Quantum Walk for Moisture Dispersion in Soil: in One and Two Dimensions*

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We simulate moisture dispersion in soil using a quantum walk framework, modeling each soil patch as a lattice site with dynamically updated coupling constants based on local gradients. This approach captures intuitive diffusion behavior while highlighting the limitations of classical simulation in higher dimensions, motivating future implementation on quantum hardware for real-time environmental control in enclosed agricultural systems.

I. INTRODUCTION

Controlled-environment agriculture, including greenhouses and indoor farms, presents a promising path toward local, efficient food production. These systems benefit from precise regulation of light, air temperature, and humidity, yet soil moisture remains a challenging variable to control. Unlike air, which obeys relatively simple thermodynamic laws, soil behaves as a complex porous medium where capillary action, gravity, root uptake, and evaporation interact in nonlinear and spatially varying ways. Understanding and predicting how water disperses through soil is crucial for optimizing irrigation, conserving water, and ensuring plant health.

A. Why Soil Moisture is Hard to Model

Soil is not a uniform medium; it exhibits nonlinear and spatially varying properties. Moisture transport is governed by capillary effects, gravity, and dynamic interactions with plant roots and watering systems. These effects are coupled and often depend on local gradients, making accurate modeling of soil moisture a computationally difficult task. Simulations must capture both global dynamics and local interactions, a requirement that scales poorly in classical computation.

B. Limitations of Classical Approaches

Traditionally, moisture dispersion is modeled using partial differential equations, such as the heat or diffusion equation. While effective in idealized systems, these models face significant limitations: they often rely on simplifications that fail to capture real soil dynamics, and their computational cost increases rapidly with the number of spatial dimensions or resolution. In particular, classical simulations of even modestly sized 2D or 3D systems can become unfeasible on standard hardware, as demonstrated by our own attempts at simulating a 5×5 grid, which led to repeated memory failures.

C. A Quantum Approach

To address these challenges, we propose using quantum walks (the quantum analog of classical random walks) to model moisture dispersion. In this framework, each patch of soil is represented by a node on a lattice, and moisture is represented by a particle undergoing a unitary evolution. Coupling constants between nodes are dynamically adjusted based on local gradients, allowing the simulation to respond to changes in moisture concentration. This approach provides a natural way to encode spatial correlations and time-dependent dynamics, with the potential for better scalability on quantum hardware.

D. Scope of This Work

In this work, we present a quantum walk model for simulating moisture dispersion in one and two dimensional soil systems. We demonstrate how local gradient information can be used to update coupling constants in real time, enabling intuitive dispersion behavior. We also discuss unphysical effects that emerge when physical constraints are not enforced, and we outline strategies for addressing these limitations. Finally, we evaluate the computational feasibility of this approach on classical machines and explore the implications for future implementation on quantum devices.

II. METHODOLOGY

A. Quantum Walk Lattice Setup

To simulate moisture dispersion, we model the soil as a discrete lattice where each site represents a fixed patch of soil. In the one-dimensional case, this lattice forms a line of N connected patches. In two dimensions, the lattice becomes a square grid with $N \times N$ sites. Each patch contains a local "moisture level," represented by a quantum amplitude. These particles then evolve over

* In 1D and 2D

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time under the influence of a Hamiltonian that governs site-to-site interactions.

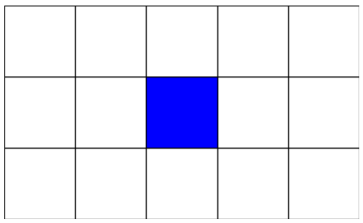

FIG. 1. Schematic of the 2D lattice used to represent soil patches. Moisture is initially concentrated in the center patch, with the amplitude represented by a a gradient of white (0) to blue (1).

