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Editorial

Virtual cells in intelligent oncology

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The idea of accurately modeling life within a computer is no longer science fiction; it is becoming a reality through the rise of the virtual cell. Over the past few years, fueled by advances in single-cell and spatial omics, artificial intelligence (AI), and high-performance computing, virtual cells have rapidly evolved from abstract concepts into practical tools with the power to reshape biomedical research. Building on earlier, more constrained attempts at integration, today's virtual cells can merge diverse data streams with sophisticated computational models, enabling comprehensive simulations of cellular structure, function, and behavior.[1,2] In doing so, they provide an unprecedented platform for reconstructing and manipulating life and open transformative opportunities for intelligent oncology. The core technical framework, data foundations, and key potential application areas of virtual cells in intelligent oncology are illustrated in Figure 1.

The value of virtual cells lies in their ability to integrate multi-scale modeling, AI, and multi-modal data, thereby reconstructing cellular dynamics and environmental interactions.[3–6] Multi-scale models can span molecular, cellular, and tissue levels to capture the complexity of tumor evolution; AI enables advances in protein structure prediction, signaling pathway modeling, and drug response simulation; and the integration of spatial omics with imaging data allows virtual cells to operate within the tumor microenvironment.[7] Recent advances further expand this paradigm through human-interpretable modeling frameworks, such as a cell behavior hypothesis grammar,[8] which translates plain-language biological rules into executable agent-based models. This both democratizes the construction of virtual cell laboratories and enables *in silico* experiments linking omics-informed hypotheses to mechanistic simulations of tumor–immune dynamics and developmental processes. Compared with conventional experiments, virtual cells offer unparalleled efficiency, reproducibility, and scalability, making them particularly suited to addressing the complexity and dynamic challenges inherent in cancer research.

In the field of intelligent oncology, the potential applications of virtual cells are rapidly emerging:

1. Reconstructing spatiotemporal dynamics in pathology. Conventional pathology relies on static tissue sections, which are unable to capture the continuous process of tumor initiation, tumor progression, and therapeutic responses. Virtual cells can integrate omics and imaging data from multiple time points to reconstruct the dynamic trajectories of tumor cell populations.[9,10] For instance, by simulating metabolic reprogramming under hypoxic conditions, scientists can model tumor progression *in silico*, offering new insights for early intervention.
2. Unraveling the complexity of the tumor microenvironment. Tumor cells do not exist in isolation; they interact with immune cells, fibroblasts, and vascular systems. Virtual cells provide a systems-level approach to studying these interactions.[8] They can predict the impact of signaling pathway perturbations on immune infiltration and simulate the systemic effects of radiotherapy or immunotherapy, thus supporting the design of individualized therapeutic strategies.
3. Accelerating research on drug response and resistance. Traditional laboratory drug testing is time-consuming and costly, whereas AI-driven virtual models generate high-probability hypotheses that are then tested in high-throughput automated labs. This closed-loop cycle of *in silico* prediction followed by experimental validation is dramatically accelerating the pace of cancer drug discovery.[11] By integrating spatial transcriptomics with virtual cell modeling, scientists can forecast drug sensitivities among tumor subpopulations at the individual cell level, thereby optimizing precision medicine strategies.
4. Simulating the dynamic processes of individual cells. By integrating multi-modal and multi-timepoint datasets, they can reconstruct cellular trajectories under exogenous drugs, endogenous genetic mutations, or microenvironmental perturbations and predict continuous state transitions as well as latent intermediate states. This enables scientists to explore how tumor cells enter dormancy under stress, acquire drug resistance through signaling network rewiring,

