

Computational Cancer Ecosystems: Artificial Intelligence for Modeling the Tumor Microenvironment and Treatment Response

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ABSTRACT:

Cancer is increasingly recognized as a dynamic ecosystem comprising malignant cells, immune populations, stromal fibroblasts, endothelial cells, extracellular matrix components, vascular networks, microbiota, metabolic pathways, and systemic host responses that collectively influence tumor evolution and therapeutic outcomes. Traditional reductionist approaches often investigate these components independently, limiting comprehensive understanding of tumor biology and treatment response. Recent advances in artificial intelligence (AI), particularly foundation models, multimodal transformers, graph neural networks, self-supervised learning, spatial computing, and generative AI, have enabled the integration of heterogeneous biomedical information into computational representations of the tumor ecosystem. These intelligent systems combine digital pathology, radiological imaging, genomics, transcriptomics, proteomics, metabolomics, spatial multi-omics, single-cell sequencing, laboratory biomarkers, electronic health records, liquid biopsy, and longitudinal clinical data to characterize complex cellular interactions and predict therapeutic response. Computational cancer ecosystems facilitate biomarker discovery, immunotherapy optimization, adaptive treatment planning, digital twin development, and intelligent clinical decision support while advancing systems oncology and precision medicine. Emerging technologies including large language models, retrieval-augmented generation, federated learning, reinforcement learning, explainable artificial intelligence, and agentic AI are further expanding the capabilities of ecosystem-based computational oncology. Despite remarkable progress, important challenges remain regarding multimodal data integration, computational scalability, interpretability, interoperability, regulatory validation, ethical governance, and clinical implementation. This review provides a comprehensive overview of computational cancer ecosystems, emphasizing artificial intelligence methodologies for modeling the tumor microenvironment and predicting treatment response in precision oncology.[1]

Keyword: Tumor microenvironment, Computational oncology, Artificial intelligence, Foundation models, Systems oncology, Multi-omics, Digital pathology, Precision medicine, Treatment response, Clinical decision support.

Received Date: 5 December 2025; **Accepted Date:** 15 December 2025; **Published Date:** 20 December 2025.

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1.Introduction

Cancer is no longer viewed as a disease driven solely by malignant cells but rather as a highly complex biological ecosystem involving

continuous interactions among tumor cells, immune populations, stromal fibroblasts, endothelial cells, extracellular matrix components, vascular networks, metabolites,

signaling molecules, and host physiological systems. These dynamic interactions influence tumor initiation, progression, metastatic dissemination, immune escape, therapeutic resistance, and clinical outcomes.[2]

The tumor microenvironment evolves continuously throughout disease progression, responding to genetic alterations, immune modulation, metabolic adaptation, hypoxia, angiogenesis, therapeutic intervention, and systemic physiological changes. Conventional analytical approaches frequently investigate individual biological components independently, thereby overlooking the systems-level interactions governing tumor behavior.[3]

Artificial intelligence has emerged as a transformative computational technology capable of integrating heterogeneous biomedical information across molecular, cellular, tissue, imaging, and clinical scales into unified representations of the cancer ecosystem. Foundation AI models, graph neural networks, multimodal transformers, and self-supervised learning now enable comprehensive modeling of tumor biology while supporting precision therapeutics and adaptive clinical decision-making.[4]

The convergence of computational oncology, systems biology, and artificial intelligence is therefore redefining precision cancer medicine by enabling holistic characterization of tumor ecosystems and personalized prediction of therapeutic response.[5]

2.Evolution of Computational Cancer Ecosystems

Early cancer research primarily focused on intrinsic characteristics of malignant cells, including histopathological morphology, genetic mutations, and proliferative capacity. Although these discoveries substantially advanced oncology, they provided only a partial understanding of the biological mechanisms governing disease progression and treatment resistance.[6]

Subsequent recognition of the importance of immune responses, stromal remodeling, angiogenesis, extracellular matrix organization,

and cellular communication expanded the conceptual framework toward tumor ecosystem biology. High-throughput sequencing technologies, digital pathology, spatial biology, radiomics, and systems biology further revealed the remarkable complexity of tumor–host interactions.

