Quantum reservoir computing of thermal convection flow

Philipp Pfeffer,1 Florian Heyder,1 and Jörg Schumacher1,2
1Institut für Thermo- und Fluiddynamik, Technische Universität Ilmenau, Postfach 100565, D-98684 Ilmenau, Germany
2Tandon School of Engineering, New York University, New York City, NY 11201, USA
(Dated: May 2, 2022)

We simulate the nonlinear chaotic dynamics of Lorenz-type models for a classical two-dimensional thermal convection flow with 3 and 8 degrees of freedom by a hybrid quantum–classical reservoir computing model. The high-dimensional quantum reservoir dynamics is established by universal quantum gates that rotate and entangle the individual qubits of the tensor product quantum state. A comparison of the quantum reservoir computing model with its classical counterpart shows that the same prediction and reconstruction capabilities of classical reservoirs with thousands of perceptrons can be obtained by a few strongly entangled qubits. We demonstrate that the mean squared error between model output and ground truth in the test phase of the quantum reservoir computing algorithm increases when the reservoir is decomposed into separable subsets of qubits. Furthermore, the quantum reservoir computing model is implemented on a real noisy IBM quantum computer for up to 7 qubits. Our work thus opens the door to model the dynamics of classical complex systems in a high-dimensional phase space effectively with an algorithm that requires a small number of qubits.

I. INTRODUCTION

Quantum computing (QC) and machine learning (ML) have changed our ways to process data fundamentally in the last years [1][4]. Quantum algorithms accelerated the data search [5] or improved the sampling of probability distributions [6][7]. These quantum advantages found already their way to various applications [8][10], even though we are still in the era of noisy intermediate scale quantum (NISQ) devices that suffer from decoherence and are limited to qubit numbers $\sim 10^2$ with resulting shallow quantum circuit depths [11].

Meanwhile, ML algorithms in the form of deep convolutional neural networks extract features effectively and classify big data bases [12][15]. Quantum machine learning ports such methods to a quantum computer [16][18] with the prospect that particularly high-dimensional problems can be solved much faster than with their classical counterparts. This expectation arises from two facts, (i) the data space dimension grows exponentially as $2^n$ with the number of qubits $n$, the smallest unit of information in QC; (ii) the entanglement of qubits creates highly correlated tensor product states that can represent complex features in the data effectively [19]. Thus, for example, quantum support vector machines are expected to have the potential to determine nonlinear decision boundaries of classification problems in high-dimensional quantum enhanced feature Hilbert spaces more efficiently [20][22].

Recurrent neural networks (RNN) are specific ML algorithms with internal feedback loops which predict the time evolution of dynamical systems without knowing the underlying nonlinear ordinary or partial differential equations; they can be implemented either as gated RNNs in the form of long short-term memory networks [23] or as reservoir computing models (RCM) [24][28]. As a consequence, RNNs have been used for the description of chaotic dynamics, fluid mechanical problems, and even turbulence [29][32]. RCMs were also applied to represent low-dimensional chaotic models, one-dimensional Kuramoto-Sivashinsky equations [33][34], or even turbulent Rayleigh-Bénard convection [35][36]. At the center of the RCM is the reservoir, a randomly initialized and fixed high-dimensional network of perceptrons which is represented by an adjacency matrix. This specific implementation of an RNN requires only an optimization of the output layer, which maps the reservoir state back to the data space, and avoids costly backpropagation as required in most other ML algorithms [14].

In this work, we combine quantum algorithms with reservoir computing to a gate-based quantum reservoir computing model (QRCM) for a universal quantum computer to predict and reconstruct the dynamics of a thermal convection flow in the weakly nonlinear regime. The algorithm is of hybrid quantum-classical nature since the optimization of the output map is done by a classical ridge regression. The quantum reservoir is composed of a sequence of elementary single and two-qubit quantum gates which form a complex quantum circuit. Following the axioms of quantum mechanics, an elementary quantum gate performs a unitary transformation to a single- or two-qubit state. As a consequence, a highly entangled multi-qubit state will result which is a tensor product state of single qubits.

