system adjusts learning rates and model architecture if necessary.

[0570] According to an aspect, tor uncertainty quantification, the method employs Bayesian online learning techniques, providing confidence intervals for its predictions. This is useful for real-time decision support, allowing the system to flag predictions with high uncertainty for human expert review. The adaptive modeling method may further comprise an automated feature importance analysis, using techniques such as, for example, SHAP (SHapley Additive explanations) values calculated in a streaming fashion, to provide interpretable insights into the factors driving model predictions.

[0571] An example application of this method in the cellular modeling platform could be directed to real-time monitoring and prediction of cancer cell responses to combination therapies in a microfluidic tumor-on-a-chip system. The method would continuously process imaging data

showing cell morphology changes, fluorescence signals indicating pathway activations, and microfluidic sensor data on metabolite concentrations. It would adapt its predictions of cell state transitions, drug efficacy, and potential resistance development in real-time, providing researchers with immediate insights into the dynamics of cancer cell populations under different treatment conditions. This real-time adaptive modeling enables rapid iteration in experimental design, allowing for on-the-fly adjustments to treatment protocols based on observed cellular responses, thereby accelerating the drug discovery and optimization process.

[0572] FIG. **37** is a flow diagram illustrating an exemplary method **3700** for providing uncertainty quantification, according to an embodiment. The uncertainty quantification process in the AI-enhanced cellular modeling and simulation platform is designed to provide robust estimates of confidence in model predictions, important for informed decision-making in cellular research and drug development. This method employs a multi-faceted approach combining Bayesian techniques, ensemble methods, and Monte Carlo simulations to capture different sources of uncertainty in cellular modeling. According to the embodiment, the process begins at step **3701** with the implementation of a variational inference system. According to an aspect, the method utilizes Bayesian Neural Networks (BNNs) where network weights are treated as probability distributions rather than point estimates. These BNNs are implemented using variational inference techniques, specifically the Bayes by Backprop algorithm, which allows for efficient training and uncertainty estimation in high-dimensional parameter spaces typical of complex cellular models. The process may further comprise defining prior distributions for network weights and optimizing variational posterior using stochastic gradient descent.

[0573] The method also incorporates ensemble techniques, specifically using Deep Ensembles, where multiple models with different random initializations are trained on the same data at step **3702**. At step **3703**, a loss function is employed to capture uncertainty in the model(s). This captures model uncertainty arising from the optimization process and helps in identifying regions of the input space where predictions are less reliable. According to an aspect, to account for aleatoric uncertainty (inherent randomness in cellular processes), the method employs a heteroscedastic loss function, allowing the model to predict both the mean and variance of the output distribution for each input. For scenarios where computational efficiency is of concern, such as real-time monitoring of cellular responses, the method may implement Monte Carlo Dropout as an approximation to Bayesian inference, providing rapid uncertainty estimates with minimal computational overhead.

[0574] To handle the multi-scale nature of cellular modeling, the method integrates uncertainties across biological scales at step **3704**. According to an embodiment, the method employs a hierarchical Bayesian approach, where uncertainties at different biological scales (e.g., molecular, cellular, tissue-level) are propagated and integrated. This is particularly important for capturing how uncertainties at lower levels (e.g., in protein-protein interactions) impact higher-level predictions (e.g., cellular phenotypes). The method also comprises sensitivity analysis at step **3705** using, for example, Sobol indices, calculated through efficient sampling techniques, to quantify how different input parameters contribute to output uncertainties. This provides valuable insights into which aspects of the cellular model are most critical for accurate predictions.

[0575] The uncertainty quantification method in the AI-enhanced cellular modeling platform goes beyond initial model training and sensitivity analysis to provide comprehensive, real-time uncertainty estimates for each prediction. At step **3706**, for each prediction task, the method generates multiple samples from the posterior distribution of model parameters, effectively creating a set of plausible models. These samples are then propagated through the model to obtain a distribution of outputs, capturing the range of possible predictions given the uncertainties in the model parameters. From this output distribution, the method calculates summary statistics such as the mean prediction, variance, and credible intervals, providing a nuanced view of the prediction's reliability.

[0576] At step **3707** the method aggregates predictions from multiple ensemble members, combining the outputs from different model initializations to capture model uncertainty. This aggregation step can use techniques like Bayesian Model Averaging, weighting the contributions of different ensemble members based on their performance on validation data. At step **3708** the system combines uncertainties from different sources (e.g., epistemic uncertainty from model parameters, aleatoric uncertainty from inherent randomness in the data, and hierarchical uncertainty from multi-scale modeling, etc.) into a unified uncertainty representation. This holistic approach ensures that all aspects of uncertainty are accounted for in the final prediction.

[0577] To make these uncertainty estimates interpretable and actionable, the method generates sophisticated visualizations at step **3709**. These can include, but are not limited to, probability distribution plots for key output variables, allowing researchers to see the full range of possible outcomes and their likelihoods. It can also produce heatmaps showing how uncertainty varies across different input conditions, helping identify regions of the input space where the model is less confident. An alert system may be implemented to flag high-uncertainty predictions that exceed predefined thresholds, prompting human expert review for critical decisions.

[0578] According to an aspect, the method continuously updates its uncertainty estimates as new data becomes available. It may use Bayesian updating to refine model parameters, incorporating new evidence to sharpen or broaden uncertainty estimates as appropriate. In cases where significant new information contradicts existing models, the system can trigger a retraining of ensemble members to ensure the uncertainty estimates remain accurate and relevant.

[0579] According to an embodiment, the method further comprises maintaining a comprehensive log of all uncertainty estimates and their sources. This logging may be used for retrospective analysis, allowing researchers to track how uncertainties evolve over time and in response to new data. It also facilitates continuous improvement of the uncertainty quantification process itself, enabling researchers to identify patterns in high-uncertainty predictions and refine the modeling approach accordingly.

[0580] This detailed approach to uncertainty quantification ensures that the AI-enhanced cellular modeling and simulation platform provides not just point predictions, but a full probabilistic understanding of cellular behaviors and responses. This is particularly vital in applications like personalized cancer therapy, where understanding the range of possible treatment outcomes and their likelihoods can significantly impact clinical decision-making.

[0581] As an example of this uncertainty quantification method in the cellular modeling platform, consider predicting the efficacy of a novel combination therapy for treatment-resistant cancer. The method would provide not just point estimates of expected tumor reduction, but comprehensive probability distributions of outcomes. It would quantify uncertainties arising from variability in patient-specific cellular characteristics, potential off-target effects of the drugs, and limitations in the underlying biological knowledge. Researchers could then visualize these uncertainties through interactive plots, showing, for instance, the probability of achieving different levels of tumor reduction along with confidence intervals. This would allow for more informed decision-making in clinical trial design, highlighting cases where additional data collection or model refinement is needed before proceeding to human trials.

[0582] FIG. **38** is a flow diagram illustrating an exemplary method **3800** for personalized treatment optimization, according to an embodiment. The personalized treatment optimization method in the AI-enhanced cellular modeling and simulation platform is designed to tailor therapeutic strategies to individual patients based on their unique cellular and molecular profiles. This method integrates multi-omics data, including, but not limited to, genomics, transcriptomics, proteomics, and metabolomics, with advanced machine learning techniques and mechanistic modeling to predict patient-specific treatment responses and optimize therapy regimens. The process begins at step **3801** by obtaining patient-specific data. This may comprise a comprehensive profiling of the patient's cells, typically involving single-cell sequencing, high-content imaging, and functional

assays to capture cellular heterogeneity and dynamic behaviors. The patient-specific data, which may comprise a plurality of multi-modal data, may be preprocessed and integrated at step **3802**

[0583] At step **3803** the system constructs a hybrid model. The core of the hybrid model combines mechanistic ordinary differential equation (ODE) models of key cellular pathways with machine learning components, particularly graph neural networks (GNNs) and recurrent neural networks (RNNs). The ODE models capture known biological mechanisms and drug-target interactions, while the GNNs model complex cellular interaction networks and the RNNs capture temporal dynamics of cellular responses. This hybrid approach allows the system to leverage prior biological knowledge while also learning complex patterns from data that may not be fully explained by current mechanistic understanding.

[0584] The optimization process utilizes reinforcement learning, specifically a variant of Deep Q-Networks (DQN) adapted for continuous action spaces, to navigate the vast space of possible treatment combinations and dosing schedules. At step **3804** the system initializes a reinforcement learning environment. The system further trains one or more reinforcement agents (algorithms) at step **3805**. The reward function for the reinforcement learning algorithm is multi-objective, considering factors such as predicted tumor reduction, minimization of side effects, and long-term survival probability. To handle the uncertainty inherent in biological systems and incomplete patient data, the method employs a robust optimization approach at step **3806**, using techniques from distributionally robust optimization to ensure that the selected treatment strategy performs well across a range of plausible scenarios.

[0585] The method also incorporates a Bayesian optimization component for fine-tuning treatment parameters, using Gaussian Process surrogates to efficiently explore the parameter space and balance exploitation of promising regions with exploration of uncertain areas. At step **3807** the system generates an initial personalized treatment plan for the patient. The platform may then simulate a plurality of treatment outcomes at step **3808**. At step **3809** the platform can implement monitoring and adaptation protocols. This may comprise defining key biomarkers and clinical indicators to track, and/or setting thresholds for triggering treatment plan updates. To account for potential changes in the patient's condition over time, the system implements an adaptive treatment strategy using model predictive control, where the treatment plan is periodically updated based on the latest patient data and model predictions at step **3810**. The platform may be configured to generate a comprehensive report which comprises one or more of: a summary of the recommended treatment plan; visualizations of predicted outcomes and uncertainties; and rationale explaining treatment decisions.

[0586] An example application of this method could be in optimizing combination immunotherapy for a patient with metastatic melanoma. The system would integrate the patient's tumor genomic profile, immune cell repertoire (from single-cell RNA sequencing), and plasma cytokine levels with data from previous patients and preclinical models. It would then simulate the patient's likely response to various combinations and schedules of immune checkpoint inhibitors, cytokine therapies, and targeted drugs. The optimization algorithm might identify a personalized treatment regimen involving a specific sequence of checkpoint inhibitors, followed by a cytokine therapy to enhance T-cell infiltration, with dynamically adjusted dosing based on predicted tumor response and immune activation markers. This personalized strategy could potentially achieve better efficacy with reduced side effects compared to standard protocols.

[0587] FIG. **39** is a flow diagram illustrating an exemplary method **3900** for cellular imaging analysis, according to an embodiment. According to the embodiment, the cellular imaging analysis process of the AI-enhanced cellular modeling and simulation platform is designed to extract comprehensive, quantitative information from complex cellular images, enabling detailed characterization of cellular morphology, behavior, and interactions. This method integrates advanced computer vision techniques with deep learning models to process and analyze various types of microscopy data, including brightfield, fluorescence, and high-content imaging. According

to an aspect, the method utilizes is a multi-stage deep learning pipeline that performs semantic segmentation, instance segmentation, and tracking of individual cells across time-series data.

