



# Quantum Computing and Digital Twin in Dentistry: A Potential Emerging Synergy

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## Abstract

The convergence of quantum computing (QC) and digital twin (DT) technology marks a transformative juncture in the evolution of precision dentistry. Digital twins virtual, data-driven replicas of oral structures offer real-time simulation, diagnostics, and personalized treatment planning. This aim of this narrative review is to explore how the synergy between QC and DT can reshape clinical workflows, from modeling craniofacial structures to simulating outcomes of orthodontic, surgical, and restorative procedures. However, their complexity demands significant computational power, which classical systems often cannot meet efficiently. Quantum computing, with its ability to process large datasets through quantum parallelism, provides an ideal solution to this limitation. We examine recent advances in quantum algorithms, such as the Quantum Approximate Optimization Algorithm (QAOA) and quantum machine learning, and their potential to enhance the predictive accuracy of digital twins. Challenges, including ethical considerations, data interoperability, and the current limitations of Noisy Intermediate-Scale Quantum (NISQ) devices, are discussed. By integrating real-time data acquisition with quantum-enhanced analysis, the fusion of DTs and QC could lead to unprecedented levels of personalization in oral healthcare. While still in its infancy, this interdisciplinary synergy holds significant promise for the future of dentistry.

**Keywords:** Quantum computing, Digital twin, Dentistry, Personalized medicine, Craniofacial modeling, Predictive diagnostics, Dental informatics.

## Introduction

The integration of advanced computational paradigms into healthcare is redefining diagnostics, personalized treatment, and predictive modeling. Among these, Digital Twin (DT) technologies have emerged as powerful tools, enabling real-time, data-driven representations of physical entities for simulation, monitoring, and prediction. In parallel, Quantum Computing (QC), though in its nascent stage, promises unprecedented computational speed and efficiency for solving complex problems unapproachable by classical computing. In dentistry, where patient-specific variability and biomolecular intricacies abound, the convergence of DT and QC opens new avenues for precision oral healthcare.

The aims and objectives of this review is to explore the conceptual foundation, current applications, and future potential of merging Quantum Computing with Digital Twins in dentistry, highlighting their complementary capabilities to enhance clinical decision-making, biomaterial research, and patient-specific simulation.

### 1.1 Digital Twin in Dentistry: State of the Art

A Digital Twin is a virtual replica of a physical entity that evolves over

time using real-time data and machine learning. In dentistry, DTs are being increasingly utilized to model craniofacial structures, orthodontic dynamics, prosthodontic workflows, and even periodontal disease progression [3]. Tools like 3Shape TRIOS, Invisalign ClinCheck, and Carestream CS software are enabling the creation of functional DTs using intraoral scans, CBCTs, and facial photographs, offering simulation environments for orthodontic and surgical planning. Current DT applications in dentistry include orthodontic simulation of tooth movement; implantology planning, including bone density modelling; TMJ biomechanical analysis; and caries risk prediction using integrated EHR and imaging data. These platforms rely heavily on computational modeling and real-time data integration. However, the complexity of modeling biochemical, biomechanical, and systemic interactions especially for large datasets or real-time responses places a burden on classical computing resources.

### 1.2 Quantum Computing: Concept and Dental Relevance

Quantum Computing is based on the principles of superposition, entanglement, and quantum interference, allowing it to process complex probabilistic models more efficiently than classical systems. Unlike classical bits, qubits can exist in multiple states simultaneously, enabling

exponential speedup for certain computations such as optimization, machine learning, and molecular modeling [2]. Although not yet mainstream in clinical dentistry, quantum computing shows promise in molecular dynamics simulations for dental biomaterials and adhesives, AI-enhanced diagnostics via quantum-enhanced machine learning, and big-data analytics particularly for genomic, transcriptomic, and oral microbiome data [1][2].

## Clinical Significance of synergy of quantum computing and Digital Twin in dentistry

The convergence of Digital Twin (DT) and Quantum Computing (QC) holds transformative potential for dentistry. Each technology individually offers substantial capabilities: DTs enable personalized, dynamic, and continuously updated simulations of the human craniofacial system; QC offers exponential computational power capable of solving problems that overwhelm classical computers. When integrated, they form a synergistic framework for predictive, optimized, and biologically detailed simulations that can revolutionize dental diagnostics, treatment planning, and research [4].