B. Hamiltonian and Coupling Constants

The time evolution of the system is governed by a Hamiltonian of the form:

$$H = \sum_{\langle i,j \rangle} J_{ij}(t) \left(\sigma_i^+ \sigma_j^- + \sigma_j^+ \sigma_i^- \right) \ . \tag{1}$$

where σ_i^+, σ_i^- are the raising and lowering operators at site are the raising and lowering operators at site i, and $J_{ij}(t)$ is the coupling constant between neighboring sites i and j at time t. These couplings are designed to encode local gradients in the moisture distribution:

$$J_{ij}(t) = f\left(\rho_i(t) - \rho_j(t)\right) \tag{2}$$

C. Simulation Procedure

The simulation proceeds in discrete time steps and follows an iterative loop:

- **Initialization:** The quantum state is prepared with X gates on the sites with full moisture, and a Hamiltonian is built creating $J_{ij}(t = 0)$ values between neighbors on the grid (based on their moisture gradient).
- **Time Evolution:** The system evolves according to the Hamiltonian for a small Trotterized time step.
- **Measurement:** A measurement is performed to extract site populations, which are interpreted as the new moisture distribution.
- **Gradient Update:** The measured distribution is used to recalculate the coupling constants $J_{ij}(t)$.
- **Repeat:** The system is reinitialized with the previous time steps, and with the updated gradient repeats the **Time Evolution** step.

This process continues over multiple iterations to simulate long-term dispersion. Because quantum measurement collapses the wavefunction, true continuous evolution is approximated via re-preparation of states based on prior measurements.

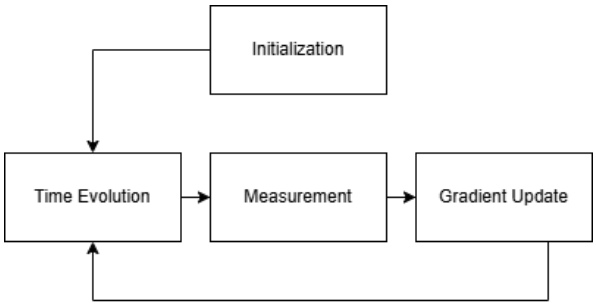

FIG. 2. Flowchart of the simulation loop

D. Implementation

The simulations were implemented using Quiskit, a Python-based quantum computing framework. Moisture levels were encoded in qubit states, and custom circuits were written to implement Hamiltonian evolution with variable couplings. Simulations were executed on a high-performance desktop designed for quantum work, but significant limitations emerged.

In 1D, the simulation ran smoothly across grids of 5 sites. However, extension to 2D proved computationally intensive. A 5×5 (25 sites) required tracking large entangled quantum states and updating $J_{ij}(t)$ after every measurement. The classical RAM and CPU constraints led to multiple simulation crashes due to memory overflow. These results suggest that while quantum walk modeling is feasible in principle, classical simulation of such systems quickly becomes intractable— motivating future implementation on real quantum hardware.

III. RESULTS

A. Observed Dispersion Behavior

The quantum walk simulation successfully produced intuitive moisture dispersion in one-dimensional lattices. Starting from an initial configuration where moisture was localized at the left edge of the lattice, the system evolved

such that particle amplitudes gradually spread to neighboring sites over successive iterations. This pattern resembled classical diffusion, with smooth population gradients and no abrupt discontinuities. The use of dynamically updated coupling constants $J_{ij}(t = 0)$,based on local differences in moisture levels, significantly improved the realism of the dispersion. Sites with greater moisture gradients exhibited stronger coupling, leading to faster redistribution of moisture in regions with large imbalances.

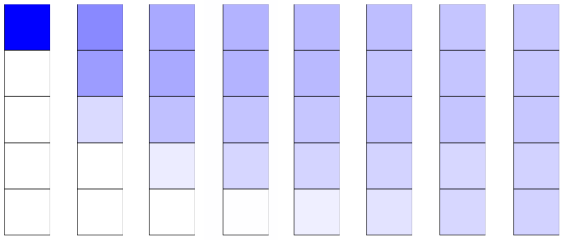

FIG. 3. Time evolution in increments of 25 iterations left to right.