[0588] The process begins at step **3901** with image preprocessing, involving techniques such as noise reduction using wavelet-based methods, illumination correction via Gaussian filtering, and contrast enhancement through adaptive histogram equalization. The preprocessed images then undergo semantic segmentation at step **3902** using, for example, a U-Net architecture with a ResNet backbone, trained on diverse cellular datasets to distinguish cell bodies, nuclei, and various subcellular structures. Instance segmentation is performed at step **3903** by using, for example, a Mask R-CNN model, allowing for the delineation of individual cells even in densely packed environments. For time-series data, cell tracking is performed at step **3904**. According to an aspect, the method comprises using a combination of deep learning and graph-based optimization, specifically employing a Siamese neural network for feature extraction and the Hungarian algorithm for track assignment.

[0589] Feature extraction is performed at step at step **3905**. This may utilize both hand-crafted features (e.g., shape descriptors, texture features) and learned features from a pre-trained convolutional neural network. These features are used to characterize cellular morphology, quantify protein expression levels, and analyze subcellular localization patterns. The method also incorporates advanced techniques at step **3906** for analyzing cellular interactions and microenvironment, including, but not limited to, spatial point pattern analysis for studying cell-cell interactions and graph-based methods for characterizing tissue architecture.

[0590] According to an aspect, to handle the heterogeneity inherent in cellular populations, the method employs unsupervised learning techniques, specifically a variational autoencoder (VAE) coupled with a Gaussian Mixture Model (GMM), to identify distinct cellular subpopulations at step **3907** based on morphological and functional features. For analyzing dynamic cellular behaviors at step **3908**, the method may utilize recurrent neural networks, particularly Long Short-Term Memory (LSTM) networks, to model temporal patterns in cellular features and predict future states.

[0591] As an example, consider the analysis of a time-lapse fluorescence microscopy experiment studying the effects of a novel drug combination on cancer cell migration and division. The method would segment and track individual cancer cells over time, quantifying changes in cell morphology, migration speed, and division rates. It would identify distinct subpopulations of cells based on their response to the treatment, potentially uncovering resistant populations. The spatial analysis components would characterize changes in cell-cell interactions and tissue organization, providing insights into the drug combination's effects on the tumor microenvironment. This comprehensive analysis would feed into the broader cellular modeling platform, informing predictions of drug efficacy and helping to optimize treatment strategies.

[0592] FIG. **40** is a flow diagram illustrating an exemplary method **4000** for providing personalized medicine, according to an embodiment. According to the embodiment, the process for providing personalized medicine begins at step **4001** with the comprehensive collection of patient-specific data, including genetic information, molecular profiles, medical history, and real-time physiological data from wearable devices. At step **4002** this diverse dataset is then integrated and processed using advanced multi-omics data integration techniques, creating a holistic view of the patient's biological state. Based on this integrated data, the system generates a personalized cellular model at step **4003** that accurately represents the patient's unique physiological characteristics at a cellular level. This model serves as the foundation for simulating various treatment responses at step **4004**, allowing the system to predict how the patient might react to different therapeutic options. The system then analyzes these simulations and prioritizes treatment options based on predicted efficacy at step **4005**, potential side effects, and the patient's individual circumstances. As treatment progresses, the system incorporates real-time monitoring data from wearable devices and periodic medical tests at step **4006**, continuously refining its predictions and recommendations. This allows

for dynamic adjustment of the treatment plan in response to the patient's evolving condition at step **4007**. Throughout the entire process, the system provides ongoing personalized care, offering insights and recommendations tailored to the patient's unique needs and responses at step **4008**.

[0593] As an example, consider a patient diagnosed with a rare form of leukemia. The AI-enhanced cellular modeling and simulation platform would first collect the patient's genomic data, transcriptomic profile of their cancer cells, proteomic data, and medical history. It would also integrate real-time data from a wearable device monitoring the patient's heart rate, activity levels, and sleep patterns. Using this comprehensive dataset, the system would generate a detailed cellular model of the patient's leukemia cells and healthy blood cells. The platform would then simulate how these cells might respond to various treatment options, including standard chemotherapy regimens, targeted therapies, and experimental treatments. By analyzing these simulations, the system might identify that a combination of a novel targeted therapy and a specific immunotherapy could be most effective for this patient's unique cancer profile. As treatment begins, the system continuously monitors the patient's response through blood tests and wearable device data. If it detects signs of increased inflammation or decreased efficacy, it might recommend adjusting the drug dosage or adding a supportive therapy to manage side effects. Throughout the treatment course, the system provides the healthcare team with ongoing insights and recommendations, enabling truly personalized and adaptive care for the patient.

[0594] FIG. **41** is a flow diagram illustrating an exemplary method **4100** for providing drug discovery using an AI-enhanced cellular modeling and simulation platform, according to an embodiment. According to the embodiment, the method for providing drug discovery begins at step **4101** with a clear definition of the target disease or condition, establishing the specific therapeutic goals. At step **4102** the system then collects and integrates data from multiple sources, including genomic databases, proteomics studies, published literature, and clinical trial results. Using this comprehensive dataset, the platform generates detailed cellular models and simulations that represent the disease state and potential drug interactions at a molecular level at step **4103**. At step **4104** the system then screens vast libraries of chemical compounds, analyzing their potential interactions with the cellular models. This process identifies promising lead compounds, which are then prioritized and optimized based on their predicted efficacy, safety profiles, and other relevant factors at step **4105**. For personalized therapies, such as cancer vaccines, the system designs and simulates treatments tailored to specific patient profiles at step **4106**. Throughout the process, the platform assesses **4107** the comprehensive impact of potential treatments, considering factors such as long-term patient outcomes, quality of life, economic viability, and healthcare accessibility. The drug discovery process is iterative, with the system continuously refining its models and predictions based on new data and feedback from experimental results.

[0595] For example, consider the discovery of a novel treatment for a specific type of treatment-resistant breast cancer. The AI-enhanced cellular modeling and simulation platform would start by integrating data on the genetic mutations common in this cancer type, proteomic profiles of tumor cells, and results from previous clinical trials of related treatments. Using this data, the system would generate detailed cellular models of the cancer cells, including their unique signaling pathways and metabolic processes. The platform would then simulate how these cells interact with a vast library of potential drug compounds, including both existing drugs and novel chemical entities. Through this process, it might identify a previously overlooked compound that shows promise in disrupting a key cellular process specific to this cancer type. The system would then optimize this lead compound, suggesting structural modifications to enhance its efficacy and reduce potential side effects. Simultaneously, it would design a personalized vaccine approach that could complement the drug treatment, targeting specific neoantigens expressed by the patient's tumor cells. The platform would simulate how this combination therapy might perform across a diverse patient population, considering factors such as genetic variations and potential resistance mechanisms. It would also assess the economic feasibility of developing this treatment, considering

manufacturing complexity and potential market size. Throughout this process, the system would continuously update its models based on new experimental data, refining its predictions and guiding researchers towards the most promising avenues for further investigation. This AI-driven approach could significantly accelerate the discovery of effective treatments for this challenging form of breast cancer, potentially bringing new hope to patients who have exhausted conventional treatment options.

[0596] FIG. **42** is a flow diagram illustrating an exemplary method **4200** for providing cellular engineering using the AI-enhanced cellular modeling and simulation platform, according to an embodiment. According to an aspect, the platform enables fascia-based cellular engineering.

[0597] According to the embodiment, the process for providing cellular engineering begins at step **4201** with a clear definition of the engineering objectives and the specific cellular system to be modified. This may comprise identifying the desired cellular functions or behaviors to be enhanced or introduced, as well as any constraints or limitations that need to be considered. Once the objectives are established, the system collects and integrates a wide range of data at step **4202**, including genomic, transcriptomic, proteomic, and structural information related to the target cells and their surrounding tissues. This comprehensive data integration creates a holistic view of the cellular environment and its functions.

[0598] Using this integrated data, the system generates detailed computational models of the cells and tissues involved at step **4203**. These models incorporate various scales, from molecular interactions to tissue-level behaviors, providing a multi-dimensional representation of the cellular system. With these models in place, the cellular engineering system then designs potential genetic or structural modifications to achieve the desired objectives at step **4204**. This may comprise, for example, designing new genetic circuits, modifying existing cellular pathways, or engineering changes to the cellular microenvironment.

[0599] At step **4205** the system simulates the behavior of the engineered cells using advanced AI and machine learning algorithms. These simulations predict how the proposed modifications will affect cellular function, interaction with surrounding tissues, and overall system behavior. Based on these simulation results, the system iteratively optimizes the design at step **4206**, refining the proposed modifications to maximize desired outcomes while minimizing potential negative effects.

[0600] Once an optimal design is achieved, the system conducts extensive in silico experiments at step **4207** to validate the design under various conditions and scenarios. This validation process helps identify potential issues or unexpected behaviors before physical implementation. At step **4208**, after validation, the system generates a detailed implementation protocol, providing step-by-step guidance for carrying out the cellular engineering in a laboratory setting.

[0601] At step **4209**, the system provides recommendations for ongoing monitoring and adjustment of the engineered cells. This can include suggestions for key parameters to track, potential issues to watch for, and strategies for fine-tuning the engineered system based on real-world performance.

[0602] As an example, consider the use of the cellular engineering system to design a modified T-cell for improved cancer immunotherapy. The system would start by defining the objective: to engineer T-cells with enhanced tumor-targeting capabilities and increased persistence in the tumor microenvironment. It would then integrate data on T-cell biology, cancer cell characteristics, and the tumor microenvironment, including information on relevant signaling pathways, surface receptors, and metabolic profiles.

[0603] Using this data, the system would generate comprehensive models of T-cells, cancer cells, and their interactions within the tumor microenvironment. It might then design genetic modifications to the T-cells, such as introducing a chimeric antigen receptor (CAR) targeting a specific tumor antigen, and engineering metabolic pathways for improved function in the nutrient-poor tumor environment.

[0604] The system would simulate how these modified T-cells would behave in the tumor microenvironment, predicting their efficacy in targeting cancer cells, their persistence, and any

potential off-target effects. Through multiple iterations, it would optimize the design, perhaps adjusting the CAR structure for improved binding affinity or introducing additional genetic modifications to enhance T-cell survival.

[0605] After extensive in silico validation, the system would generate a detailed protocol for creating these engineered T-cells, including the specific genetic constructs to be used and the optimal cell culture conditions. It would also provide guidance on how to monitor the performance of these cells in clinical trials, suggesting biomarkers to track and potential adaptive strategies based on patient responses. This comprehensive approach would significantly accelerate the development of more effective cancer immunotherapies, showcasing the power of AI-enhanced cellular modeling and simulation in advancing cellular engineering for medical applications.

[0606] FIG. **43** is a flow diagram illustrating an exemplary method **4300** for providing synthetic biology design and simulation, according to an embodiment. According to the embodiment, the process begins at step **4301** with a clear definition of the objectives and the specific medical application for the microbots or biobots. This may comprise identifying the desired functionalities, such as targeted drug delivery, tissue repair, or diagnostic imaging, as well as the physiological context in which the bots will operate. Once the objectives are established, the system utilizes its microbot design optimizer to create initial designs for the bots at step **4302**, considering factors such as size, shape, propulsion mechanism, and payload capacity.

[0607] At step **4303** the designed bots are then simulated in a virtual microenvironment using the microbot environment simulator. This step models how the bots interact with various biological structures, fluids, and barriers, providing insights into their behavior and effectiveness. At step **4304**, based on these simulations, the system optimizes the bot design and swarm dynamics using AI algorithms, refining parameters to enhance performance and coordination among multiple bots.

