Journal of Quantum Computing, Simulation and Emerging Computation

PRIME OPEN ACCESS

Volume 1, Issue 1

Research Article

Date of Submission: 06 Mar, 2026
Date of Acceptance: 30 Mar, 2026
Date of Publication: 10 Apr, 2026

Quantum-Nuclear DNA Computing: Using Nucleotide Spin States as Biological Quantum Bits for Molecular Calculations

Ndenga Lumbu Barack*

Independent Researcher, Kinshasa, Democratic Republic of the Congo

***Corresponding Author:** Ndenga Lumbu Barack, Independent Researcher, Kinshasa, Democratic Republic of the Congo.

Citation: Barack, L. N. (2026). Quantum-Nuclear DNA Computing: Using Nucleotide Spin States as Biological Quantum Bits for Molecular Calculations. *J Quant Comp Simul Emerg Comput, 1*(1), 01-05.

Abstract

This article introduces a novel and comprehensive framework for biological quantum computing, in which nucleotide spin states act as qubits for molecular calculations. By conceptualizing DNA strands as quantum registers, we explore how precise nuclear spin manipulations could enable in vivo computation within biological systems. This work develops a theoretical foundation that integrates quantum mechanics, nuclear magnetic resonance (NMR) techniques, and molecular biology. Simulation strategies are proposed to demonstrate the feasibility of encoding, processing, and measuring information directly at the molecular level. Potential applications include adaptive drug design, bioinformatics optimization, molecular cryptography, and intelligent biological systems, laying the groundwork for the ambitious Q-DNA Project.

Key Highlights Include:

- Encoding information in nucleotide spin qubits with superposition and entanglement
- Simulation protocols for mapping DNA sequences into quantum circuits
- Strategies for handling decoherence and noise in molecular systems
- Applications in computational biology and bio-quantum technologies

This framework not only presents a paradigm shift in biological computation but also opens new avenues for quantum-assisted biological research, merging theoretical physics, advanced mathematics, and molecular biology into a unified computational platform

Introduction

Recent advancements in quantum computing have showcased unprecedented computational capacities, far surpassing classical approaches for certain problem classes, including optimization, simulation, and cryptography. Simultaneously, DNA computing has proven a promising paradigm for parallel and high-density information processing, exploiting the combinatorial potential inherent in nucleotide sequences.

This work proposes an innovative fusion of these paradigms by conceptualizing the nuclear spin states of nucleotides (^{13}C, ^{15}N, ^{31}P) as biological qubits. DNA strands, in this framework, function as quantum registers capable of in vivo computations, offering a path to realize molecular-scale quantum processing.

Background and Motivation

- **Quantum Bits (Qubits):** Exploit superposition and entanglement, allowing parallel computation across a large number of states, far exceeding classical binary systems.
- **Nuclear Magnetic Resonance (NMR):** A well-established technique to manipulate nuclear spins, providing a

practical method for controlling qubits at the atomic level.

• **DNA as a Quantum Medium:** Nucleotides are naturally abundant and provide an information-dense platform for encoding, storing, and processing quantum information. Leveraging these biological molecules can potentially allow computations intrinsically embedded within living systems, opening a new frontier in bio-quantum computing.

Objectives

Establish a theoretical framework for nucleotide spin-based qubits. Develop simulation models to explore quantum operations within DNA sequences. Evaluate potential applications in biomedicine, bioinformatics, and molecular cryptography. Lay the foundation for experimental and computational follow-up studies under the Q-DNA Project.

Methodology

The methodology section describes how nucleotide spin states can be theoretically manipulated as qubits, how quantum operations can be simulated, and how the system can be analyzed for computational outcomes.

Nucleotide Spin Qubits

Each nucleotide (A, T, C, G) is conceptualized as a single qubit.
Basis states are defined as:
• $|0\rangle$: spin-up configuration
• $|1\rangle$: spin-down configuration

Superposition Allows Representation of a Linear Combination: $|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$ with $|\alpha|^2 + |\beta|^2 = 1$.
Entanglement between nucleotides enables multi-qubit operations and correlated behavior across sequences.

Quantum Gates and Operations

• **Single-Qubit Gates:** H (Hadamard), X, Y, Z, S, T, and rotation gates Rx(θ), Ry(θ), Rz(θ) applied to nucleotide spins.

• **Two-Qubit Gates:** CNOT, SWAP, and controlled-phase gates establish entanglement between nucleotide qubits.

• **Unitary Evolution:** DNA sequences evolve under Hamiltonians representing interaction energies and NMR pulse sequences.

Handling Decoherence and Noise

Decoherence times (T1 and T2) are included to model environmental effects. Kraus operators are employed to simulate noise and measurement collapse. Strategies for error mitigation and stabilization of qubit coherence are discussed.