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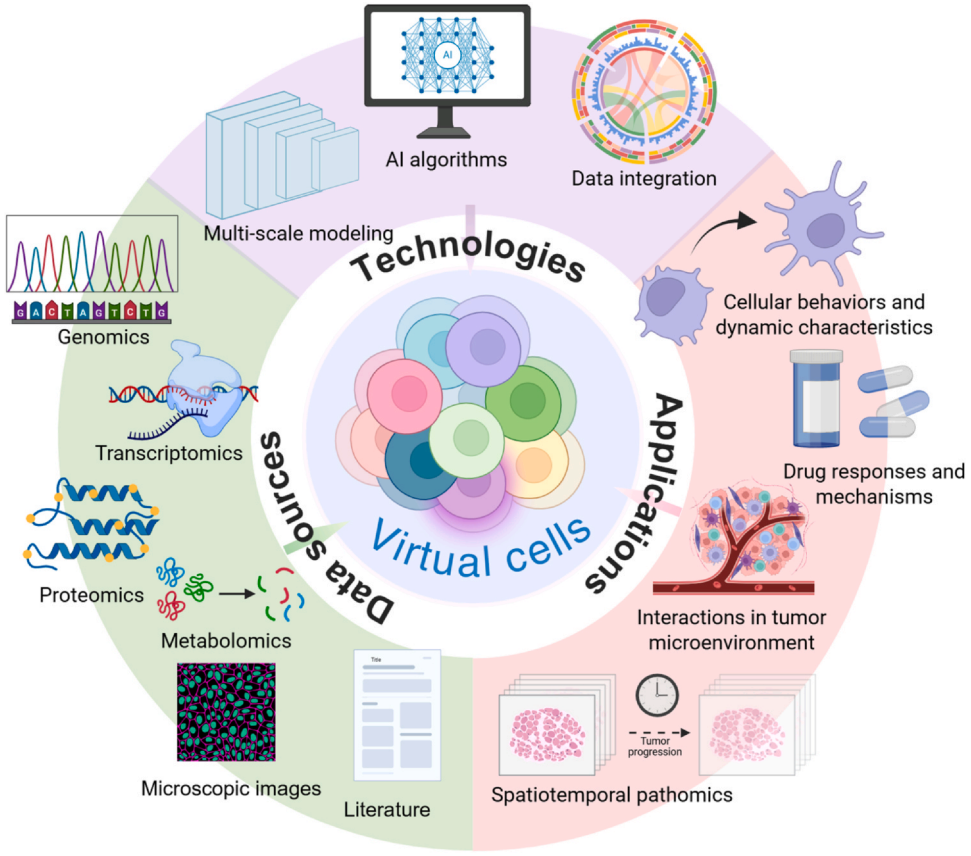


Figure 1. Conceptual framework and potential application scenarios of virtual cells in intelligent oncology.
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or migrate and evolve across ecological niches.[1] Importantly, virtual cells can link molecular mechanisms to phenotypic outcomes, which can help scientists identify the causes of cancer cell behavior and lead to the development of new approaches to therapeutic target discovery and cancer treatments.

Virtual cells are poised to play a critical role in intelligent oncology. The integration of real-time imaging and spatiotemporal pathomics will enhance the fidelity of tumor dynamics modeling. Efforts to establish universal virtual cell models may become a milestone comparable to the Human Genome Atlas Project. Interdisciplinary collaboration and open-source initiatives will accelerate global progress in this field. Virtual cells are driving oncology toward a truly data-driven and computational era.

CRediT authorship contribution statement

Jiarong Deng: Writing – original draft, Conceptualization. **Bo Xu**: Writing – review & editing, Supervision, Conceptualization.

Declaration of Competing Interest

Bo Xu is the Editor-in-Chief of Intelligent Oncology and the authors declare no conflicts of interest.

References

1. Bunne C, Roohani Y, Rosen Y, et al. How to build the virtual cell with artificial intelligence: priorities and opportunities. *Cell.* 2024;187(25):7045–7063.
2. Qian L, Dong Z, Guo T. Grow AI virtual cells: three data pillars and closed-loop learning. *Cell Res.* 2025;35(5):319–321.
3. Zheng L, Shi S, Lu M, et al. AnnoPRO: a strategy for protein function annotation based on multi-scale protein representation and a hybrid deep learning of dual-path encoding. *Genome Biol.* 2024;25(1):41.
4. Rao J, Xie J, Yuan Q, et al. A variational expectation-maximization framework for balanced multi-scale learning of protein and drug interactions. *Nat Commun.* 2024;15(1):4476.
5. Madani A, Krause B, Greene ER, et al. Large language models generate functional protein sequences across diverse families. *Nat Biotechnol.* 2023;41(8):1099–1106.
6. Ashuach T, Gabitto MI, Koodli RV, Saldi GA, Jordan MI, Yosef N. MultiVI: deep generative model for the integration of multimodal data. *Nat Methods.* 2023;20(8):1222–1231.
7. Brancato V, Esposito G, Coppola L, et al. Standardizing digital biobanks: integrating imaging, genomic, and clinical data for precision medicine. *J Transl Med.* 2024;22(1):136.
8. Johnson JAI, Bergman DR, Rocha HL, et al. Human interpretable grammar encodes multicellular systems biology models to democratize virtual cell laboratories. *Cell.* 2025;188(17):4711–4733.e37.
9. Hu D, Jiang Z, Shi J, et al. Histopathology language-image representation learning for fine-grained digital pathology cross-modal retrieval. *Med Image Anal.* 2024;95:103163.
10. Chaurasia AK, Toohey PW, Harris HC, Hewitt AW. Multi-resolution vision transformer model for histopathological skin cancer subtype classification using whole slide images. *Comput Biol Med.* 2025;196(Pt A):110724.
11. Zhang K, Yang X, Wang Y, et al. Artificial intelligence in drug development. *Nat Med.* 2025;31(1):45–59.