[0608] For applications involving drug delivery, the drug release simulator models the release kinetics and tissue interactions of therapeutic agents at step **4305**. This helps in optimizing drug loading, release mechanisms, and targeting strategies. The magnetic field simulator plans navigation pathways and control strategies at step **4306**, ensuring precise guidance of the bots to their target locations.

[0609] At step **4307** the system then conducts comprehensive virtual trials, simulating the bots' operation in various physiological conditions and potential scenarios. These trials help identify potential challenges and refine the overall strategy. Based on these simulations, the system generates detailed deployment and control protocols at step **4308**, including parameters for bot activation, navigation, and therapeutic action.

[0610] Planning for real-time monitoring and adaptive control may be an additional step, where the telemetry analyzer is configured to process live data from the bots during operation. This enables dynamic adjustments to bot behavior based on real-time physiological feedback. Additionally, the system can develop safety measures and contingency plans, considering potential complications or unexpected physiological responses.

[0611] As an example, consider using the synthetic biology system to develop a microbot-based targeted drug delivery system for treating a brain tumor. The system would start by designing microbots capable of crossing the blood-brain barrier and carrying a specific chemotherapy drug. It would then simulate these microbots in a detailed model of the brain's vascular system and tumor microenvironment. The swarm intelligence controller would optimize how the microbots navigate through blood vessels and accumulate at the tumor site. The drug release simulator would model how the chemotherapy drug is released from the microbots and diffuses through the tumor tissue.

[0612] The magnetic field simulator would design a precise navigation strategy, considering the need to guide the microbots through the complex brain vasculature. Virtual trials would simulate various scenarios, such as different tumor sizes or locations, helping to refine the approach. The system would then generate a detailed protocol for microbot deployment, including the injection site, magnetic field parameters for navigation, and drug release triggers.

[0613] It would also plan for real-time monitoring, setting up the telemetry analyzer to track microbot positions and drug release rates during the procedure. Safety measures might include protocols for removing microbots after drug delivery or responding to potential aggregation in non-target areas. This comprehensive approach would allow for the development of a highly targeted, efficient, and safe drug delivery system, potentially revolutionizing brain tumor treatment by minimizing systemic drug exposure and maximizing therapeutic effect at the tumor site.

[0614] FIG. **44** is a flow diagram illustrating an exemplary method **4400** for microbiome simulation and monitoring, according to an embodiment. According to the embodiment, the process begins at step **4401** with the collection and processing of multi-omics microbiome data. This may comprise analyzing genomic, transcriptomic, and proteomic data from microbiome samples taken from various body sites. At step **4402** the system then integrates this microbiome data with host physiological information, creating a holistic view of the microbiome-host ecosystem. Using this integrated data, the system generates comprehensive microbiome profiles for different body sites at step **4403**, characterizing the diversity and abundance of microbial species present.

[0615] The next step **4404** involves modeling the temporal dynamics of microbiome composition, tracking how these microbial communities change over time in response to various factors such as diet, medication, or environmental changes. At step **4405** the system then simulates complex microbiome-host interactions, modeling how microbial metabolites and other factors influence host physiology across multiple biological scales.

[0616] Based on these simulations and historical data, the system predicts disease risks and potential health outcomes associated with specific microbiome profiles at step **4406**. It also analyzes how the microbiome might influence drug metabolism and efficacy at step **4407**, providing valuable insights for personalized medicine approaches. Using all this information, the system designs personalized microbiome interventions at step **4408**, such as dietary recommendations or probiotic therapies, tailored to an individual's unique microbial profile and health goals.

[0617] For advanced research applications, the system can simulate the effects of gene-edited microbes at step **4409**, exploring potential therapeutic applications of engineered microbial strains. Throughout this process, the system provides ongoing monitoring and generates adaptive recommendations, continuously refining its models and predictions based on new data and observed outcomes.

[0618] As an example, consider using the microbiome simulation and monitoring system to optimize treatment for a patient with inflammatory bowel disease (IBD). The system would start by analyzing the patient's gut microbiome composition through genomic sequencing and metabolomic profiling. It would integrate this data with the patient's medical history, diet, and current symptoms. The system would then model how the patient's microbiome has changed over time, potentially identifying shifts associated with IBD flare-ups.

[0619] Using its microbiome-host interaction simulator, the system would predict how the current microbiome composition is influencing gut inflammation and overall health. It might identify an overgrowth of pro-inflammatory bacteria and a deficit in beneficial short-chain fatty acid-producing bacteria. The disease risk predictor would assess the patient's risk for complications or related conditions based on their microbiome profile.

[0620] The microbiome-drug interaction predictor would then simulate how different IBD treatments might interact with the patient's microbiome, predicting their efficacy and potential side effects. Based on these simulations, the microbiome intervention optimizer would design a personalized treatment plan. This might include a combination of targeted antibiotics to reduce pro-inflammatory bacteria, specific probiotic strains to enhance beneficial bacteria, and dietary recommendations to support a healthier microbiome composition.

[0621] The system would also simulate the potential effects of novel treatments, such as gene-edited bacteria designed to produce anti-inflammatory compounds in the gut. Finally, it would

provide a monitoring plan, recommending regular microbiome testing to track the effectiveness of the interventions and allowing for real-time adjustments to the treatment strategy.

[0622] This comprehensive approach would enable a highly personalized and adaptive treatment strategy for the IBD patient, potentially improving symptom management and long-term health outcomes by addressing the underlying microbiome imbalances contributing to their condition.

[0623] FIG. **45** is a flow diagram illustrating an exemplary method **4500** for phage dynamics analysis, according to an embodiment. According to the embodiment, the process for supporting phage dynamics analysis begins at step **4501** with the collection and processing of genomic data from both phages and their target bacteria. This may comprise analyzing genetic sequences to identify key features such as phage receptor binding sites, bacterial defense mechanisms, and potential targets for therapeutic intervention. At step **4502**, the system processes structural data using automated cryo-EM analysis, providing high-resolution information about phage and bacterial morphologies, which is important for understanding their interactions at a molecular level.

[0624] Using this integrated data, the system simulates nonlinear gene expression and protein production at step **4503**, particularly focusing on unique mechanisms like rolling circle reverse transcription observed in some phage-bacteria interactions. This step is useful for understanding how bacteria defend against phages and how phages overcome these defenses. At step **4504** the system models complex phage-bacteria interactions and infection dynamics, simulating how different phages interact with various bacterial strains under different conditions.

[0625] Based on these simulations and historical data, the system predicts potential resistance development at step **4505**, including cross-resistance between phage therapies and traditional antibiotics. This step helps in designing phage therapies that are less likely to induce resistance. At step **4506** the system engages in the design and optimization of phage proteins for therapeutic applications, using iterative processes to enhance binding affinity, stability, and specificity.

[0626] To ensure safety and efficacy, the system simulates the effects of proposed phage therapies on host tissues and organs at step **4507**, considering potential side effects and interactions with the host's immune system. At step **4508** is may assess the broader, population-level impacts of implementing phage therapy, considering factors such as the potential for widespread resistance development and changes in microbial ecosystems.

[0627] Integrating all this information, the system generates personalized phage therapy protocols, tailored to individual patients' infections and physiological conditions at step **4509**. Throughout this process, the system provides ongoing monitoring and adaptive recommendations, continuously refining its models and predictions based on new data and observed outcomes.

[0628] As an example, consider using the phage dynamics analysis system to develop a personalized phage therapy for a patient with a multi-drug resistant *Pseudomonas aeruginosa* infection. The system would start by analyzing the genomic data of the patient's *P. aeruginosa* strain, identifying potential phage binding sites and virulence factors. It would then process cryo-EM data of relevant phages and the bacterial strain, providing structural insights into their potential interactions.

[0629] The nonlinear gene expression simulator would model how the bacteria might respond to phage infection, including potential defense mechanisms like the recently discovered DRT2 system. The phage-bacteria dynamics simulator would then model how different phages might interact with this specific bacterial strain, predicting infection rates and bacterial clearance under various conditions.

[0630] Using the cross-resistance predictor, the system would assess the risk of the bacteria developing resistance to the proposed phage therapy, as well as potential impacts on antibiotic susceptibility. The recursive protein design optimizer might then be employed to engineer a cocktail of phages optimized for this specific bacterial strain, enhancing their ability to overcome bacterial defenses.

[0631] The phage-tissue interaction modeler would simulate how this phage cocktail might affect

the patient's lung tissue (assuming a respiratory infection), ensuring the therapy doesn't cause unintended damage. The societal impact simulator would consider the broader implications of using this novel phage therapy, such as its potential impact on hospital microbiomes if widely adopted.

[0632] Finally, the phage therapy protocol optimizer would integrate all this information to design a personalized treatment plan, specifying the composition of the phage cocktail, dosing schedule, and administration method. This plan would be adaptive, with recommendations for real-time monitoring and potential adjustments based on the patient's response.

[0633] This comprehensive approach would enable the development of a highly targeted, effective, and safe phage therapy, potentially offering a life-saving treatment option for a patient with an otherwise untreatable infection. The system's ability to rapidly analyze, simulate, and optimize phage therapies represents a significant advancement in the field of personalized medicine for infectious diseases.

[0634] FIG. **46** is a flow diagram illustrating an exemplary method **4600** for applying epidemiological analysis, according to an embodiment. According to the embodiment, the process begins at step **4601** with the collection and integration of diverse data from multiple sources, including, but not limited to, public health databases, clinical reports, environmental sensors, and social media. At step **4602** this comprehensive data is used to generate multi-scale disease transmission models, spanning from cellular-level interactions to global population dynamics. At step **4603** the system continuously analyzes real-time data streams to detect potential outbreak signals, employing advanced pattern recognition algorithms to identify anomalies that might indicate emerging health threats.

[0635] Based on these models and real-time data, the system predicts disease spread patterns and assesses risks at various geographical and temporal scales at step **4604**. At step **4605** it simulates multiple intervention strategies, such as vaccination campaigns, travel restrictions, or social distancing measures, optimizing them for maximum effectiveness and minimal societal disruption. At step **4606**, the system provides personalized risk assessments and recommendations to individuals, considering factors like location, health status, and behavior patterns.

[0636] According to an aspect of this method, it incorporates neuro-immune response modeling at step **4607**, simulating how individual physiological reactions to infection influence population-level disease dynamics. At step **4608** the system generates and analyzes various future outbreak scenarios, enabling long-term planning and preparedness. Throughout the process, the system visualizes results and generates detailed reports for different stakeholders at step **4609**, from policymakers to healthcare providers. Additionally, the method involves continuous updating and refinement of its models based on new data and observed outcomes, ensuring that the system's predictive power and accuracy improve over time.

[0637] As an example, consider using the epidemiological analysis system to manage a novel influenza outbreak. The system would start by integrating data from various sources, including hospital admission rates, viral surveillance from wastewater testing, social media trends indicating flu-like symptoms, and environmental data on temperature and humidity. Using this data, it would generate multi-scale models of influenza transmission, from the cellular level (modeling how the virus interacts with human respiratory cells) to the population level (simulating spread through communities and regions).

[0638] The system would continuously monitor these data streams, and might detect an unusual spike in flu-like symptoms in a particular city, triggering an early warning. It would then predict the likely spread of the outbreak, considering factors like population density, travel patterns, and seasonal influences. Based on these predictions, the system would simulate various intervention strategies, such as targeted vaccination campaigns or temporary school closures, optimizing for both effectiveness in controlling the outbreak and minimizing economic and social disruption.