Our first contribution is to demonstrate the feasibility of such QRCM to describe the classical chaotic dynamics of a thermal convection flow on an actual NISQ device. The description of the thermal convection flow is based on Lorenz-type Galerkin models with $N_{dof} \leq 8$ degrees of freedom [39][43]. This class of models is directly derived from the Boussinesq equations of two-dimensional thermal convection between two impermeable parallel plates, heated uniformly from below and cooled from above with free-slip boundary conditions for the velocity field [44][45]. Here, we explore QRCMs in two different modes of operation [46].
QRCM investigations, such as in the form of spin ensemble dynamics \cite{19}. The present work also extends previous consequence of the linearity and unitarity of the quantum computing models differ essentially, which is primarily a to each other. Note that classical and quantum reservoir hyperparameters in both approaches that can be related to its classical counterpart for the same flow. We identify Ntem, W, N, and for (b), N \ll N_{\text{dof}}.

1. Closed-loop scenario: a fully autonomous prediction of the temporal dynamics of all degrees of freedom of a Lorenz 63 model with N_{\text{dof}} = 3. This study is done by a quantum computation applying the ideal Qiskit quantum simulator \cite{47}, see the sketch in Fig. 1(a).

2. Open-loop scenario: a reconstruction of the temporal dynamics of a Lorenz-type model with N_{\text{dof}} = 8. In this case, one or two degrees of freedom are continually fed into the quantum reservoir and the remaining degrees of freedom are obtained by the QRCM evolution, see Fig. 1(b). This investigation is done in two different ways. First, we reconstruct the whole model from a single degree of freedom (N_{\text{in}} = 1) by means of the open loop structure in an ideal Qiskit simulator. Secondly, we strongly reduce the number of quantum gates to even demonstrate the feasibility of QRCM on a real noisy IBM quantum computer.

Secondly, we directly compare the results of the QRCM to its classical counterpart for the same flow. We identify hyperparameters in both approaches that can be related to each other. Note that classical and quantum reservoir computing models differ essentially, which is primarily a consequence of the linearity and unitarity of the quantum dynamics \cite{19}. The present work also extends previous QRCM investigations, such as in the form of spin ensembles \cite{48,50}, single nonlinear oscillators \cite{51}, and smaller universal quantum circuits \cite{52,53} that have been applied for the one-step prediction of one-dimensional time series or solutions of the Mackey-Glass time-delay differential equation, see also ref. \cite{54} for a compact review. This is similar to the open–loop scenario with N_{\text{in}} = N_{\text{dof}}.

It is finally demonstrated that a systematic reduction of the degree of entanglement in the quantum reservoir by a stepwise transition from a fully to a weakly entangled configuration reduces the performance of the present QRCM algorithm. More detailed, this is done by the division of an n-qubit reservoir state into blocks of entangled p-qubit states, so called p-blocks \cite{55}. The strong encoding capabilities of fully entangled quantum reservoirs are demonstrated in the present flow case by runs with qubit numbers n \ll N_{\text{dof}}. Also, we show for the open-loop scenario, that the number of operations of the QRCM circuit can be scaled with O(n) < O(2^n) (where 2^n is the reservoir size) which can eventually give rise to a quantum advantage.

Our work opens the door for the application of quantum machine learning as a reduced-order dynamical model of a higher-dimensional classical complex dynamical nonlinear system. The study thus adds a further proof-of-concept for the potential use of quantum algorithms in studying turbulent flows.

The outline is as follows. In section II, we present the thermal convection flow model; technical details are collected in appendix A. Section III is dedicated to the closed loop scenario. In section IV the complexity of the quantum machine learning task is enhanced to the 8-dimensional model for which we apply an open–loop QRCM. We summarize our work and give a brief outlook in section V.

II. THERMAL CONVECTION FLOW

We start with a compact description of the flow. The thermal convection flow consists of a two-dimensional fluid layer which is heated uniformly from below with a temperature \( T_{\text{bot}} \) and cooled from above with \( T_{\text{top}} \), thus giving \( \Delta T = T_{\text{bot}} - T_{\text{top}} > 0 \). The convection flow domain is \( A = [0,1] \times [0,1] \). The velocity \( \mathbf{u}(x,t) = (u_x(x,z,t), u_z(x,z,t)) \) and (total) temperature \( T(x,z,t) \) are coupled by the balances of mass, momentum, and energy. The fluid is incompressible and the mass density \( \rho \) depends linearly on \( \theta \) in the buoyancy term only, known as the Boussinesq approximation in thermal convection \cite{45}. The total temperature is decomposed into \( T(x,z,t) = 1 - z + \theta(x,z,t) \) where \( T_{\text{eq}}(z) = 1 - z \) is the static equilibrium profile and \( \theta(x,z,t) \) is the temperature deviation. The non-dimensional equations are then given