Simulation Protocol

• **DNA-to-Qubit Mapping:** $A \rightarrow |0\rangle, T \rightarrow |1\rangle, C \rightarrow (|0\rangle + |1\rangle)/\sqrt{2}, G \rightarrow (|0\rangle - |1\rangle)/\sqrt{2}.$

• **Circuit Generation:** DNA sequences translated into quantum circuits with defined gate operations.

Measurement and Analysis: Simulation outputs Bloch spheres, probability distributions, and circuit diagrams.

Software Implementation

• **Programming Environment:** Python 3.10+, using NumPy, SciPy, Qiskit, Matplotlib.

• **Notebooks:** Jupyter Notebook setup for interactive simulations.

• **Scenario Selection:** Multiple DNA sequences and operations tested via modular scripts.

• **Reproducibility:** Fixed random seeds and configuration files ensure consistent outcomes.

Step-by-Step Procedure

• **Install Required Packages:** pip install numpy scipy qiskit matplotlib jupyter

• Download the simulation repository.

• Launch Q DNA Simulator.ipynb in Jupyter Notebook.

• Select scenario (entanglement, algorithm test, sequence mapping).

• Execute all cells sequentially to run simulations.

• Visualize Bloch spheres, circuit diagrams, and measurement probabilities.

• Export results as images, JSON (circuits), and CSV (data).

• Modify sequences or parameters to explore different computational scenarios.

Results

The simulation results demonstrate the feasibility of using nucleotide spin states as qubits for molecular-level quantum computations. Various scenarios were analyzed, highlighting the computational potential embedded within DNA sequences.

Superposition and Entanglement

Single-qubit superposition was achieved for each nucleotide type, demonstrating the ability to maintain coherent quantum states. Entangled states between nucleotides, such as Bell states, were successfully simulated, indicating the possibility of correlated quantum operations within a DNA strand.

Algorithmic Simulation

The Deutsch–Jozsa algorithm was implemented for a two-qubit DNA system, correctly distinguishing constant and balanced functions with a single query.

Grover-type search simulations were performed on small nucleotide sequences, showcasing potential quantum speed-up in searching molecular data.

DNA-to-Circuit Mapping

Example DNA sequences (e.g., ATCGTAGC) were mapped into quantum circuits, successfully reproducing theoretical quantum behavior. Bloch sphere visualizations confirmed correct superposition and rotation of qubits. Probability distributions of measurement outcomes matched expected theoretical predictions, validating the simulation protocol.

Noise and Decoherence Analysis

Simulations under realistic decoherence models demonstrated robustness of the qubit operations for short sequences. Error rates increased with sequence length, highlighting the need for quantum error correction strategies in extended DNA computations.

Summary of Findings

DNA nucleotides can theoretically serve as functional qubits.
Quantum gates and entanglement operations can be mapped and simulated effectively. Simulation outputs confirm correct quantum behavior consistent with theoretical expectations. The methodology establishes a foundation for future experimental validation and practical implementation in molecular quantum computing.

Discussion

The results highlight the enormous potential of biological qubits for high-density information storage and quantum processing. NMR-based manipulation of nuclear spins demonstrates theoretical feasibility for performing quantum computations directly within living molecular systems.

Advantages

• **High-Density Storage:** DNA nucleotides provide a naturally dense and scalable medium for qubits.

• **Intrinsic Parallelism:** Superposition and entanglement allow simultaneous computation across multiple states.

Integration with Living Systems: Potential for in vivo computation and bio-quantum sensing.

Limitations

• **Decoherence Times:** Spin relaxation may limit the duration of coherent operations.

• **Error Correction:** Practical strategies for mitigating quantum errors at the molecular level remain challenging.

• **Experimental Realization:** Translating the theoretical model into actual biological systems requires significant technological advancement.

Comparison with Classical DNA Computing

Quantum DNA computing offers potential speed-up compared to classical DNA computing methods, particularly in search and optimization tasks. Incorporating qubits into nucleotides allows for parallel evaluation of exponentially large state spaces, beyond the capacity of conventional biochemical computation.

Future Perspectives

Development of robust bio-quantum experimental platforms. Integration of quantum error correction and noise mitigation

techniques. Exploration of complex algorithms for molecular computation, adaptive therapeutics, and bio-cryptography.

Applications and Future Work

Biomedicine

- **Programmable Molecular Responses:** DNA molecules can be engineered to adaptively modify function or structure.

- **Adaptive Drug Molecules:** Potential for molecules that adjust activity based on cellular signals or environmental inputs.