[0639] At the individual level, the system might provide personalized risk assessments and

recommendations. For instance, it could advise high-risk individuals in affected areas to avoid large gatherings or suggest optimal times for vaccination based on local virus activity and individual health status.

[0640] The system would also model how the neuro-immune response to influenza (e.g., fatigue and social withdrawal) might influence the outbreak's trajectory. It might find that these natural sickness behaviors significantly slow the spread in some communities, informing public health messaging strategies.

[0641] Throughout the outbreak, the system would generate future scenarios, such as potential mutations of the virus or its spread to new regions, allowing health authorities to prepare proactively. It would continuously update its models based on the actual progression of the outbreak and the effectiveness of interventions, improving its predictive accuracy for future events.

[0642] This comprehensive approach enables a more nuanced, responsive, and effective management of the influenza outbreak, potentially reducing its impact through early detection, optimized interventions, and personalized risk management.

[0643] FIG. **47** is a flow diagram illustrating an exemplary method **4700** for ecosystem-level analysis in cancer, according to an embodiment. According to the embodiment, the process begins at step **4701** with the comprehensive collection and integration of multi-omics data from tumor samples. This includes genomic, transcriptomic, proteomic, and metabolomic information, as well as data on the tumor microenvironment. Using this integrated data, the system generates at step **4702** a detailed cellular ecosystem model of the tumor, representing the diverse cell populations and their interactions within the tumor microenvironment.

[0644] At step **4703** the system simulates intra-tumor heterogeneity and cell-cell interactions using the GLV equations, modeling how different cancer cell subpopulations, stromal cells, and immune cells compete, cooperate, and evolve within the tumor ecosystem. This simulation captures the dynamic nature of tumor progression and helps identify key drivers of tumor growth and potential vulnerabilities.

[0645] At step **4704** the analysis of immune system interactions within the tumor ecosystem is performed. The system can model how various immune cell types infiltrate the tumor, interact with cancer cells, and potentially become suppressed or exhausted. This provides insights into immune evasion mechanisms and opportunities for enhancing anti-tumor immune responses.

[0646] Based on these simulations, the system predicts tumor evolution and treatment responses at step **4705**. It forecasts how the tumor ecosystem might change over time under different conditions, including various treatment scenarios. This predictive capability is essential for anticipating treatment resistance and identifying effective therapeutic strategies.

[0647] At step **4706** the system simulates and optimizes combination therapies, considering how different treatment modalities might synergistically disrupt the tumor ecosystem. This could involve combinations of targeted therapies, immunotherapies, and conventional treatments like chemotherapy or radiation.

[0648] At step **4707** advanced imaging data is integrated into the analysis, providing spatial information about the tumor ecosystem. This could include data from techniques like spatial transcriptomics or multiplex immunohistochemistry, allowing for a more precise mapping of cellular interactions within the tumor.

[0649] Using all this information, the system generates personalized treatment strategies tailored to the specific characteristics of each patient's tumor ecosystem at step **4708**. These strategies are designed to maximally disrupt the tumor ecosystem while minimizing harm to healthy tissues.

[0650] The method includes ongoing monitoring and adaptive treatment recommendations at step **4709**. As new data becomes available during treatment, the system continuously updates its models and adjusts treatment recommendations accordingly. This adaptive approach allows for real-time optimization of cancer therapy based on the evolving tumor ecosystem.

[0651] Throughout this process, the system continuously refines its models based on new data and

observed outcomes, improving its predictive accuracy and therapeutic recommendations over time.

[0652] As an example, consider using the ecosystem-level analysis system for a patient with advanced triple-negative breast cancer. The system would start by integrating multi-omics data from the patient's tumor biopsy, including single-cell RNA sequencing data to capture cellular heterogeneity. It would generate a cellular ecosystem model of the tumor, identifying multiple cancer cell subpopulations with different gene expression profiles, as well as various stromal and immune cell types.

[0653] Using the GLV simulator, the system would model how these different cell populations interact and compete within the tumor microenvironment. It might identify a highly proliferative cancer cell subpopulation that suppresses local immune cell activity. The immune-disease ecosystem interaction simulator would then model how different immunotherapy approaches might alter this dynamic.

[0654] The system would predict how the tumor ecosystem might evolve under different treatment scenarios. It might simulate that a combination of a CDK4/6 inhibitor (to target the proliferative subpopulation) and an immune checkpoint inhibitor (to reinvigorate suppressed immune cells) could effectively disrupt the tumor ecosystem.

[0655] The quantum-enhanced medical image analyzer would process the patient's PET-CT scans, providing spatial information about tumor heterogeneity and metabolic activity. This information would be used to refine the tumor ecosystem model and treatment predictions.

[0656] Based on all these analyses, the ecosystem-based personalized treatment optimizer would generate a tailored treatment plan. This might involve a specific sequencing of the CDK4/6 inhibitor and immunotherapy, along with recommendations for dosing and scheduling to maximize disruption of the tumor ecosystem.

[0657] As treatment progresses, the system would continuously monitor the patient's response through blood-based biomarkers and imaging, updating its model of the tumor ecosystem and adjusting treatment recommendations as needed. This might involve suggesting the addition of a third agent if resistance begins to emerge in a specific cancer cell subpopulation.

[0658] This comprehensive, adaptive approach would enable more precise and effective cancer treatment, potentially improving outcomes for this patient with a typically aggressive form of breast cancer. By considering the full complexity of the tumor ecosystem, the system can identify and exploit vulnerabilities that might be missed by more traditional approaches to cancer therapy.

[0659] FIG. **48** is a flow diagram illustrating an exemplary method **4800** for ecosystem-level analysis in endometriosis, according to an embodiment. According to the embodiment, the process begins at step **4801** with the comprehensive collection and integration of multi-omics data from endometriotic lesions and patient samples. This may comprise genomic, transcriptomic, proteomic, and metabolomic information, as well as data on the lesion microenvironment and systemic factors like hormone levels. Using this integrated data, the system generates a detailed cellular ecosystem model of the endometriotic lesions at step **4802**, representing the diverse cell populations (including endometrial-like epithelial and stromal cells, immune cells, and surrounding tissue cells) and their interactions within the lesion microenvironment.

[0660] At step **4803** the system then simulates lesion heterogeneity and cell-cell interactions using advanced modeling techniques, capturing the dynamic nature of endometriosis progression. This simulation helps identify key drivers of lesion growth, factors contributing to pain and inflammation, and potential vulnerabilities that could be targeted therapeutically.

[0661] At step **4804** the system performs analysis of immune system interactions within the endometriosis ecosystem. The system models how various immune cell types interact with endometriotic cells, contribute to inflammation, and potentially perpetuate the disease. This provides insights into immune dysregulation mechanisms and opportunities for modulating the immune response to treat endometriosis.

[0662] Based on these simulations, the system predicts lesion evolution and treatment responses at

step **4805**. It forecasts how the endometriosis ecosystem might change over time under different conditions, including various treatment scenarios. This predictive capability is essential for anticipating treatment efficacy and identifying effective therapeutic strategies.

[0663] At step **4806** the system simulates and optimizes hormone-based and/or targeted therapies, considering how different treatment modalities might disrupt the endometriosis ecosystem. This may comprise combinations of hormonal treatments, anti-inflammatory agents, and novel targeted therapies aimed at specific cellular or molecular components of the lesions.

[0664] Advanced imaging data is integrated into the analysis at step **4807**, providing spatial information about the endometriosis ecosystem. This may comprise data from techniques like high-resolution MRI or specialized ultrasound, allowing for a more precise mapping of lesion locations, sizes, and characteristics.

[0665] Using all this information, the system generates personalized treatment strategies tailored to the specific characteristics of each patient's endometriosis ecosystem at step **4808**. These strategies are designed to effectively manage symptoms, slow lesion growth, and potentially promote lesion regression while minimizing side effects.

[0666] The method comprises at step **4809** ongoing monitoring and adaptive treatment recommendations. As new data becomes available during treatment, the system continuously updates its models and adjusts treatment recommendations accordingly. This adaptive approach allows for real-time optimization of endometriosis therapy based on the evolving disease ecosystem and patient response. Throughout this process, the system continuously refines its models based on new data and observed outcomes, improving its predictive accuracy and therapeutic recommendations over time.

[0667] As an example, consider using the ecosystem-level analysis system for a patient with severe, recurrent endometriosis who has not responded well to conventional treatments. The system would start by integrating multi-omics data from the patient's lesion biopsies, including single-cell RNA sequencing data to capture cellular heterogeneity. It would also incorporate data from blood tests, including hormone levels and inflammatory markers.

[0668] The system would generate a cellular ecosystem model of the patient's endometriotic lesions, identifying multiple cell populations including endometrial-like epithelial and stromal cells, various immune cell types, and surrounding tissue cells. Using the GLV simulator, it would model how these different cell populations interact and contribute to lesion growth and symptoms.

[0669] The immune-disease ecosystem interaction simulator would model the complex immune dysregulation in the patient's endometriosis, perhaps identifying an overactive population of pro-inflammatory macrophages contributing to pain and lesion persistence. The system might predict that a combination of a hormonal treatment to suppress lesion growth and a targeted therapy to modulate macrophage activity could effectively disrupt the endometriosis ecosystem.

[0670] The quantum-enhanced medical image analyzer would process the patient's MRI scans, providing detailed spatial information about lesion locations, sizes, and characteristics. This information would be used to refine the endometriosis ecosystem model and treatment predictions, perhaps identifying deep infiltrating lesions that require special consideration in treatment planning.

[0671] Based on all these analyses, the ecosystem-based personalized treatment optimizer would generate a tailored treatment plan. This might involve a specific combination of a GnRH antagonist to suppress estrogen production, a novel macrophage-modulating agent, and a carefully timed surgical intervention for the deep infiltrating lesions. The system would also recommend lifestyle modifications and complementary therapies based on their predicted impact on the patient's endometriosis ecosystem.

[0672] As treatment progresses, the system would continuously monitor the patient's response through symptom tracking, blood-based biomarkers, and imaging, updating its model of the endometriosis ecosystem and adjusting treatment recommendations as needed. This might involve

suggesting changes in hormone therapy dosing or the addition of a new targeted therapy if certain aspects of the disease ecosystem show signs of resistance to the current treatment.

[0673] This comprehensive, adaptive approach would enable more precise and effective endometriosis treatment, potentially improving outcomes for this patient with severe, recurrent disease. By considering the full complexity of the endometriosis ecosystem, including its interactions with the patient's immune system and hormonal environment, the system can identify and exploit therapeutic opportunities that might be missed by more traditional approaches to endometriosis management.

[0674] FIG. **49** is a flow diagram illustrating an exemplary method **4900** for AI-image analysis in histology and pathology, according to an embodiment. According to the embodiment, the process begins at step **4901** with the acquisition and preprocessing of high-resolution histopathology images and corresponding spatial-omics data (e.g., spatially-aligned 'omics data). This may comprise standardizing image quality, correcting for batch effects, and ensuring proper alignment of spatial-omics data with histological features. At step **4902** the system can integrate these multi-modal data types, carefully preserving the spatial context of molecular information within the tissue architecture.

[0675] At step **4903**, the preprocessed images are analyzed using deep learning models, typically convolutional neural networks or vision transformers, to extract relevant features and classify various cellular structures and abnormalities. This analysis provides a detailed characterization of the tissue microenvironment, identifying different cell types, their spatial arrangements, and any pathological changes.

