Available online at www.sciencedirect.com

ScienceDirect

Current Opinion in Structural Biology

The next revolution in computational simulations: Harnessing AI and quantum computing in molecular dynamics

Anna Lappala

The integration of artificial intelligence, machine learning and quantum computing into molecular dynamics simulations is catalyzing a revolution in computational biology, improving the accuracy and efficiency of simulations. This review describes the advancements and applications of these technologies to process vast molecular dynamics simulation datasets, adapt parameters of simulations and gain insight into complex biological processes. These advances include the use of predictive force fields, adaptive algorithms and quantum-assisted methodologies. While the integration of artificial intelligence and quantum computing with MD simulations provides insightful and stimulating improvements to our understanding of molecular mechanisms, it could introduce new issues related to data quality, interpretability of models and computational complexity. Modern multidisciplinary approaches are needed to navigate these challenges and exploit the potential of these emerging technologies for MD simulations of biomolecular systems.

Addresses
Department of Molecular Biology, Massachusetts General Hospital, Boston, MA 02114, USA

Corresponding author: Lappala, Anna (lappala@molbio.mgh.harvard.edu)

Current Opinion in Structural Biology 2024, **89**:102919

This review comes from a themed issue on **Theory and Simulation/Computational Methods (2024)**

Edited by **Paolo Carloni** and **Karissa Y. Sanbonmatsu**

For complete overview of the section, please refer the article collection - Theory and Simulation/Computational Methods (2024)

