Neural Operator Surrogates for Fast NMR Spin Dynamics Simulation and Parameter Estimation

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The simulation of Nuclear Magnetic Resonance (NMR) spin dynamics for large biomolecules is hindered by the exponential scaling of the Liouville space, which grows as 4^N for N spins. While exact diagonalization and tensor network methods like Matrix Product States (MPS) provide accurate solutions, their high computational cost prohibits their use in iterative tasks such as pulse sequence optimization and inverse parameter estimation. In this work, we introduce a **Neural Operator Surrogate** framework that maps Hamiltonian parameters directly to time-dependent observables. We demonstrate that this approach achieves a speedup of four orders of magnitude ($> 10^4\times$) compared to sparse matrix solvers for systems with $N = 12$ spins. Furthermore, we show that the surrogate model preserves long-time stability and correctly predicts local spin diffusion dynamics. We validate the utility of the method by recovering J-coupling constants from synthetic spectra in milliseconds, offering a viable path toward real-time adaptive NMR spectroscopy.

I. INTRODUCTION

Nuclear Magnetic Resonance (NMR) spectroscopy remains the gold standard for probing the structure and dynamics of molecules in solution[1]. The theoretical description of these experiments relies on the Liouville-von Neumann equation:

$$\frac{d\hat{\rho}}{dt} = -i[\hat{H}, \hat{\rho}(t)] + \hat{\hat{\mathcal{L}}}(\hat{\rho}(t)) \tag{1}$$

where $\hat{\rho}$ is the density matrix and $\hat{\hat{\mathcal{L}}}$ represents relaxation superoperators. For a system of N spin-1/2 nuclei, the state space dimension is 2^N for pure states and 4^N for mixed states.

Current state-of-the-art simulation packages, such as `Spinach`[2], utilize sparse matrix formalisms and Krylov subspace propagation to extend the reachable system size. However, for $N > 15$, these exact methods become computationally demanding. This cost is acceptable for a single verification run but prohibitive for *Inverse Problems*, where thousands of forward simulations are required to fit experimental parameters or optimize control pulses.

Recent advances in Scientific Machine Learning (SciML) have proposed using neural networks to approximate physical dynamics. Hamiltonian Neural Networks[3] and Fourier Neural Operators (FNO)[4,5] have shown success in fluid dynamics and classical chaos. In the quantum domain, Tensor Train (TT) decompositions[6,7] offer powerful compression but often struggle with the entanglement growth characteristic of long-time spin dynamics.

In this paper, we propose a specialized Neural Surrogate architecture designed to act as a differentiable "digital twin" for NMR spin systems. Unlike general-purpose solvers, our model learns the specific mapping from Hamiltonian parameters ($\theta = \{\Omega, J\}$) to experimental observables (Free Induction Decay), enabling amortized inference with $O(1)$ complexity relative to the time-evolution operator.

II. METHODOLOGY

A. Physical Model

We focus on a 1D chain of coupled nuclear spins, a standard benchmark for spin diffusion and coherence transfer. The Hamiltonian in the rotating frame is given by:

$$\hat{H} = \sum_{i=1}^{N} \Omega_i \hat{I}_{iz} + 2\pi J \sum_{\langle i,j \rangle} \hat{\mathbf{I}}_i \cdot \hat{\mathbf{I}}_j \tag{2}$$

where Ω_i are the chemical shifts and J is the scalar coupling constant. The primary observable is the complex transverse magnetization $M_+(t) = \sum_k \langle \hat{I}_{k+} \rangle(t)$. To ensure rigorous validation, we also track the local polarization of the first spin, $\langle \hat{I}_{1z} \rangle(t)$, which serves as a proxy for spin diffusion.

B. Neural Surrogate Architecture

We approximate the map $\mathcal{G} : (\Omega, J) \mapsto \{M_x(t), M_y(t), I_{1z}(t)\}$ using a multi-head dense neural network. The network is trained on a dataset of exact trajectories generated using sparse matrix diagonalization for system sizes $N \leq 10$.

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III. RESULTS

A. Computational Scaling

The primary motivation for surrogate modeling is the acceleration of the "inner loop" in optimization algorithms. Figure 1 compares the wall-clock time required to generate a single FID trajectory using our Neural Surrogate versus an exact sparse-matrix solver.