[0676] Based on this integrated and analyzed data, the system generates comprehensive cellular ecosystem models at step **4904**. These models capture the complex interactions between different cell types and molecular factors within the tissue context. At step **4905** the system performs longitudinal analysis. This may comprise creating space-time stabilized models that account for changes in tissue structure and cellular composition over time. This step is important for tracking disease progression or treatment response at the cellular level.

[0677] Using these models, the system predicts disease progression at multiple scales at step **4906** from cellular changes to overall tissue-level effects. This multi-scale prediction provides a comprehensive view of how the disease might evolve over time. The system then leverages these predictions and spatial-omics insights to optimize treatment strategies at step **4907**, simulating how different interventions might affect the disease ecosystem.

[0678] To provide a more complete picture, the method incorporates environmental and lifestyle factors into its analysis at step **4908**, creating holistic patient models that consider the broader context of a patient's health. At step **4909**, the system synthesizes all this information to provide AI-assisted diagnostic support to pathologists, offering insights, highlighting regions of interest, and suggesting potential diagnoses. Throughout this process, the system continuously updates and refines its models based on new data and expert feedback, ensuring that it remains at the cutting edge of pathological analysis.

[0679] As an example, consider using the AI image analysis system for analyzing a series of breast cancer biopsy samples. The process would start by integrating high-resolution H&E-stained histology images with spatial transcriptomics data from the same tissue sections. The histopathology image analyzer would process these images, identifying different cell types, including various cancer cell populations, immune cells, and stromal cells. It would also detect and classify specific features like mitotic figures, nuclear pleomorphism, and tubule formation, which are crucial for cancer grading.

[0680] Simultaneously, the spatial-omics data integrator would align the transcriptomics data with the histological features, creating a comprehensive map of gene expression patterns across the tissue. The tumor microenvironment simulator would then use this integrated data to model the interactions between different cell populations, simulating how cancer cells interact with immune

cells and how this varies across different regions of the tumor.

[0681] For a patient with multiple biopsies over time, the space-time stabilized modeling engine would align these different time points, creating a model of how the tumor has evolved. This might reveal areas of the tumor that have become more aggressive or developed treatment resistance. The multi-scale disease progression predictor would use this information to forecast how the cancer might progress, potentially identifying areas at high risk of metastasis.

[0682] The spatial-omics based treatment optimizer would then simulate how different treatment options, such as various chemotherapy regimens or targeted therapies, might affect different regions of the tumor. It might, for instance, identify a subpopulation of cells likely to be resistant to the standard treatment but vulnerable to a specific targeted therapy.

[0683] Throughout this process, the holistic patient modeler would incorporate information about the patient's overall health, lifestyle, and environmental exposures, which might influence treatment efficacy or risk of recurrence. Finally, the AI-assisted diagnostic support system would present all these insights to the pathologist in an intuitive interface, highlighting key findings, suggesting a tumor grade and stage, and providing treatment recommendations based on the spatial-omics analysis. This comprehensive approach would enable a much more detailed and nuanced understanding of the patient's cancer than traditional histopathology alone, potentially leading to more accurate prognosis and more effective, personalized treatment strategies.

[0684] FIG. **50** is a flow diagram illustrating an exemplary method **5000** for quantum computing cellular modeling, according to an embodiment. According to the embodiment, the process begins at step **5001** with a clear definition of the cellular system to be studied and the specific modeling objectives. This may comprise identifying the key cellular components, processes, and interactions that need to be simulated, as well as the desired outcomes of the modeling process. Once the scope is defined, the next step **5002** is to prepare and encode the classical cellular data for quantum processing. This step may comprise transforming complex biological data into a format that can be efficiently represented in a quantum system, often using techniques like amplitude encoding or basis encoding.

[0685] With the data prepared, the quantum system is initialized with this encoded cellular information at step **5003**. This step leverages the quantum superposition principle, allowing the system to represent multiple cellular states simultaneously. At step **5004** the system applies specific quantum algorithms tailored for cellular simulation and analysis. These may include, but are not limited to, variational quantum algorithms for optimization problems, quantum Fourier transforms for analyzing periodic behaviors in cellular systems, or quantum phase estimation for determining energy states of molecular interactions within cells.

[0686] After the quantum computations are performed, the next step **5005** is to measure the quantum states and decode the results back into classical information that can be interpreted in the context of cellular biology. This step can be often challenging, requiring careful consideration of measurement strategies to extract meaningful information from the quantum system. The quantum results are then integrated with classical data and AI models at step **5006**. This hybrid approach allows for the quantum-enhanced insights to be contextualized within the broader understanding of cellular biology and leverages classical AI techniques for further analysis.

[0687] The integrated results are then analyzed and interpreted at step **5007**, translating the quantum-enhanced computations into biological insights. This often involves visualization tools and statistical analyses to make sense of the complex data. Based on these interpretations, the model is optimized and refined at step **5008**. This may involve adjusting the quantum algorithms, tweaking the encoding methods, or modifying the integration with classical models to improve accuracy and relevance.

[0688] An important step **5009** in the process is validating the quantum-enhanced model against experimental data. This ensures that the insights gained from quantum computations align with observed biological phenomena and helps in assessing the model's predictive power. Finally, the

process is iterated and scaled to address more complex cellular systems or to explore different aspects of the cellular processes under study.

[0689] As an example, consider using the quantum computing cellular modeling system to simulate and analyze the folding process of a complex protein involved in a neurodegenerative disease. The process would start by defining the specific protein and the aspects of its folding dynamics to be studied. The amino acid sequence and known structural data would be encoded into a quantum state, potentially using a basis encoding scheme where each possible folding configuration is represented by a basis state in the quantum system.

[0690] The quantum simulation engine would then apply a variational quantum algorithm, such as the Variational Quantum Eigensolver, to simulate the protein folding process. This algorithm would leverage quantum superposition to explore multiple folding pathways simultaneously, potentially uncovering folding intermediates that are difficult to detect with classical methods.

[0691] As the simulation progresses, the quantum-classical hybrid optimizer would work in tandem with the VQE to iteratively refine the quantum circuit parameters, guiding the simulation towards the most energetically favorable protein conformations. The results of these quantum simulations would then be measured and decoded, providing a distribution of probable protein conformations and their associated energies.

[0692] These quantum-derived results would be integrated with classical molecular dynamics simulations and existing structural biology data through the quantum-AI hybrid learning module. This module might employ a quantum-enhanced neural network to classify the protein conformations and identify potential misfolding patterns associated with the neurodegenerative disease.

[0693] The quantum-enhanced 3D cellular modeler would then use these results to generate detailed visualizations of the protein's folding landscape, highlighting key intermediates and potential misfolding hotspots. These insights could be useful for understanding the disease mechanism and identifying potential therapeutic strategies.

[0694] Throughout this process, the system would continuously refine its models based on comparisons with experimental data, such as cryo-EM structures or hydrogen-deuterium exchange mass spectrometry results. This iterative approach ensures that the quantum-enhanced simulations remain grounded in biological reality while pushing the boundaries of what can be computationally explored in protein folding dynamics.

[0695] This example illustrates how the quantum computing cellular modeling system can leverage quantum computational advantages to tackle complex biological problems that are challenging for classical methods alone, potentially leading to breakthroughs in our understanding of protein folding and neurodegenerative diseases.

[0696] FIG. **51** is a flow diagram illustrating an exemplary method **5100** for facilitating AI predictive oncology, according to an embodiment. According to the embodiment, the process begins at step **5101** with the comprehensive collection and integration of multi-modal patient data. This may comprise gathering clinical records, genomic profiles, imaging data, and real-time monitoring information from various sources. The clinical-genomic data harmonizer processes this diverse data, standardizing formats and resolving inconsistencies to create a unified patient profile.

[0697] Using this integrated data, the system generates a detailed digital twin of the patient at step **5102**, representing their current health status, cancer characteristics, and relevant physiological parameters. This digital twin serves as a virtual model for subsequent analyses and simulations.

[0698] The multi-token cancer progression model then applies advanced AI algorithms to predict multiple aspects of cancer evolution simultaneously at step **5103**. This model considers various 'tokens' or markers of cancer progression, providing a nuanced forecast of potential disease trajectories. The predictions account for complex interactions between genetic factors, tumor microenvironment, and treatment history.

[0699] Based on these progression predictions, the cancer treatment response simulator runs

multiple simulations to model how different treatment options might affect the patient's specific cancer at step **5104**. This step leverages the AI-enhanced cellular modeling capabilities to predict responses at both cellular and tissue levels.

[0700] The oncology treatment optimizer then processes these simulation results, along with data from previous cases and current research, to generate an optimized, personalized treatment plan at step **5105**. This plan balances predicted efficacy, potential side effects, and patient-specific factors.

[0701] Throughout this process, the oncology ai explainer provides clear, interpretable explanations for the AI's predictions and recommendations at step **5106**. This ensures that oncologists can understand and trust the system's reasoning, facilitating informed decision-making.

[0702] At step **5107** the system validates its predictions against real-world outcomes as they become available, continuously updating and refining its models to improve accuracy. This adaptive learning process allows the system to evolve with new data and research findings. At step **5108** the AI predictive oncology system integrates with existing clinical decision support systems, providing oncologists with AI-driven insights alongside traditional clinical guidelines. Furthermore, the entire process iterates and adapts based on new research, clinical feedback, and emerging treatment options, ensuring that the system remains at the cutting edge of oncology practice.

[0703] As an example, consider using the AI predictive oncology system for a patient newly diagnosed with triple-negative breast cancer (TNBC). The process would start by integrating the patient's clinical data, including tumor biopsy results, imaging studies, and full genomic sequencing, into a comprehensive digital twin. The multi-token cancer progression model would then analyze this data, predicting not just overall tumor growth, but also potential metastatic sites, changes in tumor heterogeneity, and evolving drug resistance patterns.

[0704] The system might identify a high risk of early metastasis to the lungs based on specific genetic markers and the presence of circulating tumor cells. Simultaneously, it could predict the emergence of a drug-resistant subclone within the primary tumor over the next 6-12 months.

[0705] The cancer treatment response simulator would then model various treatment scenarios. It might simulate standard chemotherapy regimens, emerging immunotherapies, and potential combination approaches. The simulation could reveal that while a standard chemotherapy approach might initially shrink the tumor, it's likely to leave behind resistant cells, leading to recurrence. In contrast, a combination of immunotherapy and a targeted agent might result in a more durable response by addressing both the bulk tumor and the potentially resistant subclones.

[0706] Based on these simulations, the oncology treatment optimizer would recommend a personalized treatment plan. This might involve starting with the immunotherapy-targeted agent combination, followed by adaptive monitoring to detect early signs of resistance or metastasis.

[0707] The oncology AI explainer would provide visualizations and explanations for these recommendations, showing how specific genetic markers in the patient's tumor correlate with predicted treatment responses and highlighting the key factors driving the AI's decision-making process.

[0708] As treatment progresses, the system would continuously update its predictions based on the patient's response, potentially suggesting modifications to the treatment plan if new resistance mechanisms emerge or if the patient experiences unexpected side effects.

[0709] This example showcases how the AI predictive oncology system can leverage advanced modeling and AI techniques to provide highly personalized, adaptive cancer care, potentially improving outcomes for patients with aggressive cancers like TNBC.