Available online 21 September 2024

https://doi.org/10.1016/j.sbi.2024.102919

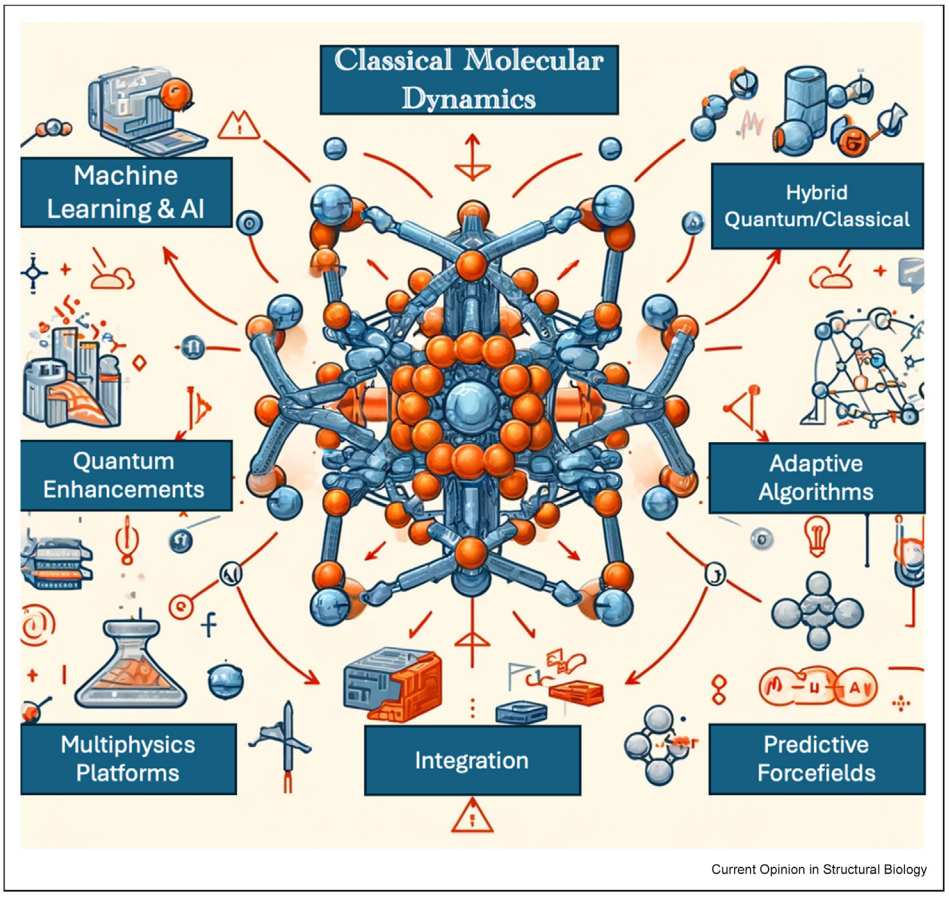
Introduction

The application of cutting-edge computational technologies such as artificial intelligence (AI), machine learning (ML), and quantum computing is revolutionizing the field of molecular dynamics (MD) simulations. These technologies are not simply enhancing existing methodologies— they are fundamentally transforming our approach to computational biology. By streamlining complex data analysis and refining simulation parameters, AI and ML enable researchers to process the extensive datasets generated by MD simulations efficiently, thereby facilitating rapid hypothesis testing and adaptation. This integration is enhancing both the precision and speed of simulations, deepening our understanding of complex biological systems as a result. In this review, we elucidate how AI, ML, and quantum computing are being integrated into MD simulations to accelerate scientific discovery. These advancements provide unprecedented insights into molecular mechanisms and open new avenues for innovation in drug discovery, disease modeling, and fundamental biological research. Furthermore, we address the challenges and complexities involved in integrating these sophisticated computational tools into traditional MD simulation frameworks, emphasizing the need for a multidisciplinary approach to fully realize their potential and overcome inherent limitations. This discussion aims to provide a comprehensive overview of the current state and future directions of AI and quantum-enhanced MD simulations, underscoring their transformative impact on biological modeling and simulation (Figure 1).

Integration with machine learning and artificial intelligence

The integration of ML and AI with MD simulations is not just enhancing existing computational methodologies but is fundamentally changing the field of computational biology [1–3]. AI's capability to automate complex data analysis from simulations is transformational. Typically, MD simulations generate vast amounts of data that can be convoluted and time-consuming to analyze. Machine learning algorithms can rapidly process this data, identifying patterns and relationships that might not be immediately apparent. This automation accelerates the research process, allowing for rapid adjustment of hypotheses. AI and ML are instrumental in optimizing simulation parameters. In traditional MD simulations, selecting appropriate parameters such as time step size, temperature conditions, and force fields can significantly affect the accuracy and efficiency of the simulation. Machine learning models can predict the most effective parameters based on the simulation goals and the characteristics of the molecular system under study. This

Figure 1



An overview of the integration of current and advanced technologies, methods and applications that provide an outlook on potential future developments in biological computer simulations. Partially produced with the assistance of Artificial Intelligence.

optimization not only improves the quality of the simulations but also makes them more computationally efficient, reducing the time and resources needed for extensive trial-and-error testing [4].

One of the most exciting prospects in the integration of AI with MD simulations is the development of predictive force fields. Force fields are physical models that describe the potential energy of a system of atoms, and they are crucial for accurately predicting molecular interactions and behaviors. Traditional force fields are derived from empirical data and theoretical principles, which can limit their accuracy or applicability to novel molecules or conditions not covered by existing data. ML models, trained on large datasets of molecular dynamics simulations, could potentially predict new force fields tailored to specific types of molecules or specific conditions, thereby expanding the scope and accuracy of simulations [5–7].

AI can also contribute to the design of entirely new types of simulations. By analyzing data from a range of simulation types and outcomes, ML algorithms can learn to identify which simulation methods are most effective under various conditions. This capability could lead to the development of adaptive simulation algorithms that dynamically adjust their methods based on real-time results, significantly advancing the field's ability to tackle complex biological problems. The potential of AI and ML to transform MD simulations extends beyond mere efficiency improvements. These technologies could enable entirely new ways of exploring molecular dynamics, leading to deeper insights into biological processes at the molecular level. As these tools become more sophisticated and integrated into computational biology, they promise to unlock scientific discoveries and enhance our understanding of the fundamental mechanisms that govern biological complexity [8].