Artificial intelligence subsequently enabled automated integration of these diverse biomedical datasets, while foundation AI models introduced generalized multimodal representation learning capable of characterizing entire cancer ecosystems rather than isolated biomarkers.[7]

Today, computational cancer ecosystems represent an integrated systems-oncology framework that combines biological complexity with advanced computational intelligence to support personalized cancer care.[8]

3.Principles of Computational Cancer Ecosystems

Computational cancer ecosystems are founded upon the principle that tumor behavior emerges from interactions among numerous interconnected biological components rather than from individual molecular abnormalities. Artificial intelligence serves as the computational engine integrating these diverse biological processes into coherent predictive models.[9]

These systems incorporate genomic sequencing, transcriptomics, proteomics, metabolomics, immunomics, spatial biology, digital pathology, radiological imaging, laboratory biomarkers, liquid biopsy, wearable technologies, and electronic health records into unified computational representations.

Graph neural networks model relationships among malignant cells, immune populations, fibroblasts, endothelial cells, cytokines, extracellular matrix proteins, vascular structures, signaling pathways, therapeutic targets, and clinical outcomes, enabling systems-level reasoning regarding tumor evolution and therapeutic response.[10]

4.Computational Architecture

Modern computational cancer ecosystem platforms consist of multiple interconnected

computational layers responsible for multimodal biomedical data acquisition, preprocessing, biological representation learning, ecosystem modeling, predictive analytics, and intelligent clinical decision support.[11]

The acquisition layer continuously integrates radiological imaging, digital pathology, genomic sequencing, transcriptomics, proteomics, metabolomics, spatial transcriptomics, single-cell sequencing, laboratory investigations, liquid biopsy, wearable physiological monitoring, medication history, and longitudinal electronic health records. Advanced preprocessing pipelines normalize imaging studies, harmonize molecular datasets, encode clinical documentation through natural language processing, and synchronize temporal patient information.

Foundation AI models generate generalized computational embeddings representing molecular biology, cellular populations, tissue architecture, imaging phenotypes, physiological status, and clinical trajectories. Graph neural networks subsequently model dynamic interactions across the tumor ecosystem while supporting predictive systems oncology.[12]

5.Artificial Intelligence for Cellular Ecosystem Modeling

The tumor ecosystem consists of highly heterogeneous cellular populations exhibiting distinct biological functions and continuously evolving interactions. Malignant cells coexist with cytotoxic T lymphocytes, regulatory T cells, macrophages, dendritic cells, natural killer cells, cancer-associated fibroblasts, endothelial cells, adipocytes, and numerous additional stromal components that collectively determine disease progression.[13]

Artificial intelligence integrates single-cell RNA sequencing, multiplex immunohistochemistry, imaging cytometry, spatial transcriptomics, and computational pathology into comprehensive representations of cellular ecosystems. Machine learning identifies biologically significant cellular subpopulations associated with immune escape, metastatic dissemination, angiogenesis, therapeutic resistance, and recurrence.

Graph neural networks characterize communication among neighboring cellular populations, enabling systems-level understanding of tumor-immune interactions while supporting individualized therapeutic strategies.[14]

6.Multi-Omics Integration

Comprehensive characterization of computational cancer ecosystems requires integration of genomics, transcriptomics, proteomics, metabolomics, epigenomics, immunomics, microbiomics, lipidomics, and single-cell sequencing into unified molecular representations of tumor biology.[15]

Foundation AI models utilize multimodal transformers, biological knowledge graphs, and graph neural networks to identify complex relationships among genes, proteins, metabolites, signaling pathways, immune responses, microbiota, and therapeutic targets that remain difficult to identify using conventional analytical approaches.

Integrated multi-omics substantially improves biomarker discovery, molecular subtype classification, therapeutic response prediction, systems biology research, and precision medicine while enabling comprehensive understanding of ecosystem-level biological interactions.[16]

7.Spatial Biology and Digital Pathology

Digital pathology and spatial biology provide high-resolution characterization of tissue architecture and cellular organization within the tumor ecosystem. Whole-slide imaging, spatial transcriptomics, multiplex immunofluorescence, and imaging mass cytometry reveal spatial relationships among malignant cells, immune populations, fibroblasts, vascular structures, and extracellular matrix components.[17]

Foundation AI models trained on large-scale histopathological datasets automatically learn generalized tissue representations while graph neural networks quantify spatial interactions and cellular neighborhoods. These computational approaches identify immune niches, stromal remodeling, angiogenesis, hypoxic regions, and invasion fronts that influence therapeutic response and disease progression.

