Artificial Intelligence-Assisted Design and Virtual Diagnostic for the Initial Condition of a Storage-Ring-Based Quantum Information System

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ABSTRACT

Developments in Artificial Intelligence (AI) are helping to solve complex physical problems that otherwise may be too computationally demanding to solve using traditional approaches. Universal Approximation Theorems tell us that we can model any physical system if we can approximate the system with some continuous function (i.e., compact convergence topology and algorithmically generated sets of functions, such as the convolutional neural network), whether for an arbitrary depth or arbitrary width neural network. We consider the problem of solving a set of $N$ coupled algebraic equations as $N$ becomes very large and apply machine learning (ML) to solve this problem for any value of $N$. The physical problem we are focusing on is to model the equilibrium positions of ions in an ion trap. A storage ring quantum computer could contain well over tens of thousands of ions. Quickly determining the equilibrium positions will be important to minimize the time to target and observe each ion. As each ion serves as a single qubit, this is important for setting and measuring the individual qubit states. The phonon modes from a collection of ions acts as another qubit, useful for gate operations. Measuring the phonon modes, where ions are oscillating around their respective equilibrium positions also means understanding the equilibrium positions very well. Turning all of this into a virtual diagnostic allows real time prediction and comparison to ensure unique definition of each ion.

INDEX TERMS

Curve fitting, ion beams, lasers, machine learning, nonlinear equations, particle accelerators, phonons, quantum computing, storage rings.

I. INTRODUCTION

Quantum information systems (QIS) refers to developing technologies, such as quantum communication and quantum computing (QC) [1]. QIS promises to revolutionize our current communication and computational paradigms; this has prompted a race between countries and institutions alike towards building practical QIS. The United States, for example, launched in 2018 a national initiative on developing technologies that will help enable QIS [2]. The technological leap...
enabled by QIS comes from harnessing the quantum properties of atomic, electronic, and photonic systems, to perform calculations that are virtually impossible even with state-of-art computational systems.

In classical computing, information is encoded and streamlined as binary bits that can exist in one of two mutually exclusive states, generally represented by the digits 0 and 1. More complex logical gates can be formed from this binary set to process complex information and to perform calculations. The computational power of classical computers comes from their ability to perform numerous consecutive tasks very fast. Quantum computing is fundamentally different in that it exploits the principle of superposition. The principle of superposition in quantum mechanics (QM) is conceptually different than in classical physics [3]. Here we describe it in the context of the QM mathematical framework. In QM, it is postulated that measurements can affect the state of the system and they are mathematically described with Hermitian operators [4]. The operator $M$ has eigenvectors $|m_k\rangle$ and eigenvalues $m_k$. If the general state of a system is represented by the state-vector $|\psi\rangle$ and we perform the measurement $M$, then it is useful to re-write the initial state as a linear combination of the eigenvectors of $M$ [4]:

$$|\psi\rangle = \sum_k a_k |m_k\rangle.$$  

Performing the measurement $M$ on the system will force the initial state-vector to “collapse” into $|m_k\rangle$ with probability proportional to the modulus square of the coefficient $a_k$. Equation (1) can be interpreted as the original state of the system existing as a superposition of all the possible states corresponding to the measurement $M$, the eigenvectors of $M$. In the context of QC, a quantum bit, or qubit, exists as a superposition of the normal states represented by $|0\rangle$ and $|1\rangle$. Measuring the qubit will result in either 0 or 1. Note how this situation is different from classical computing, where the state of the classical bit is either 0 or 1 at any specific time, but not both of them.

QM deals with the smallest physical systems: atoms, electrons and photons [5]. Consequently, different QIS can be built based on different qubits, e.g., electronic spin, photon polarization, and trapped ions. For a thorough review on the current state of QC technology, see [6]. This work concerns a particular QIS: the storage ring quantum computer (SRQC) [7], which uses an unprecedented long chain of ions as qubits.

### A. THE STORAGE RING QUANTUM COMPUTER

Ions have been trapped and studied for years using Paul [8], [9] and Penning traps [10]. These experiments use electromagnetic fields and laser pulses to isolate and manipulate ions [11]. Similarly, storage rings use electromagnetic fields to accumulate and to store beams of charged particles in a closed trajectory. The SRQC is effectively an ion trap based QC that can potentially store thousands of ions in a rotating frame. Using ions as qubits is particularly interesting since they have longer coherence time [7]. The SRQC has many advantages over conventional ion traps, e.g., it can store a significantly higher number of ions and it opens up the possibility of storing multiple ion chains.