The integration of machine learning with molecular dynamics simulations has significantly enhanced the precision and efficiency of simulations through various methodologies. For instance, neural network potentials like SchNet and ANI-1 [9], trained on quantum mechanical data, have improved the accuracy of predicting molecular properties, outperforming traditional force fields in certain applications. Enhanced sampling techniques, such as Deep Potential Molecular Dynamics (DPMD) [10], utilize deep learning to generate potential energy surfaces, enabling the study of complex systems like water with quantum-level accuracy. Adaptive simulation algorithms [11], like those used in Adaptive Biasing Force (ABF) and Metadynamics, benefit from reinforcement learning, optimizing parameters in real-time to enhance the exploration of free energy landscapes. Predictive force fields, such as Gaussian Approximation Potentials (GAP) [12], trained on high-fidelity quantum mechanical calculations, have been successfully applied in materials science, providing accurate predictions of complex materials' behaviors under stress. Additionally, self-optimizing force fields like Reactive Force Fields (ReaxFF) have been improved through ML techniques, optimizing parameters in real-time for simulations involving chemical reactions [6]. Quantum-assisted force fields, integrating quantum mechanical calculations with classical force fields in Quantum Mechanical/Molecular Mechanical (QM/MM) approaches, enable dynamic switching between QM and MM treatments, crucial for accurately modeling enzyme reactions [13]. These examples illustrate the transformative impact of integrating ML with MD simulations, enabling new methodologies and unveiling insights previously unachievable.

Integrating machine learning and artificial intelligence with molecular dynamics simulations presents several challenges. A primary concern is the dependency on high-quality, substantial data sets for training AI models; inaccurate or biased training data can lead to flawed predictions, and the computational expense of generating large datasets is significant. Additionally, many ML models lack interpretability, a critical factor in scientific fields where understanding the underlying mechanisms is as important as the outcomes. There is also the risk of overfitting, where models tuned too closely to specific datasets fail to generalize to novel scenarios, limiting their applicability across different molecular systems. Technically and scientifically integrating ML with MD simulations involves layers of complexity. Software and computational frameworks must not only be compatible but also optimized for efficient interaction, which often necessitates extensive development. Moreover, these integrations must respect the fundamental physical and chemical principles that govern molecular dynamics, requiring a deep interdisciplinary expertise.

Resource intensity is another issue; while ML can reduce computational costs by predicting outcomes without full simulations, training sophisticated ML models requires significant computational resources, including high-performance computing systems or graphics processing units (GPUs). Ethical and security concerns also arise, particularly regarding the privacy and security of data, which is especially pertinent when dealing with sensitive or proprietary information. Addressing these multifaceted challenges will require a collaborative approach involving experts in computational biology, machine learning, and ethics to enhance the reliability and applicability of integrated ML-MD tools responsibly.

Enhanced^2 sampling techniques

Enhanced sampling techniques in molecular dynamics simulations are essential for exploring the vast conformational spaces of biological molecules and capturing their dynamic behaviors over biologically relevant timescales. The integration of Artificial Intelligence, Machine Learning, and quantum computing can significantly refine these techniques, leading to more efficient algorithms and more comprehensive exploration strategies.

AI and ML can transform enhanced sampling by introducing adaptive algorithms that adjust sampling parameters in real time based on the outcomes of previous simulations. This adaptive sampling allows the system to "learn" from accumulating data, focusing computational resources on exploring less understood or more critical regions of the conformational space. Furthermore, machine learning models trained on datasets from previous MD simulations can predict likely transition states and identify rare events, guiding the simulations to explore these states more thoroughly. Techniques like principal component analysis (PCA) or t-distributed stochastic neighbor embedding (t-SNE) can be used to reduce the dimensionality of simulation data [14]. Dimensional reduction simplifies complex, high-dimensional data generated by MD simulations, making it easier to identify and interpret key patterns and states. Relating dimensional reduction to Markov State Models (MSM) [15] is particularly valuable, as techniques like time-lagged Independent Component Analysis (tICA) and Uniform Manifold Approximation and Projection (UMAP) [16] can be used to identify slow modes and metastable states, which are fundamental for constructing accurate MSMs. These methods have been increasingly applied in MD simulation analysis for their ability to capture long-timescale dynamics and produce meaningful low-dimensional representations that facilitate the identification of critical conformational states and transitions in complex biomolecular systems.