[0710] FIG. **52** is a flow diagram illustrating an exemplary method **5200** for simulating basal cognition, according to an embodiment. According to the embodiment the process begins at step **5201** with a clear definition of the cellular system to be studied and the specific basal cognition objectives. This may comprise identifying the types of cells involved, their basic properties, and the collective behaviors or problem-solving abilities to be simulated. Once the scope is defined, the

next step **5202** is to initialize a multi-agent cellular environment where each cell is represented as an individual agent with its own set of properties and potential actions.

[0711] A component of the simulation is the implementation of bioelectric signaling mechanisms at step **5203**. This may comprise modeling how cells generate, transmit, and respond to electrical signals, which play a role in coordinating collective behaviors. The system then models individual cell decision-making processes at step **5204**, incorporating factors such as gene expression, protein interactions, and responses to environmental cues.

[0712] With individual cell behaviors established, the simulation focuses on intercellular communication and collective behavior. This step **5205** models how cells share information and coordinate their actions, leading to emergent behaviors at the group level. The system then applies external stimuli or perturbations to the cellular environment at step **5206**, such as changes in nutrient availability, introduction of toxins, or physical disturbances, to observe how the cellular collective responds and adapts.

[0713] As the simulation runs, the system observes and analyzes at step **5207** the emergent behaviors that arise from the collective actions of the cells. This may comprise identifying patterns of self-organization, problem-solving strategies, or adaptive responses to environmental changes. Based on these observations, the model is iteratively refined to better capture the observed behaviors and to explore different scenarios at step **5208**.

[0714] At step **5209** the system validates the simulation against experimental data from real cellular systems exhibiting basal cognition. This ensures that the model's predictions align with observed biological phenomena and helps in assessing the model's accuracy and predictive power. Finally, the validated model is scaled up to simulate larger, tissue-level systems, allowing for the exploration of how basal cognition principles apply at more complex organizational levels.

[0715] As an example, consider using the oncology simulation and regenerative medicine system to simulate basal cognition in the context of wound healing and potential cancer initiation. The process would start by defining a cellular system representing a section of epithelial tissue, including various cell types such as epithelial cells, fibroblasts, and immune cells.

[0716] The multi-agent environment would be initialized, with each cell represented as an agent with properties like position, gene expression profile, and bioelectric potential. The bioelectric communication modeler would simulate the propagation of electrical signals across the tissue, representing the natural bioelectric gradients present in healthy tissue.

[0717] Individual cell behaviors would be modeled, including responses to damage, proliferation, and differentiation. The cellular cooperation breakdown simulator would be used to introduce the potential for some cells to deviate from normal behavior, simulating the early stages of potential cancer formation.

[0718] The simulation would then model how cells communicate and coordinate their actions during the wound healing process. This might involve simulating the release of cytokines, the formation of new blood vessels, and the migration of cells to close the wound. External stimuli, such as the introduction of a wound or carcinogenic factors, would be applied to the system.

[0719] As the simulation progresses, the system would observe emergent behaviors such as the collective migration of cells to close the wound, the formation of new tissue structures, or the potential emergence of aberrant cell growths. The Basal cognition-based disease evolution simulator would analyze how changes in cellular collective behaviors might lead to successful wound healing or, alternatively, the initiation of a tumor.

[0720] The simulation would be iteratively refined based on the observed patterns, potentially adjusting parameters like the strength of bioelectric signaling or the sensitivity of cells to environmental cues. The results would be validated against experimental data on wound healing and early cancer formation in epithelial tissues.

[0721] Finally, the validated model could be scaled up to simulate larger sections of tissue or even entire organs, providing insights into how basal cognition principles influence tissue homeostasis,

repair, and potential disease initiation across different scales.

[0722] This example demonstrates how the oncology simulation and regenerative medicine system can leverage basal cognition principles to provide new insights into complex biological processes like wound healing and cancer initiation, potentially leading to novel therapeutic strategies or early intervention techniques.

[0723] FIG. **53** is a flow diagram illustrating an exemplary method **5300** for advanced image analysis and simulation, according to an embodiment. According to the embodiment, the process begins at step **5301** with the acquisition and preprocessing of multi-modal medical imaging data. This may comprise collecting various types of medical images such as MRIs, CT scans, and ultrasounds, and preparing them for analysis through techniques like noise reduction, normalization, and registration. At step **5302** the system performs AI-driven image analysis using deep learning models to detect anomalies, segment structures, and extract relevant features from the images.

[0724] At step **5303** the imaging results are integrated with other patient health data, including electronic health records, genetic profiles, and lab results. This integration creates a comprehensive view of the patient's health status. Using this integrated data, the system generates a spatiotemporal patient model at step **5304**, representing the patient's physiology and anatomy in a dynamic, time-evolving framework.

[0725] Based on this patient model, the system simulates potential disease progression paths and treatment responses at step **5305**. This may comprise using AI algorithms to predict how the patient's condition might evolve over time under different scenarios. At step **5306** the system optimizes personalized treatment strategies by simulating various interventions and their potential outcomes.

[0726] Throughout this process, the system incorporates real-time patient data from wearable devices and medical equipment at step **5307**, continuously updating the patient model to reflect the most current health status. At step **5308** the system synthesizes insights from multiple medical disciplines, considering all the analyzed data and simulation results to provide a holistic view of the patient's condition.

[0727] At step **5309**, the system visualizes the results and generates comprehensive reports for clinicians. These visualizations might include 3D renderings of anatomical structures, time-lapse simulations of disease progression, and interactive treatment planning tools. The entire process iterates and refines based on clinical feedback and observed outcomes, continuously improving the system's accuracy and effectiveness.

[0728] As an example, consider using the advanced image analysis and simulation system for a patient with suspected early-stage lung cancer. The process would start by ingesting the patient's recent chest CT scans, PET scans, and previous X-rays. The AI-driven image analysis would detect and characterize any suspicious nodules, using convolutional neural networks trained on large datasets of lung cancer images.

[0729] The system would then integrate these imaging results with the patient's smoking history, genetic risk factors, and recent blood test results. Using this comprehensive data, it would generate a spatiotemporal model of the patient's lungs, including the detected nodules and surrounding tissues.

[0730] The disease progression simulator would then model potential growth trajectories of the suspicious nodules, considering factors like their size, shape, and metabolic activity from the PET scan. It might predict, for instance, that one nodule has a 70% chance of becoming malignant within the next year based on its characteristics and the patient's risk factors.

[0731] The treatment response simulator would then model various intervention strategies, such as surgical resection, radiation therapy, or watchful waiting with regular screenings. It might simulate how each approach could affect the patient's lung function and overall health over time.

[0732] Throughout this process, the system could incorporate real-time data from a wearable

device monitoring the patient's respiratory function and physical activity levels. This data could be used to refine the patient model and treatment simulations continuously.

[0733] The multi-disciplinary insight synthesizer would then compile insights from oncology, radiology, and pulmonology perspectives, presenting a comprehensive view of the patient's condition and treatment options.

[0734] Finally, the system would generate visualizations showing the detected nodules, their predicted growth, and the potential outcomes of different treatment approaches. This would be presented to the oncologist through an interactive interface, allowing them to explore different scenarios and make an informed decision about the best course of action for the patient.

[0735] This example demonstrates how the advanced image analysis and simulation system can provide a comprehensive, personalized approach to cancer diagnosis and treatment planning, potentially leading to earlier interventions and more effective treatment strategies.

Exemplary Computing Environment

[0736] FIG. **56** illustrates an exemplary computing environment on which an embodiment described herein may be implemented, in full or in part. This exemplary computing environment describes computer-related components and processes supporting enabling disclosure of computer-implemented embodiments. Inclusion in this exemplary computing environment of well-known processes and computer components, if any, is not a suggestion or admission that any embodiment is no more than an aggregation of such processes or components. Rather, implementation of an embodiment using processes and components described in this exemplary computing environment will involve programming or configuration of such processes and components resulting in a machine specially programmed or configured for such implementation. The exemplary computing environment described herein is only one example of such an environment and other configurations of the components and processes are possible, including other relationships between and among components, and/or absence of some processes or components described. Further, the exemplary computing environment described herein is not intended to suggest any limitation as to the scope of use or functionality of any embodiment implemented, in whole or in part, on components or processes described herein.

[0737] The exemplary computing environment described herein comprises a computing device **10** (further comprising a system bus **11**, one or more processors **20**, a system memory **30**, one or more interfaces **40**, one or more non-volatile data storage devices **50**), external peripherals and accessories **60**, external communication devices **70**, remote computing devices **80**, and cloud-based services **90**.

[0738] System bus **11** couples the various system components, coordinating operation of and data transmission between those various system components. System bus **11** represents one or more of any type or combination of types of wired or wireless bus structures including, but not limited to, memory busses or memory controllers, point-to-point connections, switching fabrics, peripheral busses, accelerated graphics ports, and local busses using any of a variety of bus architectures. By way of example, such architectures include, but are not limited to, Industry Standard Architecture (ISA) busses, Micro Channel Architecture (MCA) busses, Enhanced ISA (EISA) busses, Video Electronics Standards Association (VESA) local busses, a Peripheral Component Interconnects (PCI) busses also known as a Mezzanine busses, or any selection of, or combination of, such busses. Depending on the specific physical implementation, one or more of the processors **20**, system memory **30** and other components of the computing device **10** can be physically co-located or integrated into a single physical component, such as on a single chip. In such a case, some or all of system bus **11** can be electrical pathways within a single chip structure.

[0739] Computing device may further comprise externally-accessible data input and storage devices **12** such as compact disc read-only memory (CD-ROM) drives, digital versatile discs (DVD), or other optical disc storage for reading and/or writing optical discs **62**; magnetic cassettes, magnetic tape, magnetic disk storage, or other magnetic storage devices; or any other medium

which can be used to store the desired content and which can be accessed by the computing device **10**. Computing device may further comprise externally-accessible data ports or connections **12** such as serial ports, parallel ports, universal serial bus (USB) ports, and infrared ports and/or transmitter/receivers. Computing device may further comprise hardware for wireless communication with external devices such as IEEE 1394 ("Firewire") interfaces, IEEE 802.11 wireless interfaces, BLUETOOTH® wireless interfaces, and so forth. Such ports and interfaces may be used to connect any number of external peripherals and accessories **60** such as visual displays, monitors, and touch-sensitive screens **61**, USB solid state memory data storage drives (commonly known as "flash drives" or "thumb drives") **63**, printers **64**, pointers and manipulators such as mice **65**, keyboards **66**, and other devices **67** such as joysticks and gaming pads, touchpads, additional displays and monitors, and external hard drives (whether solid state or disc-based), microphones, speakers, cameras, and optical scanners.