The SRQC concept has two pairs of inner electrodes to tailor a quadrupolar electric field that helps to focus the beam transversely. In the longitudinal direction, the beam is not bounded, but radiofrequency potentials can be introduced to break the beam into many parts, opening the possibility to parallel computing [7]. The dynamics of individual ions in the beam is driven by external fields and by interactions with other ions. The statistical motion of the ions forming the beam is the thermal energy of the beam [12]. For SRQC to be feasible, we need to reduce the beam thermal energy to a level where it is possible to identify and manipulate the external and internal quantum states of individual ions. Laser pulses can be used for beam cooling. For example, Doppler cooling [13], a process in which an ion absorbs and re-emits photons, results in a lower energy state of the ion [11]. By cooling the ion beam below the Doppler limit, but not to the point of the Lamb Dicke limit [7], the thermal motion is reduced so that the dominant interaction force is the Coulomb interaction, and a crystalline beam is formed [14]. If the crystalline beam is cooled enough and it is possible to identify phonon modes, then an Ion Coulomb Crystal (ICC) is formed. The SRQC will store an ICC, and use both the external and internal quantum states as qubits. The external modes are the phonon modes, and the internal modes are the hyperfine spin states [7].

The use of a storage ring for trapping an ion crystalline beam was investigated in LMU Munich in 2002. The experiment, PAul Laser coolIng Accelerator System (PALLAS), stored a beam of $^{24}$Mg$^+$, and cooled it enough to produce a crystalline beam [15]. For the SRQC, we expect to produce homogeneous beams of $^{24}$Mg$^+$ or $^7$Li$^+$ [7], and cool them to form an Ion Coulomb Crystal (ICC).$^3$

### B. ARTIFICIAL INTELLIGENCE FOR SRQC

The use of Artificial intelligence (AI) in support of experimental facilities has been identified as a competitive technology [16]. The use of AI-enabled controllers, for example, has resulted in enhanced beam quality and performance at large-scale particle accelerators [17]–[19]. Here we discuss possible applications of AI to SRQC [20]–[23], particularly on manipulating an unprecedented large number of ions and on storing multiple ICC. One example of a task that the SRQC should perform regularly is a reset of the ICC to its baseline state: if the ICC is in an arbitrary excited state, the lasers should be accurately triggered to lower the energy state of the

$^1$The Hermitian condition ensures the eigenvalues of the operator are real, as expected for any physical system.

$^2$Since it is virtually impossible to completely isolate the qubits from the rest of the Universe, quantum decoherence is a limitation of QC and there is an overarching quest to achieve longer coherence times.

$^3$The ICC abbreviation will be used to denote either single or multiple crystals.
ICCs, i.e., phonon excitations are suppressed and individual ions return to their equilibrium positions.

Random variations in the different sub-systems of the SRQC will produce different ICCs every time. The simplest difference is in the number of ions forming the ICC.\footnote{Other possibilities include, for example, a 2D ICC or having multiple ion species.} We envision a physics informed [24], virtual diagnostic tool [25, 26], that can accurately predict when a specific ion is approaching the SRQC window so that the corresponding laser can be triggered to excite the ion. A virtual diagnostic tool can be enabled by multiple supervised Machine Learning (ML) algorithms, such as Neural Networks (NN), and the accuracy of the ML model depends on the quality of data used for training, i.e., there should be a good amount of data that correctly represents the expected solutions, particularly as the number of ions becomes large.

II. ION COULOMB CRYSTAL

In the crystalline beam state, individual ions are locked into their corresponding equilibrium positions and can exhibit vibrations around this point. In the ICC state, the ion vibrations are small enough that the phonon modes of the crystal become dominant. The phonon modes are important for QC [27]. In general, the ICC is free to form a crystal in 2 or 3 dimensions and exhibits topological phase transitions [28]–[30]. If the ions are strongly bounded by the transverse fields, then the ions form a longitudinal 1D ICC, or an ion chain, where the distance between adjacent ions is determined only by the trap and Coulomb potentials. Qualitatively, we expect the behavior of the ion chain to be as follows: ions near the center of the chain experience a quasi-symmetric Coulomb interaction from both sides, becoming equidistant by a minimum distance \( u_{\text{min}} \). However, the ions closer to the edges of the chain are less bounded by Coulomb interaction and are spaced farther apart. We will restrict the rest of our discussion to the 1D ICC, which is the ideal ICC case to have in SRQC.