Quantum computing offers a different set of enhancements to sampling techniques. For instance, quantum-assisted metadynamics can leverage the unique capabilities of quantum computers to calculate the free energy landscapes of molecular systems more efficiently than classical computers. This rapid generation of free energy maps can guide simulations to more relevant conformational changes, avoiding unnecessary computational efforts on well-understood or less significant areas. Quantum metadynamics presents several compelling advantages over classical metadynamics, primarily in accuracy and the ability to incorporate quantum mechanical effects, such as tunneling, electron correlation, and quantum entanglement, which are often inaccessible to classical methods. These quantum effects are particularly important in accurately modeling reactions involving small energy barriers or rare events, where quantum phenomena significantly influence the system's behavior. Moreover, as quantum computing technology progresses, quantum metadynamics is expected to provide considerable speed improvements by enabling the simultaneous exploration of multiple pathways and energy states, reducing the computational time needed to achieve high-resolution free energy landscapes. This could revolutionize the study of complex systems, such as protein folding, enzymatic reactions, and material phase transitions, where both speed and accuracy are critical for gaining deeper insights into the underlying molecular dynamics. Similarly, quantum algorithms could optimize the selection of Monte Carlo moves in hybrid Monte Carlo/MD simulations based on a quantum evaluation of potential energy changes, making informed decisions about exploring conformational space. Moreover, direct quantum simulations of large biological systems can provide a nuanced view of molecular behaviors, especially for quantum mechanical phenomena like electron correlation and tunneling effects that classical simulations do not account for. This could reveal new interactions that are crucial for understanding complex biochemical processes [17,18]. Combining AI/ML with quantum computing, such as through Quantum Machine Learning (QML), could further optimize sampling decisions. A quantum neural network, for example, might be trained to predict the most informative conformational changes, merging the computational power of quantum computing with the predictive capabilities of machine learning. This approach would allow simulations to adapt more effectively, focusing on novel or crucial areas of the conformational space [19,20].

By harnessing AI, ML, and quantum computing, enhanced sampling in molecular dynamics simulations will not only become faster but also more accurate and effective. This synergy is poised to drive significant advancements in computational biology, facilitating discoveries and offering deeper insights into biological processes at the molecular level.

High-performance and quantum computing

Current MD simulation protocols rely on classical computing paradigms and as a result, confront substantial scalability limitations and are not designed to accurately simulate quantum mechanical phenomena due to computational demands that scale exponentially with increases in system size and simulation time-scales. Such constraints not only limit the size of systems that can be studied but also restrict the accuracy and temporal scope of simulations. Quantum computing is poised to revolutionize molecular dynamics simulations. It offers a fundamentally different approach by leveraging the principles of superposition, entanglement, and quantum interference. These features enable quantum computers to perform multiple calculations simultaneously, potentially solving complex problems at speeds unattainable by classical computers which could allow for the simulation of larger and more complex molecular systems over extended timescales with unprecedented precision. Quantum computers are intrinsically capable of modeling quantum phenomena directly, offering a more accurate representation of molecular and chemical reactions. This capability is particularly crucial for advancing our understanding in fields such as drug discovery, where precise knowledge of molecular interactions is essential [21—25]. The integration of existing MD simulation frameworks with emerging quantum computing technologies has already seen some promising developments. For example, hybrid quantum-classical algorithms such as the Variational Quantum Eigensolver (VQE) have been successfully implemented to calculate molecular ground states with higher accuracy and efficiency than purely classical methods [26]. Additionally, Quantum Monte Carlo (QMC) methods have been integrated with MD frameworks to solve many-body problems in materials science, offering insights that are challenging to achieve with classical algorithms alone [27]. Furthermore, Quantum Molecular Dynamics (QMD), which utilizes quantum computers to solve the Schrödinger equation for molecular systems, has provided a more accurate depiction of molecular interactions, advancing our understanding of complex chemical processes [28]. These examples highlight the progress made in combining quantum computing with MD simulations, illustrating how quantum technologies are beginning to enhance the accuracy, scope, and efficiency of molecular simulations.