### 2.1. Predictive Personalized Oral Health Modeling

A core promise of DT in dentistry lies in its ability to create patient-specific models that reflect the biological, functional, and anatomical status of a patient. These models are built using intraoral scans, CBCT data, electronic health records (EHRs), and even genetic and salivary biomarkers. However, incorporating and analyzing such multi-source, high-dimensional data in real time is computationally intense. Here, QC can provide breakthrough capabilities. Using quantum-enhanced machine learning (QML) and quantum support vector machines (QSVM), DTs can integrate diverse datasets from microbiome profiles to occlusal wear patterns to forecast the progression of diseases such as periodontal disease, caries susceptibility, and temporomandibular joint disorders [5]. Quantum algorithms can model these complex interactions with greater depth and reduced computational cost than traditional AI frameworks, potentially allowing real-time risk scoring and simulation of disease trajectories.

### 2.2. Quantum-Aided Biomaterial Design and Dental Drug Discovery

Dental material science is another domain that can benefit from the synergy between DT and QC. Materials like glass ionomers, zirconia ceramics, and composite resins involve complex molecular structures and reactions with the oral environment. Digital twins of these materials can simulate wear, fatigue, and bonding over time under different clinical scenarios. However, classical molecular dynamics simulations can be limited by scale and precision. Quantum computing allows quantum chemistry modeling through algorithms like Variational Quantum Eigensolver (VQE) or Quantum Phase Estimation to predict molecular properties, reactivity, and stability with unmatched accuracy [6,7]. Combined with DTs of the patient’s oral biomechanical environment, QC can help simulate how adhesive molecules interact with etched enamel/dentin, optimize the formulation of bioactive or antimicrobial dental resins, and model long-term degradation of prosthetic materials under pH, temperature, and mechanical load conditions.

### 2.3. Optimizing Orthodontic Mechanics and Treatment Planning

Orthodontics heavily relies on biomechanical modeling of tooth movement and force systems. Existing DT platforms simulate this using finite element methods (FEM) and historical patient data. However, modeling the craniofacial complex including alveolar bone remodeling, periodontal ligament behavior, and anchorage mechanics is extremely

nonlinear and sensitive to biological variability. QC can address these challenges through quantum optimization algorithms, such as the Quantum Approximate Optimization Algorithm (QAOA), to find ideal force vectors and appliance configurations for individual patients, predict root resorption or unintended movement based on simulated biological feedback, and dynamically adjust treatment stages based on intra-treatment digital scans [8].

### 2.4. Real-Time Twin Updates with Quantum Machine Learning

One of the key promises of digital twins is their real-time adaptability i.e., being continuously updated with new patient data during and after treatment. However, streaming large-scale multimodal data (e.g., from intraoral sensors, wearables, environmental logs, or microbiome assays) and updating a simulation in near real-time is a massive computational task. Quantum machine learning (QML) models trained on these data streams can recognize evolving trends in patient behavior or physiology (e.g., bruxism episodes during sleep), update the DT’s internal model to reflect new predictions, and trigger alerts or treatment plan adaptations (e.g., early signs of appliance breakage, changes in pH causing enamel demineralization) [5]. This results in a living digital twin, capable of co-evolving with the patient and offering proactive interventions marking a shift from reactive to anticipatory dentistry.

### 2.5. Multiscale Modeling from Molecules to the Maxillofacial System

Another synergistic frontier lies in multiscale modeling where DTs model the macroscopic anatomy (jaw, teeth, muscles) and QC tackles the microscopic scale (cellular, molecular, genetic). For instance, a DT of a cleft lip/palate patient can include anatomical geometry from CBCT. Simultaneously, a QC engine can simulate genetic mutations affecting osteoblast function. The combined model predicts growth patterns, healing response to grafts, or orthodontic movement stability. This unification could vastly enhance craniofacial anomaly modeling, bone graft planning, and post-surgical prognosis areas where traditional modeling often fails to capture biological variance [4].

### 2.6. Ethical Digital Twins Powered by Secure Quantum Encryption

Patient-specific digital twins raise significant concerns about data privacy and cybersecurity. Quantum computing also contributes through quantum encryption (e.g., Quantum Key Distribution - QKD), ensuring end-to-end secure transmission and storage of health data within DT frameworks. This is particularly critical when dealing with sensitive patient imaging, genetic data, and long-term treatment simulations stored in cloud platforms [4].