A. THE EQUILIBRIUM POSITIONS OF AN ION CHAIN

In the SRQC, it will be useful to distinguish between individual ions in the ICC. We use ordered labels: if \( z_k(t) \) is the position of ion \( k \) in the ICC, then \( z_{k+1}(t) \geq z_k(t) \). The potential \( V \) for an ion chain with \( N \) ions is [9, 30]:

\[
V = \sum_{k=1}^{N} \frac{1}{2} m \omega^2 z_k^2(t) + \sum_{k \neq n}^{N} \frac{e^2}{8 \pi \varepsilon_0} \frac{1}{|z_n(t) - z_k(t)|},
\]

(2)

where the first term corresponds to the trap potential and the second term to the Coulomb interaction between any pair of ions. In (2), \( m \) is the mass of the ions, \( e \) the fundamental electric charge, \( \varepsilon_0 \) the permittivity of free space, and \( \omega \) the trap frequency, which quantifies the strength of the trap potential [9]. The equilibrium positions of the ions in the chain, where \( z_k^0 \) corresponds to the equilibrium position of ion \( k \), are such that they minimize the potential (2), i.e.,

\[
\frac{\partial V}{\partial z_k}(z_k^0) = 0.
\]

(3)

When evaluating explicitly for the potential \( V \) in (3), it is convenient to introduce a length scale \( l \) that groups all the constants, where \( l^3 = e^2/4\pi \varepsilon_0 m \omega^2 \). This results in dimensionless coordinates

\[
u_k = \frac{z_k}{l}.
\]

(4)

For a given \( N \), the equilibrium position \( u_k \) of ion \( k \) in the ICC can be determined by simultaneously solving the nonlinear system of algebraic equations:

\[
u_k - \sum_{n=1}^{k-1} \frac{1}{(u_k - u_n)^2} + \sum_{n=k+1}^{N} \frac{1}{(u_k - u_n)^2} = 0,
\]

(5)

for \( k = 1, \ldots, N \).

B. NUMERICAL SOLUTION

We solve (5) using a nonlinear equation solver based on a minimization of least squares with the Levenberg-Marquardt method [31]. For representative values of \( N \), Fig. 1 shows the corresponding solutions \( u_1, \ldots, u_N \), where the vertical axis is the equilibrium position \( u_k \), and there is a common horizontal axis for comparison. Fig. 2 shows the normalized equilibrium positions \( u_k / u_{\text{max}} \), with \( u_{\text{max}} \) the position of the last ion in the chain.

Fig. 3 shows the separation between adjacent ions,

\[
\Delta u_k = u_{k+1} - u_k,
\]

(6)

where the ions near the ICC center converge to a minimum separation value [9]

\[
\Delta u_{\text{min}} \approx \frac{2.018}{N^{0.559}},
\]

(7)

and the ions near the edge of the chain are spaced farther apart from each other.
FIGURE 2. The normalized equilibrium positions of ICC, which are more convenient for processing.

FIGURE 3. The distance between adjacent ions in the ICC for different values of $N$. Note that $\Delta u_k$ converges to a finite distance as $N$ becomes larger.

III. RAPID CALCULATION OF THE ICC BASELINE STATE USING A NEURAL NETWORK

One alternative calculation approach to solve (5) faster is to use ML tools like NN. NN are non-linear mappings between the input variables and the target output [32]. NN have a fixed topology [7] with layers of interconnected unit cells. Each unit cell corresponds to a non-linear function, called activation function, and the connections between unit cells are characterized by a weight. Training a NN means finding appropriate weight values so that the NN correctly reproduces the target output of the training data examples [32]. Once trained, the NN should accurately predict generalized solutions not present in the training set. To populate a training data set for the NN, we solve (5) for different cases of $N$ using numerical methods [31]. For the NN to learn the relevant data features, the training data set needs to be representative of the range of solutions that we are interested for SRQC.

Finally, Fig. 4 shows the time needed to solve (5) as a function of $N$.

This numerical approach quickly becomes impractical as the computation time grows as $\sim N^3$, which is expected for matrices with $N^2$ elements. This motivates the exploration of alternative methods to determine the equilibrium positions of ions in an ICC. This is important for SRQC, which will manipulate long ICC formed by thousands of ions.

For this work, we used two different CPU computation systems to expedite the calculations; a workstation (Intel Core i9, 8 cores, 3.6 GHz), and the THETA supercomputer at the Argonne Leadership Computer Facility (ALCF) [6] (Intel Xeon Phi 2nd generation, various core allocations). We find similar computation times with these two processors, as shown in Fig. 4.

5 Matrix inversion typically needs $O(n^3)$ floating point operations, where $n$ is the number of elements of the matrix.

6 The ALCF is a U.S. Department of Energy User Facility. It provides an invaluable computational resource that enables a multidisciplinary scientific and engineering community with the expertise and supercomputing resources to support large-scale projects in order to solve some of the world’s most complex and challenging scientific problems, including those involving artificial intelligence.