B. Emergent Pathologies and Corrections

Initial simulations using $f(x) = |x|$ as the gradient-based coupling function produced unexpected and unphysical dynamics. Instead of resembling moisture flow, the evolution displayed behaviors characteristic of wave interference or resonance. In some cases, the system showed a runaway effect where certain sites accumulated excessive amplitudes rather than dispersing evenly. This was traced back to the absolute value function eliminating directional information from the gradient, thus encouraging feedback loops in the coupling constants.

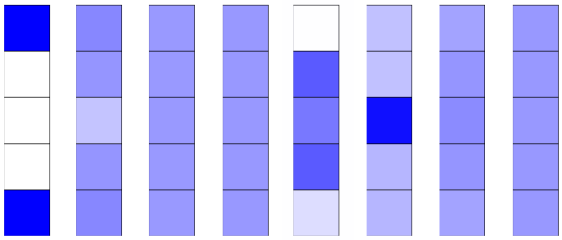

FIG. 4. Time evolution in increments of 25 iterations left to right, note the wave like interference from the gradient runaway effect.

To resolve this, the function $f(x)$ was redefined to drop the absolute value and preserve the sign of the gradient:

$$f(x) \propto x \tag{3}$$

This adjustment restored directionality and significantly improved the stability of the system. With this change, moisture flowed from regions of high concentration to low concentration, as expected, and the overall system returned to physically plausible diffusion-like behavior.

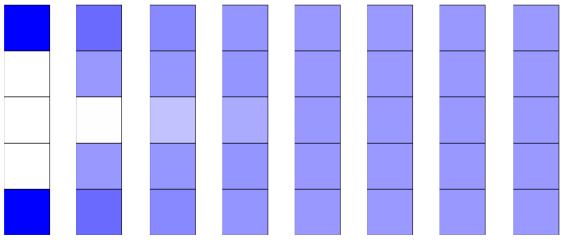

FIG. 5. Time evolution in increments of 25 iterations left to right, with a corrected $f(x)$ that prevents a runaway effect.

C. Simulation Scalability Limits

While the algorithm performed well in one-dimensional systems, scaling to two-dimensional grids proved infeasible on classical hardware. A 5×5 lattice (modest in physical size) resulted in excessive memory usage due to the exponential growth of the Hilbert space and the need to update all pairwise couplings $J_{ij}(t)$ after each iteration. For this 2D system, when evolution reached 12 iterations, the program repeatedly crashed due to memory overflow. This suggests that the iterative update-and-prepare cycle accumulates computational overhead nonlinearly with time, especially as the state becomes more entangled and the number of nonzero amplitudes increases.

The observed crashing occurred despite running on a high-performance desktop specifically built for quantum simulation, with 48 GB of RAM and a modern multi-core processor. These limitations highlight the steep cost of even modestly complex quantum walk simulations when run classically, reinforcing the motivation to transition to real quantum hardware, where such dynamics could be natively implemented without exponential memory scaling.

IV. DISCUSSION

A. Interpretation of Results

The quantum walk-based model captures key features of moisture dispersion, particularly the intuitive spreading of particles from high to low concentration regions. By dynamically updating coupling constants based on local gradients, the simulation introduces a physically motivated feedback mechanism. Once the gradient function

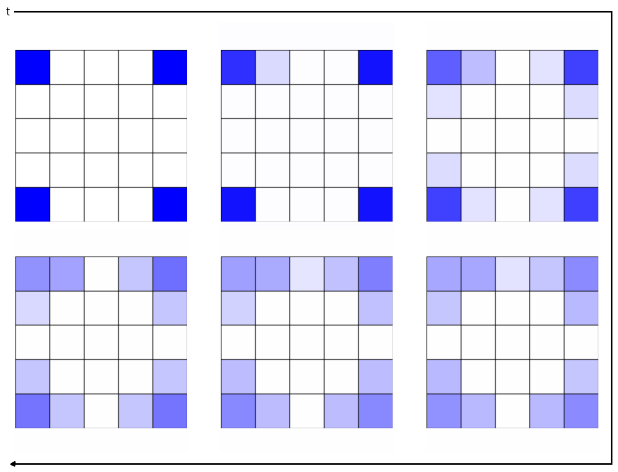

FIG. 6. Time evolution in increments of 2 iterations left to right, top to bottom. These charts represent the 12 iterations before memory overload that results in a crash.

was corrected to preserve directionality, the walk behaved in a manner consistent with classical diffusion, indicating that the approach can replicate essential features of soil moisture transport. Although not identical to real capillary and gravitational soil behavior, the evolution is suggestive of an underlying framework that can be tuned to fit real-world parameters.