[0740] Processors **20** are logic circuitry capable of receiving programming instructions and processing (or executing) those instructions to perform computer operations such as retrieving data, storing data, and performing mathematical calculations. Processors **20** are not limited by the materials from which they are formed or the processing mechanisms employed therein, but are typically comprised of semiconductor materials into which many transistors are formed together into logic gates on a chip (i.e., an integrated circuit or IC). The term processor includes any device capable of receiving and processing instructions including, but not limited to, processors operating on the basis of quantum computing, optical computing, mechanical computing (e.g., using nanotechnology entities to transfer data), and so forth. Depending on configuration, computing device **10** may comprise more than one processor. For example, computing device **10** may comprise one or more central processing units (CPUs) **21**, each of which itself has multiple processors or multiple processing cores, each capable of independently or semi-independently processing programming instructions based on technologies like complex instruction set computer (CISC) or reduced instruction set computer (RISC). Further, computing device **10** may comprise one or more specialized processors such as a graphics processing unit (GPU) **22** configured to accelerate processing of computer graphics and images via a large array of specialized processing cores arranged in parallel. Further computing device **10** may be comprised of one or more specialized processes such as Intelligent Processing Units, field-programmable gate arrays or application-specific integrated circuits for specific tasks or types of tasks. The term processor may further include: neural processing units (NPUs) or neural computing units optimized for machine learning and artificial intelligence workloads using specialized architectures and data paths; tensor processing units (TPUs) designed to efficiently perform matrix multiplication and convolution operations used heavily in neural networks and deep learning applications; application-specific integrated circuits (ASICs) implementing custom logic for domain-specific tasks; application-specific instruction set processors (ASIPs) with instruction sets tailored for particular applications; field-programmable gate arrays (FPGAs) providing reconfigurable logic fabric that can be customized for specific processing tasks;

[0741] processors operating on emerging computing paradigms such as quantum computing, optical computing, mechanical computing (e.g., using nanotechnology entities to transfer data), and so forth. Depending on configuration, computing device **10** may comprise one or more of any of the above types of processors in order to efficiently handle a variety of general purpose and specialized computing tasks. The specific processor configuration may be selected based on performance, power, cost, or other design constraints relevant to the intended application of computing device **10**.

[0742] System memory **30** is processor-accessible data storage in the form of volatile and/or nonvolatile memory. System memory **30** may be either or both of two types: non-volatile memory and volatile memory. Non-volatile memory **30***a* is not erased when power to the memory is removed, and includes memory types such as read only memory (ROM), electronically-erasable

programmable memory (EEPROM), and rewritable solid state memory (commonly known as "flash memory"). Non-volatile memory **30***a* is typically used for long-term storage of a basic input/output system (BIOS) **31**, containing the basic instructions, typically loaded during computer startup, for transfer of information between components within computing device, or a unified extensible firmware interface (UEFI), which is a modern replacement for BIOS that supports larger hard drives, faster boot times, more security features, and provides native support for graphics and mouse cursors. Non-volatile memory **30***a* may also be used to store firmware comprising a complete operating system **35** and applications **36** for operating computer-controlled devices. The firmware approach is often used for purpose-specific computer-controlled devices such as appliances and Internet-of-Things (IoT) devices where processing power and data storage space is limited. Volatile memory **30***b* is erased when power to the memory is removed and is typically used for short-term storage of data for processing. Volatile memory **30***b* includes memory types such as random-access memory (RAM), and is normally the primary operating memory into which the operating system **35**, applications **36**, program modules **37**, and application data **38** are loaded for execution by processors **20**. Volatile memory **30***b* is generally faster than non-volatile memory **30***a* due to its electrical characteristics and is directly accessible to processors **20** for processing of instructions and data storage and retrieval. Volatile memory **30***b* may comprise one or more smaller cache memories which operate at a higher clock speed and are typically placed on the same IC as the processors to improve performance.

[0743] There are several types of computer memory, each with its own characteristics and use cases. System memory **30** may be configured in one or more of the several types described herein, including high bandwidth memory (HBM) and advanced packaging technologies like chip-on-wafer-on-substrate (CoWoS). Static random access memory (SRAM) provides fast, low-latency memory used for cache memory in processors, but is more expensive and consumes more power compared to dynamic random access memory (DRAM). SRAM retains data as long as power is supplied. DRAM is the main memory in most computer systems and is slower than SRAM but cheaper and more dense. DRAM requires periodic refresh to retain data. NAND flash is a type of non-volatile memory used for storage in solid state drives (SSDs) and mobile devices and provides high density and lower cost per bit compared to DRAM with the trade-off of slower write speeds and limited write endurance. HBM is an emerging memory technology that provides high bandwidth and low power consumption which stacks multiple DRAM dies vertically, connected by through-silicon vias (TSVs). HBM offers much higher bandwidth (up to 1 TB/s) compared to traditional DRAM and may be used in high-performance graphics cards, AI accelerators, and edge computing devices. Advanced packaging and CoWoS are technologies that enable the integration of multiple chips or dies into a single package. CoWoS is a 2.5D packaging technology that interconnects multiple dies side-by-side on a silicon interposer and allows for higher bandwidth, lower latency, and reduced power consumption compared to traditional PCB-based packaging. This technology enables the integration of heterogeneous dies (e.g., CPU, GPU, HBM) in a single package and may be used in high-performance computing, AI accelerators, and edge computing devices.

[0744] Interfaces **40** may include, but are not limited to, storage media interfaces **41**, network interfaces **42**, display interfaces **43**, and input/output interfaces **44**. Storage media interface **41** provides the necessary hardware interface for loading data from non-volatile data storage devices **50** into system memory **30** and storage data from system memory **30** to non-volatile data storage device **50**. Network interface **42** provides the necessary hardware interface for computing device **10** to communicate with remote computing devices **80** and cloud-based services **90** via one or more external communication devices **70**. Display interface **43** allows for connection of displays **61**, monitors, touchscreens, and other visual input/output devices. Display interface **43** may include a graphics card for processing graphics-intensive calculations and for handling demanding display requirements. Typically, a graphics card includes a graphics processing unit (GPU) and video RAM

(VRAM) to accelerate display of graphics. In some high-performance computing systems, multiple GPUs may be connected using NVLink bridges, which provide high-bandwidth, low-latency interconnects between GPUs. NVLink bridges enable faster data transfer between GPUs, allowing for more efficient parallel processing and improved performance in applications such as machine learning, scientific simulations, and graphics rendering. One or more input/output (I/O) interfaces **44** provide the necessary support for communications between computing device **10** and any external peripherals and accessories **60**. For wireless communications, the necessary radio-frequency hardware and firmware may be connected to I/O interface **44** or may be integrated into I/O interface **44**.

[0745] Non-volatile data storage devices **50** are typically used for long-term storage of data. Data on non-volatile data storage devices **50** is not erased when power to the non-volatile data storage devices **50** is removed. Non-volatile data storage devices **50** may be implemented using any technology for non-volatile storage of content including, but not limited to, CD-ROM drives, digital versatile discs (DVD), or other optical disc storage; magnetic cassettes, magnetic tape, magnetic disc storage, or other magnetic storage devices; solid state memory technologies such as EEPROM or flash memory; or other memory technology or any other medium which can be used to store data without requiring power to retain the data after it is written. Non-volatile data storage devices **50** may be non-removable from computing device **10** as in the case of internal hard drives, removable from computing device **10** as in the case of external USB hard drives, or a combination thereof, but computing device will typically comprise one or more internal, non-removable hard drives using either magnetic disc or solid state memory technology. Non-volatile data storage devices **50** may store any type of data including, but not limited to, an operating system **51** for providing low-level and mid-level functionality of computing device **10**, applications **52** for providing high-level functionality of computing device **10**, program modules **53** such as containerized programs or applications, or other modular content or modular programming, application data **54**, and databases **55** such as relational databases, non-relational databases, object oriented databases, NoSQL databases, vector databases, key-value databases, document oriented data stores, and graph databases.

[0746] Applications (also known as computer software or software applications) are sets of programming instructions designed to perform specific tasks or provide specific functionality on a computer or other computing devices. Applications are typically written in high-level programming languages such as C, C++, Scala, Erlang, GoLang, Java, Scala, Rust, and Python, which are then either interpreted at runtime or compiled into low-level, binary, processor-executable instructions operable on processors **20**. Applications may be containerized so that they can be run on any computer hardware running any known operating system. Containerization of computer software is a method of packaging and deploying applications along with their operating system dependencies into self-contained, isolated units known as containers. Containers provide a lightweight and consistent runtime environment that allows applications to run reliably across different computing environments, such as development, testing, and production systems facilitated by specifications such as containerd.

[0747] The memories and non-volatile data storage devices described herein do not include communication media. Communication media are means of transmission of information such as modulated electromagnetic waves or modulated data signals configured to transmit, not store, information. By way of example, and not limitation, communication media includes wired communications such as sound signals transmitted to a speaker via a speaker wire, and wireless communications such as acoustic waves, radio frequency (RF) transmissions, infrared emissions, and other wireless media.

[0748] External communication devices **70** are devices that facilitate communications between computing device and either remote computing devices **80**, or cloud-based services **90**, or both. External communication devices **70** include, but are not limited to, data modems **71** which facilitate

data transmission between computing device and the Internet **75** via a common carrier such as a telephone company or internet service provider (ISP), routers **72** which facilitate data transmission between computing device and other devices, and switches **73** which provide direct data communications between devices on a network or optical transmitters (e.g., lasers). Here, modem **71** is shown connecting computing device **10** to both remote computing devices **80** and cloud-based services **90** via the Internet **75**. While modem **71**, router **72**, and switch **73** are shown here as being connected to network interface **42**, many different network configurations using external communication devices **70** are possible. Using external communication devices **70**, networks may be configured as local area networks (LANs) for a single location, building, or campus, wide area networks (WANs) comprising data networks that extend over a larger geographical area, and virtual private networks (VPNs) which can be of any size but connect computers via encrypted communications over public networks such as the Internet **75**. As just one exemplary network configuration, network interface **42** may be connected to switch **73** which is connected to router **72** which is connected to modem **71** which provides access for computing device **10** to the Internet **75**. Further, any combination of wired **77** or wireless **76** communications between and among computing device **10**, external communication devices **70**, remote computing devices **80**, and cloud-based services **90** may be used. Remote computing devices **80**, for example, may communicate with computing device through a variety of communication channels **74** such as through switch **73** via a wired **77** connection, through router **72** via a wireless connection **76**, or through modem **71** via the Internet **75**. Furthermore, while not shown here, other hardware that is specifically designed for servers or networking functions may be employed. For example, secure socket layer (SSL) acceleration cards can be used to offload SSL encryption computations, and transmission control protocol/internet protocol (TCP/IP) offload hardware and/or packet classifiers on network interfaces **42** may be installed and used at server devices or intermediate networking equipment (e.g., for deep packet inspection).

[0749] In a networked environment, certain components of computing device **10** may be fully or partially implemented on remote computing devices **80** or cloud-based services **90**. Data stored in non-volatile data storage device **50** may be received from, shared with, duplicated on, or offloaded to a non-volatile data storage device on one or more remote computing devices **80** or in a cloud computing service **92**. Processing by processors **20** may be received from, shared with, duplicated on, or offloaded to processors of one or more remote computing devices **80** or in a distributed computing service **93**. By way of example, data may reside on a cloud computing service **92**, but may be usable or otherwise accessible for use by computing device **10**. Also, certain processing subtasks may be sent to a microservice **91** for processing with the result being transmitted to computing device **10** for incorporation into a larger processing task. Also, while components and processes of the exemplary computing environment are illustrated herein as discrete units (e.g., OS **51** being stored on non-volatile data storage device **51** and loaded into system memory **35** for use) such processes and components may reside or be processed at various times in different components of computing device **10**, remote computing devices **80**, and/or cloud-based services **90**.