Integration of spatial biology with molecular profiling substantially strengthens ecosystem modeling while supporting precision oncology and computational pathology.[18]

8.Imaging Intelligence and Ecosystem Phenotyping

Radiological imaging provides macroscopic characterization of the cancer ecosystem by visualizing tumor morphology, vascularity, metabolism, perfusion, heterogeneity, organ involvement, and metastatic dissemination. Artificial intelligence integrates radiomics with digital pathology, genomics, spatial biology, laboratory biomarkers, and clinical outcomes into unified computational representations of ecosystem phenotypes.[19]

Multimodal foundation models identify relationships between imaging characteristics and underlying biological mechanisms, enabling prediction of immune infiltration, molecular alterations, angiogenesis, metabolic activity, and treatment sensitivity directly from non-invasive imaging studies. These integrated ecosystem phenotypes facilitate comprehensive diagnosis, prognostic prediction, therapeutic planning, and longitudinal monitoring throughout the cancer care continuum.[20]

9.Artificial Intelligence for Predicting Treatment Response

One of the principal objectives of computational cancer ecosystems is accurate prediction of therapeutic response through comprehensive modeling of interactions occurring within the tumor microenvironment. Foundation AI models integrate radiological imaging, digital pathology, genomics, transcriptomics, proteomics, metabolomics, spatial biology, laboratory biomarkers, liquid biopsy, and longitudinal clinical information into unified computational representations capable of predicting treatment efficacy across multiple therapeutic modalities.[21]

Unlike conventional predictive models based on isolated biomarkers, ecosystem-based AI simultaneously evaluates immune-cell infiltration, stromal remodeling, angiogenesis, metabolic adaptation, clonal evolution, extracellular matrix

organization, and molecular signaling pathways that collectively determine therapeutic outcomes. These intelligent systems estimate responsiveness to chemotherapy, targeted therapy, endocrine therapy, immunotherapy, radiation therapy, cellular therapies, and multimodal treatment combinations while continuously updating predictions as new clinical information becomes available.

10.Modeling Immunotherapy Response

The remarkable success of immunotherapy has highlighted the importance of accurately characterizing the tumor immune ecosystem. Response to immune checkpoint inhibitors, adoptive cellular therapies, cancer vaccines, and bispecific antibodies depends upon highly dynamic interactions among malignant cells, cytotoxic lymphocytes, macrophages, dendritic cells, fibroblasts, endothelial cells, cytokines, chemokines, and stromal architecture.[22]

Artificial intelligence integrates computational pathology, spatial transcriptomics, immunomics, radiomics, laboratory biomarkers, and clinical outcomes into comprehensive computational models capable of identifying immune phenotypes associated with therapeutic responsiveness and resistance. Graph neural networks simulate communication among immune populations and malignant cells, enabling increasingly accurate prediction of immune activation, immune escape, and long-term clinical benefit.

These ecosystem-based computational models substantially strengthen precision immuno-oncology while supporting individualized therapeutic selection.

11.Digital Twins and Virtual Tumor Ecosystems

Digital twin technology represents one of the most advanced applications of computational cancer ecosystems. AI-powered digital twins integrate molecular biology, cellular interactions, tissue architecture, imaging phenotypes, laboratory biomarkers, treatment history, wearable physiological monitoring, and longitudinal clinical outcomes into continuously evolving virtual representations of individual patients.[23]

These virtual ecosystems remain synchronized with biological tumors throughout diagnosis, treatment, follow-up, and survivorship. Artificial intelligence simulates tumor evolution, immune responses, therapeutic efficacy, drug resistance, recurrence, metastatic dissemination, and treatment-related toxicity before clinical intervention occurs.

Virtual therapeutic simulations allow clinicians to evaluate multiple treatment strategies while optimizing individualized care based upon continuously evolving ecosystem biology.

12.Adaptive Learning and Real-Time Oncology

Cancer ecosystems evolve continuously under selective pressures imposed by therapy, immune surveillance, metabolic adaptation, and genetic instability. Consequently, predictive computational models must also evolve to remain clinically relevant. Continuous learning artificial intelligence enables adaptive refinement of ecosystem models using newly acquired biomedical information throughout patient management.[24]

Longitudinal radiological imaging, digital pathology, circulating tumor DNA, laboratory investigations, wearable physiological monitoring, electronic health records, and patient-reported outcomes are continuously incorporated into computational models that update predictions regarding disease progression, therapeutic response, toxicity, and recurrence.

This adaptive learning framework transforms computational oncology from static prediction toward continuously evolving ecosystem intelligence capable of supporting real-time precision medicine.

13.Intelligent Clinical Decision Support

Computational cancer ecosystems provide the computational foundation for next-generation clinical decision-support systems capable of integrating heterogeneous biomedical information into comprehensive patient-centered recommendations. Imaging studies, digital pathology, molecular diagnostics, laboratory investigations, medication history, wearable technologies, physician documentation, and

evidence-based clinical guidelines are harmonized into unified computational environments supporting multidisciplinary oncology practice.[25]

Interactive clinical dashboards generate individualized diagnostic summaries, ecosystem analyses, molecular interpretations, therapeutic recommendations, toxicity estimates, recurrence predictions, and survival probabilities while facilitating collaboration among oncologists, pathologists, radiologists, surgeons, immunologists, molecular biologists, and computational scientists.