B. Limitations of the Approach

The model remains idealized in several ways. First, the simulation does not account for noise, decoherence, or gate errors, which would affect performance on real quantum hardware. Second, quantum measurement collapses the state, so each iteration requires re-preparation based on prior outcomes. This breaks the illusion of continuous evolution and introduces approximation error. Third, and most significantly, the model currently does not enforce thermodynamic principles such as entropy. For example, under certain gradient conditions, the system may evolve in ways that suggest spontaneous upconcentration of moisture, violating conservation logic. While sign-preserving gradients solved this issue for the distributions tested, further constraints may be required to guarantee physicality when scaling up to larger systems.

C. Toward More Realistic Models

Future work could address these limitations through the addition of entropy-like terms to the evolution or by embedding the walk within a larger quantum optimization loop. Perturbations such as root water uptake or new irrigation pulses could be modeled by mid-cycle adjustments to qubit populations. One proposal is to group blocks to represent one larger patch, sum block amplitudes within that patch, adjusting the total moisture by the perturbation amount, and reinstating the system by filling those patches from the center outwards until we reach the new total moisture. This would naturally introduce some error as we would only be able to fill in integers amounts of sub-moisture, but for large enough groups where sub-blocks each hold a smaller and smaller fraction of one unit of moisture, the error would decrease.

Another proposed solution is to use ancilla qubits to flip population configurations without needing full reinitialization. Through this we could flip any qubit completely to 1 or 0 regardless of its current amplitude, but this method would similarly introduce error as it limits the exact amount of moisture we can add/remove from the system. Additionally, incorporating effects like gravity-driven asymmetry or temperature-sensitive mobility can be implemented into the system through the definition of the function used in our coupling dynamic coupling constants $J_{ij}(t)$. This $f(x)$ could be fit to match real world data that incorporates all these effects, which would make the simulation more applicable to real agricultural systems.

V. CONCLUSION

This project demonstrates the viability of using quantum walks as a framework for simulating moisture dispersion in soil. By encoding soil patches as lattice sites and updating coupling constants dynamically based on local gradients, the system reproduces key features of diffusion-like behavior. The approach is intuitive, flexible, and capable of incorporating physically meaningful parameters such as directionality and local imbalance.

However, the work also reveals the steep computational cost of simulating such systems classically, especially in two dimensions or over long timescales. Memory limitations and cumulative resource demands highlight the value of transitioning to real quantum hardware, where entanglement and unitary evolution occur natively. Furthermore, addressing challenges such as thermodynamic consistency, entropy constraints, and real-time perturbations will be essential to refining the model for practical use.

Looking forward, this quantum walk-based simulation could be expanded and integrated into quantum optimization frameworks to inform adaptive irrigation strategies, particularly in climate-controlled agricultural systems. The ability to accurately and efficiently predict moisture dynamics has clear implications for sustainable farming, food security, and environmental control in constrained growing environments.

VI. REFERENCES

This work was inspired in part by the approach taken in Ref. [1] to the modeling of the heat equation, and an overview of quantum walks in Ref. [2]. While our model differs in methodology and application, the idea of encoding spatial diffusion in a quantum walk owes conceptual debt to their framework.

[1] B. Daribayev, A. Mukhanbet, N. Azatbekuly, and T. Imankulov, A quantum approach for exploring the numerical results of the heat equation, Algorithms **17**, 327 (2024).

[2] R. Duda, M. N. Ivaki, I. Sahlberg, K. Pöyhönen, and T. Ojanen, Quantum walks on random lattices: Diffusion, localization, and the absence of parametric quantum speedup, Phys. Rev. Res. **5**, 023150 (2023).