However, the integration of quantum computing into MD simulations is in its early stages and faces several challenges. Presently, quantum hardware is limited by issues such as low qubit counts, short coherence times, and high error rates, which pose significant obstacles to conducting large-scale and accurate quantum simulations. Furthermore, the development of quantum algorithms that can effectively and efficiently simulate molecular dynamics is an ongoing area of research.

These algorithms must capture the complexity of molecular systems and be robust enough to manage the errors and limitations of early-stage quantum processors [29].

To address potential problems, hybrid systems that combine classical and quantum computing represent a promising direction. In such systems, quantum computers would handle specific tasks that can exploit quantum acceleration— such as calculating the properties of highly complex molecules— while classical computers would manage other aspects of the simulations. This hybrid approach could provide immediate benefits and serve as an intermediary step toward fully quantum MD simulations. Additionally, the development of software and integration tools to bridge existing MD simulation frameworks with emerging quantum computing technologies is critical. Such tools will enable the practical application of quantum computing in the field and help realize its potential to enhance our understanding of molecular systems [13].

Despite the challenges, the advancements in quantum computing hold the promise of significant breakthroughs in molecular dynamics simulations. As technology matures and more robust algorithms and tools are developed, integration of quantum computing into molecular dynamics is expected to become a pivotal driver of scientific innovation and discovery, substantially enhancing our capabilities in molecular biology, pharmacology, and materials science.

Representation of complex environments

The advancement of multiphysics platforms such as COMSOL [30] and ANSYS [31] is significantly enhancing our ability to represent and study complex environments at the cellular level. By integrating different physical processes—mechanical, electrical, and chemical—these platforms allow for a more comprehensive understanding of the multifaceted nature of biological phenomena [32].

Multiphysics simulations are particularly valuable because biological cells are inherently complex systems where various types of physical interactions occur simultaneously and influence each other. For example, the mechanical properties of cellular structures can affect how biochemical reactions proceed; the rigidity or flexibility of a cellular membrane might influence the binding of molecules or the opening and closing of ion channels. Similarly, electrical fields generated by ion gradients across membranes play a crucial role in nerve impulse propagation and can affect the behavior of other charged particles and molecules within the cell [32–34].

One of the key contributions of multiphysics simulations is their ability to model these interactions in a unified framework. This capability is essential for studying phenomena such as electrophoresis, where electrical fields cause the movement of biomolecules, or mechanotransduction, where mechanical stress leads to biochemical responses within the cell. These simulations help to bridge the gap between the microscopic molecular interactions and the macroscopic behaviors observed in biological tissues. Moreover, the crowded and heterogeneous nature of cellular interiors poses additional challenges that multiphysics simulations are uniquely equipped to tackle. In these environments, traditional MD simulations might fail to account for the influence of varied physical forces acting simultaneously. By incorporating multiphysics models, one can simulate molecular behavior in realistically complex conditions. Multiphysics simulations have significantly advanced our understanding of biological systems by demonstrating how molecular crowding impacts biological processes such as protein folding and function, revealing critical insights into cellular processes such as enzyme activity and signal transduction. Furthermore, these simulations have elucidated how changes in pH and ion concentrations influence ion channel gating and the stability of biomolecular complexes, which are essential for maintaining cellular homeostasis and understanding drug interactions.

The future of MD simulations lies in their integration with other types of simulations to create multiscale models that can seamlessly connect atomic-level details provided by MD with larger scales relevant to whole biological systems, such as tissues or even organisms. Multiphysics simulations that incorporate different types of physical processes provide more comprehensive models of biological systems, enabling a deeper understanding of how these systems function under various conditions. Integrating ML and AI with multiphysics platforms like COMSOL or ANSYS could significantly improve the accuracy and efficiency of simulations by automating the complex task of parameter optimization and data analysis across different physical processes. For example, AI algorithms can be used to predict the optimal conditions for simulating interactions between mechanical, electrical, and chemical processes within biological systems, thus reducing the need for extensive trial-and-error testing. Furthermore, ML techniques like dimensionality reduction can simplify the analysis of high-dimensional simulation data, allowing one to focus on the most critical variables influencing system behavior. Quantum computing could further revolutionize multiphysics simulations by providing the computational power needed to model quantum mechanical phenomena directly, which is particularly valuable for accurately simulating complex systems such as molecular interactions in crowded cellular environments. The combination of quantum algorithms with classical multiphysics simulations could enable more precise and scalable models of biological systems, potentially leading to breakthroughs in areas like drug

design, tissue engineering, and understanding fundamental biological processes.