These intelligent systems reduce fragmentation of biomedical information while improving workflow efficiency and evidence-based clinical decision-making.

14.Explainability, Validation, and Ethical Implementation

Despite remarkable advances in ecosystem-based artificial intelligence, successful clinical implementation requires transparency, interpretability, reproducibility, and rigorous validation. Explainable artificial intelligence (XAI) enables clinicians to understand computational reasoning through attention visualization, saliency maps, SHAP (Shapley Additive Explanations), feature attribution analysis, uncertainty estimation, and counterfactual explanations identifying the biological variables responsible for predictive outputs.[26]

Clinical deployment also requires standardized multimodal datasets, interoperable computational infrastructure, prospective multicenter validation, continuous monitoring for algorithmic bias, cybersecurity safeguards, external benchmarking, and compliance with evolving international regulatory frameworks governing AI-enabled healthcare technologies.

Ethical considerations—including patient privacy, informed consent, transparency, accountability, equitable access, and responsible governance—remain fundamental to ensuring trustworthy implementation of computational cancer ecosystem models.

15.Future Perspectives

Future computational cancer ecosystems will increasingly integrate multimodal foundation models, large language models, agentic artificial intelligence, federated learning, reinforcement learning, digital twins, spatial multi-omics, liquid biopsy, Internet of Medical Things (IoMT) technologies, quantum computing, cloud-native healthcare infrastructure, and autonomous clinical reasoning systems into unified intelligent oncology ecosystems.[27]

These next-generation computational platforms will continuously integrate molecular biology, cellular dynamics, tissue architecture, imaging phenotypes, laboratory medicine, wearable physiological monitoring, environmental exposures, electronic health records, and real-world clinical outcomes while autonomously coordinating diagnostic workflows, optimizing therapeutic strategies, generating personalized patient communication, and supporting continuous biomedical evidence synthesis.

Such intelligent ecosystems are expected to transform precision oncology from episodic disease management toward predictive, preventive, adaptive, and continuously learning cancer care.

16. Discussion

Computational cancer ecosystems represent a major paradigm shift in systems oncology by modeling tumors as dynamic biological networks rather than collections of isolated malignant cells. Foundation AI models integrate molecular biology, cellular interactions, tissue architecture, imaging phenotypes, laboratory biomarkers, and longitudinal clinical information into unified computational frameworks capable of supporting precision therapeutics, biomarker discovery, adaptive treatment planning, and intelligent clinical decision support.[28]

Applications spanning computational pathology, radiogenomics, spatial biology, digital twins, immunotherapy optimization, adaptive learning, ecosystem phenotyping, and systems biology illustrate the extraordinary potential of artificial intelligence to transform personalized oncology. Nevertheless, widespread implementation requires continued advances in multimodal data harmonization, explainable artificial intelligence,

computational infrastructure, interoperability, regulatory science, cybersecurity, ethical governance, and multidisciplinary collaboration.

As increasingly comprehensive biomedical datasets become available, ecosystem-based computational oncology is expected to become a cornerstone of future precision cancer medicine.

17. Conclusion

Artificial intelligence is redefining precision oncology by enabling computational cancer ecosystems that integrate molecular, cellular, tissue, imaging, physiological, and clinical information into unified computational representations capable of modeling the tumor microenvironment and predicting treatment response throughout the cancer care continuum.[29]

Advances in foundation models, transformer architectures, graph neural networks, multimodal learning, digital twins, federated learning, reinforcement learning, large language models, agentic AI, and generative artificial intelligence are expected to further strengthen ecosystem-level computational reasoning while enabling increasingly accurate diagnosis, biomarker discovery, therapeutic optimization, continuous disease monitoring, and evidence-based clinical decision-making.

Although important scientific, technical, ethical, regulatory, and implementation challenges remain, sustained collaboration among oncologists, pathologists, radiologists, immunologists, molecular biologists, biomedical engineers, computer scientists, healthcare organizations, and regulatory agencies will accelerate responsible implementation of computational cancer ecosystems. These innovations have the potential to improve patient outcomes, enhance therapeutic precision, reduce healthcare disparities, and establish a new era of intelligent, adaptive, and personalized cancer care worldwide.[30]

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