[0750] In an implementation, the disclosed systems and methods may utilize, at least in part, containerization techniques to execute one or more processes and/or steps disclosed herein. Containerization is a lightweight and efficient virtualization technique that allows you to package and run applications and their dependencies in isolated environments called containers. One of the most popular containerization platforms is containerd, which is widely used in software development and deployment. Containerization, particularly with open-source technologies like Docker and container orchestration systems like Kubernetes, is a common approach for deploying and managing applications. Containers are created from images, which are lightweight, standalone, and executable packages that include application code, libraries, dependencies, and runtime. Images are often built from a Dockerfile or similar, which contains instructions for assembling the

image. Dockerfiles are configuration files that specify how to build a Docker image. Systems like Kubernetes also support containerd or CRI-O. They include commands for installing dependencies, copying files, setting environment variables, and defining runtime configurations. Docker images are stored in repositories, which can be public or private. Docker Hub is an exemplary public registry, and organizations often set up private registries for security and version control using tools such as Hub, JFrog Artifactory and Bintray, Gitlab, Github Packages or Container registries. Containers can communicate with each other and the external world through networking. Docker provides a bridge network by default, but can be used with custom networks. Containers within the same network can communicate using container names or IP addresses.

[0751] Remote computing devices **80** are any computing devices not part of computing device **10**. Remote computing devices **80** include, but are not limited to, personal computers, server computers, thin clients, thick clients, personal digital assistants (PDAs), mobile telephones, watches, tablet computers, laptop computers, multiprocessor systems, microprocessor based systems, set-top boxes, programmable consumer electronics, video game machines, game consoles, portable or handheld gaming units, network terminals, desktop personal computers (PCs), minicomputers, mainframe computers, network nodes, virtual reality or augmented reality devices and wearables, and distributed or multi-processing computing environments. While remote computing devices **80** are shown for clarity as being separate from cloud-based services **90**, cloud-based services **90** are implemented on collections of networked remote computing devices **80**.

[0752] Cloud-based services **90** are Internet-accessible services implemented on collections of networked remote computing devices **80**. Cloud-based services are typically accessed via application programming interfaces (APIs) which are software interfaces which provide access to computing services within the cloud-based service via API calls, which are pre-defined protocols for requesting a computing service and receiving the results of that computing service. While cloud-based services may comprise any type of computer processing or storage, three common categories of cloud-based services **90** are serverless logic apps, microservices **91**, cloud computing services **92**, and distributed computing services **93**.

[0753] Microservices **91** are collections of small, loosely coupled, and independently deployable computing services. Each microservice represents a specific computing functionality and runs as a separate process or container. Microservices promote the decomposition of complex applications into smaller, manageable services that can be developed, deployed, and scaled independently. These services communicate with each other through well-defined application programming interfaces (APIs), typically using lightweight protocols like HTTP, protobuffers, gRPC or message queues such as Kafka. Microservices **91** can be combined to perform more complex or distributed processing tasks. In an embodiment, Kubernetes clusters with containerd resources is used for operational packaging of system.

[0754] Cloud computing services **92** are delivery of computing resources and services over the Internet **75** from a remote location. Cloud computing services **92** provide additional computer hardware and storage on as-needed or subscription basis. Cloud computing services **92** can provide large amounts of scalable data storage, access to sophisticated software and powerful server-based processing, or entire computing infrastructures and platforms. For example, cloud computing services can provide virtualized computing resources such as virtual machines, storage, and networks, platforms for developing, running, and managing applications without the complexity of infrastructure management, and complete software applications over public or private networks or the Internet on a subscription or alternative licensing basis, or consumption or ad-hoc marketplace basis, or combination thereof.

[0755] Distributed computing services **93** provide large-scale processing using multiple interconnected computers or nodes to solve computational problems or perform tasks collectively. In distributed computing, the processing and storage capabilities of multiple machines are leveraged to work together as a unified system. Distributed computing services are designed to

address problems that cannot be efficiently solved by a single computer or that require large-scale computational power or support for highly dynamic compute, transport or storage resource variance over time requiring scaling up and down of constituent system resources. These services enable parallel processing, fault tolerance, and scalability by distributing tasks across multiple nodes.

[0756] Although described above as a physical device, computing device **10** can be a virtual computing device, in which case the functionality of the physical components herein described, such as processors **20**, system memory **30**, network interfaces **40**, NVLink or other GPU-to-GPU high bandwidth communications links and other like components can be provided by computer-executable instructions. Such computer-executable instructions can execute on a single physical computing device, or can be distributed across multiple physical computing devices, including being distributed across multiple physical computing devices in a dynamic manner such that the specific, physical computing devices hosting such computer-executable instructions can dynamically change over time depending upon need and availability. In the situation where computing device **10** is a virtualized device, the underlying physical computing devices hosting such a virtualized computing device can, themselves, comprise physical components analogous to those described above, and operating in a like manner. Furthermore, virtual computing devices can be utilized in multiple layers with one virtual computing device executing within the construct of another virtual computing device. Thus, computing device **10** may be either a physical computing device or a virtualized computing device within which computer-executable instructions can be executed in a manner consistent with their execution by a physical computing device. Similarly, terms referring to physical components of the computing device, as utilized herein, mean either those physical components or virtualizations thereof performing the same or equivalent functions.

[0757] The skilled person will be aware of a range of possible modifications of the various aspects described above. Accordingly, the present invention is defined by the claims and their equivalents.

Claims

1. A computing system for designing personalized cancer vaccines using AI-enhanced cellular modeling and simulation, the computing system comprising: one or more hardware processors configured for: compiling cellular data comprising genomic, transcriptomic, proteomic, and metabolomic information from cancer cells and healthy cells; generating one or more cellular models based on the compiled cellular data; simulating interactions between potential vaccine candidates and the generated cellular models; visualizing and analyzing cellular responses to vaccine candidates across different cellular regions and time points; linking observed cellular responses to known biological pathways and previous research findings; quantifying uncertainty in vaccine efficacy predictions; iteratively optimizing vaccine design based on multiple factors including efficacy, cellular stress, and genetic stability; running multiple in silico experiments testing various combinations of vaccine components; and outputting a personalized cancer vaccine design based on the optimized vaccine design and in silico experiment results.

2. The computing system of claim 1, wherein the one or more hardware processors are further configured for: identifying potential vaccine candidates based on specific cellular characteristics of a patient's cancer cells by inverting the simulation process.

3. The computing system of claim 1, wherein simulating interactions between potential vaccine candidates and the generated cellular models further comprises: predicting off-target interactions and influence on gene expression patterns over time for each vaccine candidate.

4. The computing system of claim 1, wherein the one or more hardware processors are further configured for: incorporating whole-slide imaging data for enhanced cancer subtyping and mutation prediction to refine the generated cellular models.

5. The computing system of claim 1, wherein the one or more hardware processors are further

configured for: generating a comparative analysis of potential treatment options based on predicted health outcomes, quality of life considerations, and economic factors associated with the outputted personalized cancer vaccine design.

6. A computer-implemented method executed on a cellular modeling and simulation platform for designing personalized cancer vaccines using AI-enhanced cellular modeling and simulation, the computer-implemented method comprising: compiling cellular data comprising genomic, transcriptomic, proteomic, and metabolomic information from cancer cells and healthy cells; generating one or more cellular models based on the compiled cellular data; simulating interactions between potential vaccine candidates and the generated cellular models; visualizing and analyzing cellular responses to vaccine candidates across different cellular regions and time points; linking observed cellular responses to known biological pathways and previous research findings; quantifying uncertainty in vaccine efficacy predictions; iteratively optimizing vaccine design based on multiple factors including efficacy, cellular stress, and genetic stability; running multiple in silico experiments testing various combinations of vaccine components; and outputting a personalized cancer vaccine design based on the optimized vaccine design and in silico experiment results.

7. The computer-implemented method of claim 6, further comprising: identifying additional potential vaccine candidates by inverting the simulation process based on specific cellular characteristics of the patient's cancer cells.

8. The computer-implemented method of claim 6, further comprising: predicting off-target interactions and influence on gene expression patterns over time for each vaccine candidate.

9. The computer-implemented method of claim 6, further comprising: refining the generated cellular models by integrating whole-slide imaging data for enhanced cancer subtyping and mutation prediction.

10. The computer-implemented method of claim 6, further comprising: generating a comparative analysis of treatment scenarios to evaluate the final personalized cancer vaccine design against alternative treatment options based on predicted health outcomes, quality of life considerations, and economic factors.

11. A system for designing personalized cancer vaccines using AI-enhanced cellular modeling and simulation, comprising one or more computers with executable instructions that, when executed, cause the system to: compile cellular data comprising genomic, transcriptomic, proteomic, and metabolomic information from cancer cells and healthy cells; generate one or more cellular models based on the compiled cellular data; simulate interactions between potential vaccine candidates and the generated cellular models; visualize and analyze cellular responses to vaccine candidates across different cellular regions and time points; link observed cellular responses to known biological pathways and previous research findings; quantify uncertainty in vaccine efficacy predictions; iteratively optimize vaccine design based on multiple factors including efficacy, cellular stress, and genetic stability; run multiple in silico experiments testing various combinations of vaccine components; and output a personalized cancer vaccine design based on the optimized vaccine design and in silico experiment results.

12. The system of claim 11, wherein the system is further caused to: identify potential vaccine candidates based on specific cellular characteristics of a patient's cancer cells by inverting the simulation process.

13. The system of claim 11, wherein simulating interactions between potential vaccine candidates and the generated cellular models further comprises: predict off-target interactions and influence on gene expression patterns over time for each vaccine candidate.

14. The system of claim 11, wherein the system is further caused to: incorporate whole-slide imaging data for enhanced cancer subtyping and mutation prediction to refine the generated cellular models.

15. The system of claim 11, wherein the system is further caused to: generate a comparative

analysis of potential treatment options based on predicted health outcomes, quality of life considerations, and economic factors associated with the outputted personalized cancer vaccine design.

16. Non-transitory, computer-readable storage media having computer-executable instructions embodied thereon that, when executed by one or more processors of a computing system employing a cellular modeling and simulation platform for designing personalized cancer vaccines using AI-enhanced cellular modeling and simulation, cause the computing system to: compile cellular data comprising genomic, transcriptomic, proteomic, and metabolomic information from cancer cells and healthy cells; generate one or more cellular models based on the compiled cellular data; simulate interactions between potential vaccine candidates and the generated cellular models; visualize and analyze cellular responses to vaccine candidates across different cellular regions and time points; link observed cellular responses to known biological pathways and previous research findings; quantify uncertainty in vaccine efficacy predictions; iteratively optimize vaccine design based on multiple factors including efficacy, cellular stress, and genetic stability; run multiple in silico experiments testing various combinations of vaccine components; and output a personalized cancer vaccine design based on the optimized vaccine design and in silico experiment results.

17. The non-transitory, computer-readable storage media of claim 16, wherein the computing system is further caused to: identify potential vaccine candidates based on specific cellular characteristics of a patient's cancer cells by inverting the simulation process.

18. The non-transitory, computer-readable storage media of claim 16, wherein simulating interactions between potential vaccine candidates and the generated cellular models further comprises: predict off-target interactions and influence on gene expression patterns over time for each vaccine candidate.

19. The non-transitory, computer-readable storage media of claim 16, wherein the computing system is further caused to: incorporate whole-slide imaging data for enhanced cancer subtyping and mutation prediction to refine the generated cellular models.

20. The non-transitory, computer-readable storage media of claim 16, wherein the computing system is further caused to: generate a comparative analysis of potential treatment options based on predicted health outcomes, quality of life considerations, and economic factors associated with the outputted personalized cancer vaccine design.