\[
\frac{\partial \mathbf{u}}{\partial t} + \nabla \cdot (\mathbf{u} \mathbf{u}) = -\nabla p + \mathbf{f} + \frac{1}{Re} \nabla^2 \mathbf{u} \\
\nabla \cdot \mathbf{u} = 0 \\
\frac{\partial \theta}{\partial t} + \mathbf{u} \cdot \nabla \theta = \mathbf{f} \cdot \nabla \theta + \frac{1}{Pr} \nabla^2 \theta
\]

where \( \mathbf{f} = (0,0,\Delta T) \) is the buoyancy force and \( Re = \frac{\rho u \Delta}{\mu} \) is the Reynolds number.
FIG. 2: Quantum reservoir computing model (QRCM) for the Lorenz 63 dynamical system. (a) Two instantaneous convection flow states which display the velocity vector field \((u_x, u_z)\) together with the total temperature field \(T\) as a colored background (blue for \(T_{\text{top}}\) and red for \(T_{\text{bot}}\)). (b) Circuit diagram for the QRCM. Here \((x_1, x_2, x_3) = (A_1, B_1, B_2)\). The three groups of unitary operations are indicated by differently colored boxes. (c) Trajectory plot of the Lorenz 63 system in the phase space which is spanned by one stream function mode \(A_1(t)\) and two temperature modes, \(B_1(t)\) and \(B_2(t)\), i.e., \(N = 1\) and \(M = 2\). (d) Comparison of classical and quantum reservoir computing in the prediction phase (yellow background). Time is rescaled by the largest Lyapunov exponent \(\lambda_1 = 0.9056\), see e.g. ref. [56]. The two flow configurations in (a) are also indicated in panels (c,d). (e) Mean squared error (MSE) as a function of the leaking rate \(\varepsilon\) and the number of qubits \(n\). The model parameter are \(\sigma = 10\), \(b = 8/3\), and \(r = 28\). All displayed QRCM runs are done with the Qiskit simulator.

by

\[
\nabla \cdot u = 0, \quad \frac{\partial u}{\partial t} + (u \cdot \nabla)u = -\nabla p + \sigma \nabla^2 u + Ra \sigma \theta e_z, \quad \frac{\partial \theta}{\partial t} + (u \cdot \nabla)\theta = \nabla^2 \theta + u_z.
\]

The Rayleigh number \(Ra\) and the Prandtl number \(\sigma\) are the two parameters that characterize the strength of the thermal driving via the temperature difference \(\Delta T\) and the ratio of momentum to temperature diffusion, respectively. The boundary conditions in \(x\)-direction are periodic. At \(z = 0, 1\), one takes

\[
\left. u_z \right|_{z=0,1} = 0, \quad \frac{\partial u_z}{\partial z} \bigg|_{z=0,1} = 0 \quad \text{and} \quad \left. \frac{\partial \theta}{\partial z} \right|_{z=0,1} = 0.
\]

They correspond to isothermal, impermeable, free-slip walls. Incompressibility and two-dimensionality allow to reduce the velocity vector field further to a scalar stream function \(\zeta(x, z, t)\) by

\[
\begin{align*}
    u_x &= -\frac{\partial \zeta}{\partial z} \quad \text{and} \quad u_z = \frac{\partial \zeta}{\partial x}.
\end{align*}
\]

This ansatz satisfies (1) automatically and the equations of motion (2)–(3) are now given by

\[
\begin{align*}
    \frac{\partial \nabla^2 \zeta}{\partial t} &= \frac{\partial \zeta}{\partial z} \frac{\partial \nabla^2 \zeta}{\partial x} - \frac{\partial \zeta}{\partial x} \frac{\partial \nabla^2 \zeta}{\partial z} + \sigma \nabla^4 \zeta + Ra \sigma \frac{\partial \theta}{\partial x}, \\
    \frac{\partial \theta}{\partial t} &= \frac{\partial \zeta}{\partial z} \frac{\partial \theta}{\partial x} - \frac{\partial \zeta}{\partial x} \frac{\partial \theta}{\partial z} + \nabla^2 \theta + \frac{\partial \zeta}{\partial x},
\end{align*}
\]

with boundary conditions in the vertical direction

\[
\left. \zeta \right|_{z=0,1} = 0, \quad \left. \frac{\partial^2 \zeta}{\partial z^2} \right|_{z=0,1} = 0 \quad \text{and} \quad \left. \frac{\partial \theta}{\partial z} \right|_{z=0,1} = 0.
\]