The enhancement of MD simulations through multiphysics platforms represents a significant stride forward in computational biology. It allows for a better representation of the complex cellular environments, leading to more accurate predictions and deeper insights into the fundamental mechanisms that govern biological processes. This approach is paving the way for new scientific discoveries and has profound implications for drug design, disease modeling, and our overall understanding of life at the molecular level.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

No data was used for the research described in the article.

Acknowledgements

The author thanks the generous support from the U.S. Department of Energy, Office of Science, through the Biological and Environmental Research (BER) and the Advanced Scientific Computing Research (ASCR) programs under contract number 89233218CNA000001 and NSF (MCB 2337393).

References

Papers of particular interest, published within the period of review, have been highlighted as:

* of special interest
** of outstanding interest

1. Shah HA, *et al.*: **Review of machine learning methods for the prediction and Reconstruction of metabolic pathways**. *Front Mol Biosci* 2021, **8**, 634141.

2. Pyrkov A, *et al.*: **Quantum computing for near-term applications in generative chemistry and drug discovery**. *Drug Discov Today* 2023, **28**, 103675.

3. Han R, *et al.*: **Revolutionizing medicinal chemistry: the application of artificial intelligence (AI) in early drug discovery**. *Pharmaceuticals* 2023, **16**.

4. Greener JG, Jones DT: **Differentiable molecular simulation can learn all the parameters in a coarse-grained force field for proteins**. *PLoS One* 2021, **16**, e0256990.

5. Chmiela S, *et al.*: **Towards exact molecular dynamics simulations with machine-learned force fields**. *Nat Commun* 2018, **9**, 3887.

6. Mudedla SK, Braka A, Wu S: **Quantum-based machine learning and AI models to generate force field parameters for drug-like small molecules**. *Front Mol Biosci* 2022, **9**, 1002535.

7. Wang Z, *et al.*: **Improving machine learning force fields for molecular dynamics simulations with fine-grained force metrics**. *J Chem Phys* 2023, **159**.

8. Zhang L, *et al.*: **Editorial: combined artificial intelligence and molecular dynamics (AI-MD) methods**. *Front Mol Biosci* 2022, **9**, 1012785.

9. Smith JS, *et al.*: **The ANI-1ccx and ANI-1x data sets, coupled-cluster and density functional theory properties for molecules**. *Sci Data* 2020, **7**, 134.

10. Jia W, *et al.*: *Pushing the limit of molecular dynamics with ab initio accuracy to 100 million atoms with machine learning. SC20: international conference for high performance computing, networking, storage and analysis*. 2020:1–14.

11. Comer J, *et al.*: **The adaptive biasing force method: everything you always wanted to know but were afraid to ask**. *J Phys Chem B* 2015, **119**:1129–1151.

12. * Deringer VL, *et al.*: **Gaussian process regression for materials and molecules**. *Chem Rev* 2021, **121**:10073–10141.
Work by Deringer et al. discusses the application of Gaussian Process Regression in modeling materials and molecules, emphasizing its ability to provide accurate predictions of complex chemical properties and behaviors, thereby advancing computational approaches in materials science and molecular chemistry.

13. * Fedorov DA, *et al.*: **Ab initio molecular dynamics on quantum computers**. *J Chem Phys* 2021, **154**, 164103.
Work by Fedorov et al. presents advancements in ab initio molecular dynamics simulations on quantum computers, highlighting how quantum computing can enhance the accuracy and efficiency of simulating molecular interactions and chemical processes at a fundamental level.

14. Tribello GA, Gasparotto P: **Using dimensionality reduction to analyze protein trajectories**. *Front Mol Biosci* 2019, **6**:46.

15. Schwantes CR, Pande VS: **Improvements in Markov state model construction reveal many non-native interactions in the folding of NTL9**. *J Chem Theory Comput* 2013, **9**: 2000–2009.