A. TRAINING ON A PARAMETERIZED MODEL

Here we describe a NN implementation using PyTorch [33] that quickly produces the solutions to (5) given a limited amount of explicitly calculated solutions. This NN takes the...
number of ions $N$ as input and returns a set of five fitting parameters. We exploit the symmetry of the solutions, see Fig. 1 or Fig. 2, by training the NN to predict the five fitting parameters that accurately fit the positive half of the solution, reducing the NN training time.

1) MODEL FITTING

We use the non-linear least-squares method fitting package `lmfit` [34] to approximate the positive side of the solutions shown in Fig. 2. We use a model

$$g_N(x) = a_N x^2 + b_N x + c_N + d_N \exp(x/f_N),$$  \hspace{1cm} (8)

with quadratic and exponential terms to fit the non-linear behavior far from the chain center. Fig. 6 shows the resulting normalized fitting parameters as a function of the number of ions $N$. Using a polynomial fit alone is not ideal since it gives oscillating values around the points at the edge of the curve, which increases the error in the fitting. Similarly, trying to extrapolate to different values of $N$ from the model $g_N$ alone does not perform as well as using NN [35]. The NN is effectively a model describing more complex features than the fitting model $g_N$.

2) DATA PROCESSING

After fitting the solutions in the training data set according to the model (8), we find that some data points change significantly with respect to the general trend. If this change is more than 50% relative to the adjacent point, we remove it from the data set. The resulting data set is then split randomly so that 70% of the data points are used for training, and the remaining 30% are used for validation of the NN, i.e. to test that the trained NN model correctly predicts the examples on the validation set. Fig. 6 also shows which data points were used for training and for validation.

3) NEURAL NETWORK AND PREDICTIONS

We propose a single layer feed-forward NN that takes the single input $N$ into a hidden layer with 64 unit cells and then into an output layer with 5 output cells, one for each of the fitting parameters ($a_N$, $b_N$, $c_N$, $d_N$, $f_N$). We choose the hyperbolic tangent $\tanh$ as the activation function. This gives almost identical results as the sigmoid function, while the commonly used Rectified Linear Unit (ReLU) function is not well suited for shallow networks.

The non-linear properties of a NN using ReLU appear when several layers are added. Therefore ReLU does not add a lot of non-linearity for a single layer NN.
Once the NN model is trained, we can make predictions on the fitting parameters that correspond to the input $N$ of our choice. Figs. 7 and 8 show the results for $N = 1000$ and $N = 2000$, correspondingly. The top plot in both figures shows the numerical solution, compared to the resulting approximated solution that uses the NN-predicted fitting parameters. The bottom plots in both figures show the three errors, defined as the following simple differences: between predicted and true, between fitted and true, and between fitted and predicted solutions. It can be noted that the errors are more significant at the edge of the chain and are more accurate at the center. Similarly, the error is larger when the fitted model is used, i.e., when reconstructing the real solution. Fig. 9 shows the error distribution for the two examples of reconstructed solutions. The corresponding sum of squared errors for $N = 1000$ and $N = 2000$ is 3.41 and 8.65 respectively. This error becomes larger for increasing values of $N$, possibly due to less available training data in this regime.

IV. DISCUSSION
Quantum computers based on ion traps are limited by the small number of ions that can be used as qubits. The storage ring quantum computer can potentially store thousands of ions to form an Ion Coulomb Crystal in a closed trajectory. For SRQC, we anticipate unique challenges associated with the unprecedented large number of ions in the ICC. For example, on timing the laser pulses to efficiently cool the ICC beam to its equilibrium energy configuration, from which ion manipulations can be initiated.

The solutions to the equilibrium positions of the ICC can be solved numerically for an arbitrary $N$, but they quickly become lengthy and impractical as $N \gg 1$, taking from hours to days. Here we described a simple NN that is able to predict the equilibrium positions of ions in the ICC, given a limited amount of numerical solutions available for training. Our NN model can predict multiple solutions within the range of the existing training data. Training the NN takes approximately two hours on a laptop (Nvidia GeForce GTX 1050 GPU). With the NN trained, prediction of the fitting parameters and reconstruction of the equilibrium positions takes only a few seconds, thus proving a valuable resource for determining multiple solutions that have not been calculated using numerical methods, e.g., all the possible solutions in between the ones used for training the NN, which took long times as illustrated in Fig. 4. The error in the NN prediction grows as the requested solution drifts away from the training data set. We are looking into extrapolating the NN prediction range to numbers beyond the range of available training data. We are also interested in expanding our model to include deviations from the ideal 1D ICC.

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