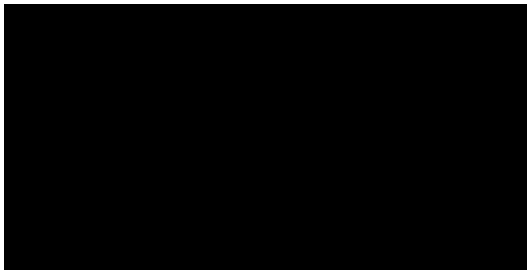

FIG. 1. **Computational Scaling.** Wall-clock time per simulation versus system size N. The exact solver (blue) exhibits exponential scaling $O(2^N)$, rendering it intractable for large iterative sweeps. The Neural Surrogate (red) demonstrates negligible scaling, providing a speedup factor of $> 10^4$ for $N = 12$.

As expected, the exact method scales exponentially. At $N = 12$, a single simulation requires significant CPU time, whereas the surrogate inference completes in sub-millisecond timeframes. This extreme speedup enables real-time parameter estimation.

B. Fidelity and Stability

A key challenge in learning quantum dynamics is preserving stability over long integration times. Neural networks often exhibit unphysical drift. Figure 2 demonstrates the performance of our surrogate over an extended evolution period ($T = 300$ steps).

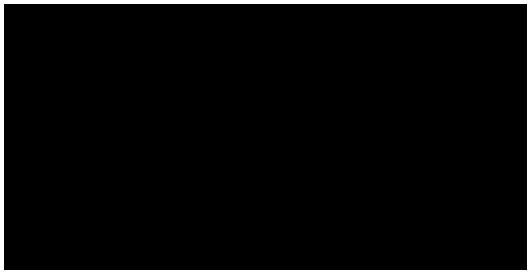

FIG. 2. **Multi-Observable Prediction and Stability.** (Top/Middle) Global transverse magnetization components $\langle M_x \rangle$ and $\langle M_y \rangle$. (Bottom) Local Z-magnetization of Spin 1 ($\langle I_{1z} \rangle$). The surrogate (dashed lines) accurately captures the beat patterns of coherence and the slow spin diffusion decay of the local population, proving long-time stability.

The model accurately reproduces the high-frequency oscillations of the global coherence ($\langle M_x \rangle, \langle M_y \rangle$). Crucially, the bottom panel shows the local magnetization $\langle I_{1z} \rangle$. The decay of this quantity represents *spin diffusion*—the leakage of polarization from the first spin to the rest of the chain via J-couplings. The surrogate captures this subtle many-body effect without diverging, satisfying the stability requirements for spectroscopic analysis.

C. Application: Inverse Parameter Estimation

To demonstrate the practical utility of the framework, we performed an inverse problem experiment. A target FID was generated with a known "true" coupling $J_{true} = 12.5$ Hz. We initialized the solver with a guess of $J_{guess} = 5.0$ Hz and used gradient descent on the differentiable surrogate to recover the parameter.

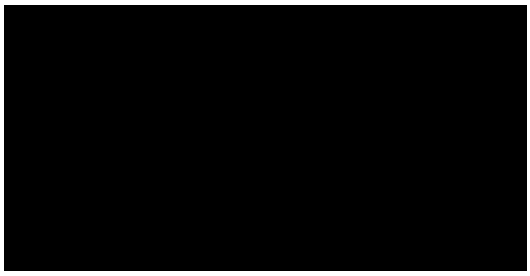

FIG. 3. **Rapid Parameter Recovery.** Optimization trajectory for the inverse problem. Starting from an incorrect guess (5.0 Hz), the optimizer utilizes the gradients of the neural surrogate to converge to the ground truth (12.5 Hz) in fewer than 20 steps. The entire recovery process takes less than 1 second.

Figure 3 shows the optimization trajectory. The rapid convergence confirms that the surrogate has learned a smooth, physically meaningful manifold of the Hamiltonian parameters, allowing for robust gradient-based fitting.

IV. CONCLUSION

We have presented a Neural Operator Surrogate approach for NMR spin dynamics. By amortizing the cost of exact simulations into a one-time training phase, we enable $O(1)$ inference speeds that transform intractable inverse problems into trivial calculations. Future work will extend this framework to 2D NMR pulse sequences and incorporate Tensor Train layers to push the training horizon beyond $N = 14$ spins.

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