Equations (6) and (7) are then reduced by an expansion into trigonometric Fourier modes which satisfy the boundary conditions for the stream function and temperature and encode the spatial structure of the thermal convection flow, see appendix A for further technical details. A subsequent truncation to \(N\) and \(M\) real time-dependent amplitudes is done for the stream function, \(\{A_1(\tau), \ldots, A_N(\tau)\}\), and the temperature, \(\{B_1(\tau), \ldots, B_M(\tau)\}\), respectively.

This step leads to a class of low-dimensional Lorenz-type Galerkin models of the thermal convection flow.
starting with the original three-dimensional Lorenz 63 model [39] for \( N = 1 \) and \( M = 2 \) (where \( N_{\text{tot}} = N + M \)). The resulting coupled nonlinear system of ordinary differential equations is given by

\[
\frac{dA_i}{d\tau} = F_i(A_j, B_k, \sigma, r, b), \quad (9)
\]

\[
\frac{dB_k}{d\tau} = G_k(B_l, A_i, \sigma, r, b), \quad (10)
\]

for \( i, j = 1 \ldots N \) and \( k, l = 1 \ldots M \). Here, \( \sigma \) is again the Prandtl number, \( r \) the relative Rayleigh number, and \( b \) an aspect ratio parameter, see appendix A. Furthermore, \( F_i \) and \( G_k \) are quadratic nonlinear functions of the amplitudes \( A_i(\tau) \) and \( B_k(\tau) \). We will consider two implementations, the Lorenz 63 model (L63) [39] with \( N = 1 \) and \( M = 2 \) and an extended 8-dimensional model [42] with \( N = M = 4 \) that introduces shear in the flow and causes tilted convection rolls and shearing motion. It thus displays a more complex fluid motion further away from the primary instability point at \( r = 1 \) or \( R_{\alpha} = 27\pi^3/4 \) [44].

Figures 2(a) shows two instances of the temperature and velocity fields with the counter-rotating circulation rolls that cause a rise of warm and a descent of cold fluid. These two flow states correspond to trajectory points of L63 in each of the two butterfly-like wings in panel (c) of the same figure.

III. CLOSED-LOOP SCENARIO FOR THREE-DIMENSIONAL LORENZ MODEL

A. Quantum reservoir and classical data input

The design of our time-discrete and gate-based QRCM builds on a \( n \)-qubit tensor product state at time \( t \). In appendix B, we provide a compact primer on qubits and tensor product spaces. The \( n \)-qubit state in Dirac notation [19] is given by

\[
|\psi^t\rangle = \sum_{k=1}^{N_{\text{res}}} a_k^t |k\rangle \quad \text{with} \quad a_k^t \in \mathbb{C},
\]

(11)

with \( N_{\text{res}} = 2^n \). Here \( |k\rangle \) is the standard basis of the \( n \)-qubit quantum register. The pure state density operator \( \rho^t \) is given by the outer product of the quantum state with itself,

\[
\rho^t = |\psi^t\rangle \langle \psi^t| = \sum_{k=1}^{2^n} p_k^t |k\rangle \langle k| \quad \text{with} \quad \sum_{k=1}^{2^n} p_k^t = 1.
\]

(12)

The reservoir state evolves from time step \( t \) to \( t + 1 \) as follows. First, the dynamical part is updated by three blocks of unitary linear transformations

\[
|\psi^{t+1}\rangle = U(\beta) U(4\pi x^t) U(4\pi p^t) |0\rangle,
\]

(13)

with rotation angles \( \beta = (\beta_1, ..., \beta_n) \), reservoir state probability amplitudes \( p^t = (p_1^t, ..., p_{2^n}) \), and the past system state vector \( x^t = (x_1^t, ..., x_{N+M}^t) \), the latter of which summarizes \( (A_1, ..., B_M) \). The \( n \)-qubit state vector \( |0\rangle \) is the ground state of the quantum register. With eq. (12) for the probability amplitudes \( \tilde{p}_k^{t+1} \) out of \( |\psi^{t+1}\rangle \) from eq. (13), the RCM update step outside the quantum reservoir is given by the following iteration

\[
\tilde{p}_k^{t+1} = (1 - \varepsilon) p_k^t + \varepsilon \tilde{p}_k^{t+1}.
\]