Bioinformatics

- **Rapid Pattern Recognition:** Exploiting quantum superposition to identify nucleotide sequence motifs efficiently.

- **Large-Scale Data Analysis:** Parallel computation within DNA sequences accelerates genomics and proteomics studies.

Cryptography

- **Molecular-Level Secure key Generation:** DNA qubits enable inherently secure encryption schemes.

- **Quantum-Resistant Protocols:** Combining biological qubits with cryptographic algorithms for enhanced security.

Further Research

- **Experimental NMR Validation:** Testing theoretical models with real nucleotide spin systems.

- **Scalable Qubit Networks:** Expanding beyond small DNA sequences to complex qubit architectures.

- **Integration with Synthetic Biology:** Creating hybrid bio-quantum systems for advanced computation and adaptive molecular technologies.

Conclusion

The Q-DNA Project represents a groundbreaking conceptual framework, establishing DNA strands as quantum registers via nucleotide spin qubits. Simulations demonstrate the theoretical feasibility of computation within biological systems, despite experimental challenges such as decoherence and error correction. This framework lays the foundation for future interdisciplinary research, bridging quantum physics, molecular biology, and computational sciences. The project opens promising avenues in quantum biology, molecular computing, adaptive therapeutics, and intelligent biological systems, highlighting the transformative potential of integrating quantum computation into living molecular structures [1-17].

References

1. Adleman, L. M. (1994). Molecular computation of solutions to combinatorial problems. science, 266(5187), 1021-1024.
2. Benenson, Y. (2012). Biomolecular computing systems: principles, progress and potential. Nature Reviews Genetics, 13(7), 455-468.
3. Lloyd, S. (2011, July). Quantum coherence in biological systems. In Journal of physics-conference series (Vol. 302, No. 1, p. 012037).
4. Mohseni, M., Omar, Y., Engel, G. S., & Plenio, M. B. (Eds.). (2014). Quantum effects in biology. Cambridge University Press.
5. Suter, D., & Álvarez, G. A. (2016). Colloquium: Protecting quantum information against environmental noise. Reviews of Modern Physics, 88(4), 041001.
6. Feynman, R. P. (1982). Simulating physics with computers. International Journal of Theoretical Physics, 21(6–7), 467–488.
7. Zhang, S., Wang, L., & Wang, J. (2020). DNA as a quantum information carrier: prospects and challenges. Quantum Information Processing, 19(7), 207.
8. Gershenfeld, N. A., & Chuang, I. L. (1997). Bulk spin-resonance quantum computation. science, 275(5298), 350-356.
9. Winfree, E., Liu, F., Wenzler, L. A., & Seeman, N. C. (1998). Design and self-assembly of two-dimensional DNA crystals. Nature, 394(6693), 539-544.
10. Nielsen, M. A., & Chuang, I. L. (2010). Quantum computation and quantum information. Cambridge university press.
11. Barack, N. L. (2025). Numerical Simulation of the 3D Navier-Stokes Equations using the Finite Volume Method–Clay University Submission. Zenodo..
12. Barack, N. L. (2025). AutoEvoChem V2. 0–An Intelligent Molecular Simulation and Synergistic AI Toolkit for Computational Chemists and Biopharmaceutical Researchers. Zenodo (2025, June 28 and 30).
13. Ndenga Lumbu Barack. (2025, June 28). Electron-free nuclear matter: magnetic confinement and bonding of bare nuclei in extreme fields. Zenodo, DOI:
14. https://doi.org/10.5281/zenodo.15764734

15. Ndenga Lumbu, B. (2025). NanoDisqueChimique RDC-1000: A new molecular approach for low-cost data storage through colorimetric coding (Version v1). Zenodo.
16. Ndenga, B. (2025). Autoevolving Nanodisk with Unlimited Memory: A Bioinspired and Quantum-Spiritual Approach.
17. Ndenga, B. (2025). Self-Adaptive Photosynthetic Quantum Crystal: A Bioinspired Innovation for Intelligent Light Harvesting and Energy Conversion

Document prepared for conceptual demonstration and academic discussion; no in vivo experimentation conducted.

Appendix: Detailed Instructions for Accessing and Using the Simulation

1. Clone or download the repository containing the Q-DNA Project simulation files.

2. Install dependencies using pip as listed above.

3. Launch the Jupyter Notebook Q DNA Simulator.ipynb.

4. Select the desired scenario (D1, D2, D3).

5. Execute all cells sequentially to run simulations.

6. Observe outputs including Bloch spheres, circuit diagrams, and probability tables.

7. Export visualizations and data using the provided functions.

8. Modify DNA sequences or noise parameters to test different configurations.

9. Use the provided random seed for reproducibility.

10. Document results for further analysis or publication purposes.