#### Summary of Synergistic Applications

Application	Digital Twin Role	Quantum Computing Contribution
Predictive disease modeling	Real-time simulation of oral disease progression	Accelerated machine learning, high-dimensional analysis
Material design and testing	Mechanical and chemical simulation in oral setting	Quantum chemistry for molecular property prediction
Orthodontic force optimization	Biomechanical modeling of tooth movement	Quantum optimization of force vectors and appliance stages

Application	Digital Twin Role	Quantum Computing Contribution
Real-time decision support	Live data updating of treatment models	Quantum learning from streaming patient data
Multiscale anomaly simulation	Macro-scale anatomy tracking	Micro/molecular level biological modeling
Data security	Patient-specific dynamic models	Quantum encryption of health records and simulations

This synergy is not hypothetical. As cloud-based QC services (e.g., IBM Q, Google Sycamore, D-Wave) become more accessible and hybrid classical-quantum models evolve, the implementation of quantum-enhanced dental digital twins is no longer a distant dream but a research frontier rapidly coming into focus.

Future Directions and Limitations

The convergence of quantum computing and digital twin technology offers an exciting frontier in dentistry, yet its clinical realization remains distant. Multiple challenges technical, infrastructural, and ethical must be addressed before this vision can move from theory to practice. A central obstacle is the immaturity of quantum hardware. Current quantum processors, limited by short coherence times, low qubit counts, and high error rates, belong to the Noisy Intermediate-Scale Quantum (NISQ) era [8]. These limitations hinder complex simulations required for real-time, clinically relevant digital twins. While platforms like IBM and Google offer cloud-based quantum access, they are not yet capable of supporting robust, large-scale dental applications such as quantum-enhanced orthodontic planning or biomaterial modeling. Data integration presents another major barrier. Dentistry relies on highly heterogeneous data 3D imaging, radiographs, genomics, microbiome profiles, and lifestyle metrics often stored in siloed, non-standardized formats. Building a dynamic, quantum-compatible digital twin requires seamless interoperability, standardized ontologies, and redesigned data pipelines, which are currently lacking [9]. An equally pressing challenge is the lack of interdisciplinary expertise. Dental professionals typically have minimal exposure to quantum computing, while quantum scientists are unfamiliar with clinical workflows and biological systems. Bridging this divide will require joint training programs, translational research hubs, and cross-sector collaboration. Regulatory and ethical concerns further complicate implementation. As digital twins incorporate predictive analytics, including genomic and behavioral data, issues of data privacy, consent, and algorithmic transparency become critical. The opaque nature of quantum algorithms raises questions about clinical accountability and trust. Establishing frameworks for explainability and governance is essential for responsible deployment [10]. Despite these hurdles, progress in adjacent fields such as quantum-assisted protein folding and cardiovascular digital twins indicates feasibility. Dentistry, already advancing in digital diagnostics and treatment planning, is poised to adopt modular quantum subroutines that enhance tasks like image segmentation, aligner staging, or implant optimization. These incremental applications can pave the way for broader adoption. Looking ahead, the future lies in secure, cloud-based ecosystems where a patient’s digital twin is continuously updated with sensor data and clinical inputs. Quantum computing would be dynamically employed to simulate treatment outcomes, predict complications, and personalize care. Such integration could shift dentistry from reactive interventions to predictive and preventive strategies. While significant challenges remain, the transformative potential ranging from precision oral healthcare to accelerated material discovery warrants strategic

investment and interdisciplinary innovation. The pace of adoption will depend on advancing hardware, data infrastructure, education, and ethical oversight.

Conclusion

The convergence of digital twin technology and quantum computing presents a transformative shift in dental care. Digital twins already enhance diagnostics and treatment planning through real-time, patient-specific simulations, but are limited by the computational demands of modeling complex biological systems. Quantum computing, with its capacity for high-speed processing and advanced simulations, addresses these limitations enabling deeper, faster, and more accurate predictions. Together, they offer a powerful tool for advancing dentistry toward a predictive, personalized, and preventive model. Key challenges remain, including immature quantum hardware, fragmented dental data, and unresolved ethical concerns. Progress will depend on cross-disciplinary collaboration, regulatory support, and investment in infrastructure and education. Despite these barriers, the trajectory is clear: intelligent, adaptive systems will shift dentistry from reactive treatment to proactive care anticipating and preventing disease before it starts.

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