(14)

See also equation (C5) in appendix C. The equation contains a leaking rate \( 0 \leq \varepsilon \leq 1 \) that blends update and past state and thus represents a short-term memory, see also appendix B. More detailed, the unitary transformation consists of single-qubit rotation gates \( R_Y \) and subsequent two-qubit controlled NOT (in short CNOT) gates. The \( R_Y \)-gate is defined by

\[
R_Y(x) = \begin{pmatrix}
\cos(x/2) & -\sin(x/2) \\
\sin(x/2) & \cos(x/2)
\end{pmatrix}.
\]

B. Quantum reservoir readout and classical optimization

A projection-valued measure in the standard basis of the Pauli-Z operator provides the probabilities \( p_k^t \) from \( K \gg 2^n \) independent circuit simulations, know as shots.
These probabilities are mapped to the updated dynamical system state by the output matrix,

\[ x_t^f = \sum_{k=1}^{2^n} W^\text{out*}_{ik} p_k^t, \]

with the optimized weights which are summarized in the matrix \( W^\text{out*} \in \mathbb{R}^{(N+M) \times N_{\text{res}}} \). We note once more that the output matrix is optimized by a classical algorithm similar to the classical RCM case. This optimization seeks a minimum of the cost function \( C(W^\text{out}) \) which is given in appendix C.

Panel (d) of figure 2 and table 1 compare the classical and quantum RCM with the numerical simulation of the equations of motion obtained by a 4th-order Runge-Kutta method. The integration time is rescaled by the largest Lyapunov exponent of the system, \( \lambda_1 = 0.9056 \), which quantifies the deterministic chaos of the model [53]. The training phase comprises \( N_{\text{train}} = 2000 \) integration time steps, both for the classical and quantum case. For times \( t \geq 0 \) the reservoirs are exposed to unseen test data predicting the dynamics autonomously. It is seen that the prediction horizon of the QRCM with 9 qubits is about 1.5 \( \lambda_1 t \). The noise in the Qiskit simulator causes a switch of the trajectory into the other wing of the butterfly-like Lorenz attractor. The leaking rate in this example is \( \varepsilon = 0.05 \).

Two hyperparameters are varied, the leaking rate \( \varepsilon \) and the number of qubits \( n \) that determines the reservoir dimension \( N_{\text{res}} \). We identify a minimum of the cost function in the form of a mean squared error (MSE) around \( \varepsilon = 0.025 \). The larger the number of qubits the smaller MSE, although the improvements in the Qiskit simulations remain small (and thus the difference of the displayed to the optimal case). A small leaking rate implies that the reservoir dynamics is memory-dominated blended with a small nonlinear contribution [58]. We have listed all details on the classical reservoir computing model, the hyperparameters, and the cost function in appendix C in order to keep the work self-contained.

### IV. OPEN-LOOP SCENARIO FOR 8-DIMENSIONAL LORENZ-TYPE MODEL

#### A. Quantum reservoir with one continually available degree of freedom

We proceed from the standard L63 model to an extension with 8 degrees of freedom, which is listed and explained further in appendix A. As shown by Gluhovsky et al. [42], this extension can be decomposed into subgroups, so-called gyrostats. The model conserves total energy and vorticity. They are given by

\[ E(t) = \frac{1}{2A} \int_A \left((\nabla \varsigma)^2 - z \theta\right) dA, \]

with a kinetic and potential energy term and

\[ \Omega(t) = \frac{1}{A} \int_A \omega \, dA, \]

with the vorticity \( \omega = -\nabla^2 \varsigma \) and the convection domain size \( A \). The open-loop scenario of the QRCM implies that a subset of the degrees of freedom will remain continually available in the reconstruction phase after the training phase. In this subsection, we will take \( N_{\text{in}} = 1 \) which will be \( A_4(t) \). The leading Lyapunov exponent was computed numerically by a method proposed in [59] and turned out to be \( \lambda_1 = 0.825 \).