16. Sainburg T, McInnes L, Gentner TQ: **Parametric UMAP embeddings for representation and semisupervised learning**. *Neural Comput* 2021, **33**:2881–2907.

17. Ivanov SD, Grant IM, Marx D: **Quantum free energy landscapes from ab initio path integral metadynamics: double proton transfer in the formic acid dimer is concerted but not correlated**. *J Chem Phys* 2015, **143**, 124304.

18. Zhang L, Wang H, E W: **Reinforced dynamics for enhanced sampling in large atomic and molecular systems**. *J Chem Phys* 2018, **148**, 124113.

19. ** Pal S, *et al.*: **Quantum computing in the next-generation computational biology landscape: from protein folding to molecular dynamics**. *Mol Biotechnol* 2024, **66**:163–178.
This work examines the transformative potential of quantum computing in computational biology, specifically highlighting its applications and advancements in complex processes such as protein folding and molecular dynamics simulations.

20. Mazzola G: **Quantum computing for chemistry and physics applications from a Monte Carlo perspective**. *J Chem Phys* 2024, **160**.

21. Chen M, *et al.*: **The emergence of machine learning force fields in drug design**. *Med Res Rev* 2024, **44**:1147–1182.

22. Choudhury C, Arul Murugan N, Priyakumar UD: **Structure-based drug repurposing: traditional and advanced AI/ML-aided methods**. *Drug Discov Today* 2022, **27**:1847–1861.

23. Sajjan M, *et al.*: **Quantum machine learning for chemistry and physics**. *Chem Soc Rev* 2022, **51**:6475–6573.

24. Velmurugan D, Pachaiappan R, Ramakrishnan C: **Recent trends in drug design and discovery**. *Curr Top Med Chem* 2020, **20**: 1761–1770.

25. Yu W, Weber DJ, MacKerell Jr AD: **Computer-Aided drug design: an update**. *Methods Mol Biol* 2023, **2601**:123–152.

26. Peruzzo A, *et al.*: **A variational eigenvalue solver on a photonic quantum processor**. *Nat Commun* 2014, **5**:4213.

27. Boixo S, *et al.*: **Evidence for quantum annealing with more than one hundred qubits**. *Nat Phys* 2014, **10**:218–224.

28. Aspuru-Guzik A, *et al.*: **Simulated quantum computation of molecular energies**. *Science* 2005, **309**:1704–1707.

29. Gong Q, *et al.*: **Simulating chemical reaction dynamics on quantum computer**. *J Chem Phys* 2024, **160**.
** This work explores the use of quantum computers to simulate chemical reaction dynamics, demonstrating the potential of quantum algorithms to accurately model complex chemical processes, which could significantly enhance the understanding and prediction of molecular behaviors beyond the capabilities of classical computing methods.

30. *COMSOL Multiphysics® v. 5.6*. COMSOL AB; 2021.

31. *ANSYS® academic research, release 2021 R2*. ANSYS, Inc; 2021.

32. Sego TJ, *et al.*: **Tissue Forge: interactive biological and biophysics simulation environment**. *PLoS Comput Biol* 2023, **19**, e1010768.
** Tissue Forge is an interactive simulation environment designed for biological and biophysics research. It enables detailed modeling of systems ranging from individual cells to multicellular structures, which facilitates the study of complex biological interactions and phenomena in a versatile and user-friendly platform.

33. Hu M, Ling Z, Ren X: **Extracellular matrix dynamics: tracking in biological systems and their implications**. *J Biol Eng* 2022, **16**:13.
* Work by Hu, Ling, and Ren explores the dynamics of the extracellular matrix within biological systems, discussing the methods for tracking these dynamics and their significant implications for understanding various biological processes and disease mechanisms.

34. Crossley RM, *et al.*: **Modeling the extracellular matrix in cell migration and morphogenesis: a guide for the curious biologist**. *Front Cell Dev Biol* 2024, **12**, 1354132.
* Work by Crossley et al. provides an in-depth guide on modeling the extracellular matrix's role in cell migration and morphogenesis, offering valuable insights for biologists interested in understanding the complex interactions between cellular processes and the extracellular environment.