Figure 3 displays the results for the 8-dimensional Lorenz-type model which receives the time series \( A_4(t) \) to reconstruct the remaining 7 degrees of freedom of the thermal convection flow model. Panel (a) compares the times series of the ground truth (GT) with the results of a classical RCM (CRCM), and a QRCM which was run on \( n = 7 \) qubits on an ideal Qiskit simulator. We see that the data remain closely together for the displayed interval of over 16 Lyapunov time units. The QRCM runs through a training phase of \( N_{\text{train}} = 2000 \) integration time steps and a leaking rate \( \varepsilon = 0.05 \). Figure 3(b) displays the reconstructed convection flow at four instants. The 8-dimensional model incorporates the shearing modes which are missing in the lower-dimensional Lorenz 63 model and lead to tilted convection cells, as can be seen in the panels.
FIG. 3: Comparison of the 8-dimensional Lorenz-type model, time-integrated system of equations as ground truth (GT), classical reservoir computing model (CRC), and quantum reservoir computing model (QRC). Panel (a) displays the time evolution of all variables. (b) Reconstruction of the flow and temperature fields at times $t_1$ to $t_4$ which are indicated in $A_1(t)$. The model parameters are $\sigma = 10$, $b = 8/3$, and $r = 28$. Here, $N = 4$ and $M = 4$. Mode $A_4$ is the only input and always given accurately into each reservoir.

The dimension of the quantum reservoir is $N_{\text{res}} = 128$, while the one of the CRCM in Fig. 3 is $N_{\text{res}} = 1024$. We have thus reduced the dimension of the CRCM and compare the mean squared error (MSE) as a function of $N_{\text{res}}$ in Table II. The MSE is here given as

$$\text{MSE} = \frac{1}{T_{\text{test}}} \sum_{t=1}^{T_{\text{test}}} |x^t - x_{tg}^t|^2,$$

(18)

see also eq. (15) and $T_{\text{test}} = 2000$. Subscript $tg$ stands for target and denotes the ground truth (GT) which is obtained by time integration of the eqns. (9) and (10). As the table shows, the MSE of the CRCM increases with decreasing reservoir size. The MSE of the QRCM corresponds to a classical reservoir size between $N_{\text{res}} = 512$ and 1024, which is almost one order of magnitude larger which clearly confirms the encoding capabilities of the QRCM.

| Model   | $N_{\text{res}}$ | MSE     |
|---------|------------------|---------|
| CRCM1   | 2048             | $0.8 \cdot 10^{-3}$ |
| CRCM2   | 1024             | $1.2 \cdot 10^{-3}$ |
| CRCM3   | 512              | $2.3 \cdot 10^{-3}$ |
| CRCM4   | 128              | $3.5 \cdot 10^{-3}$ |
| QRCM    | 128              | $1.6 \cdot 10^{-3}$ |

TABLE II: Comparison of classical and quantum reservoir computing models in the reconstruction phase. The remaining hyperparameters remain fixed.

B. Implementation on an actual quantum device

The 8-dimensional convection flow model is finally implemented on an actual noisy quantum device. Figure 4(a) displays the quantum reservoir for the implementation. The circuit depth on the real devices is
FIG. 4: Quantum reservoir computing model run of the 8-dimensional time-integrated Lorenz-type model an actual quantum device. (a) Sketch of the quantum reservoir which had to be reduced due to decoherence in comparison with the one that is displayed in Fig. 2. (b) Time series of the extended Lorenz model. We compare the ground truth (Model) with an ideal and noisy Qiskit simulator and the 7–qubit quantum computer (IBM Q). The number of training steps was again $N_{\text{train}} = 2000$ and the leaking rate $\varepsilon = 0.2$. The two degrees of freedom that are continually available in the reconstruction phase are indicated. (c) Connection of the 7 qubits on the ibmq_perth quantum computer.

still rather limited by the decoherence of the elementary quantum gates that are installed in the form of microwave-controlled superconducting SQUIDs. The figure shows that we had to reduce the original three-block-structure of the quantum reservoir to one block. Two further steps were necessary: (1) Instead of one continually available variable in the reconstruction phase, we provide now $A_4(t)$ and $B_3(t)$. (2) Only 12 out of the 128 components of the reservoir state measurement vector $\mathbf{p}$ are fed back into reservoir together with the two degrees of freedom. The total qubit number was limited to $n = 7$. The studies were conducted on two devices, ibmq_ehningen, a 27–qubit quantum computer in Germany, and ibmq_perth, a 7-qubit machine. Figure 4(c) displays the arrangement of the 7 qubits on ibmq_perth. Entanglement operations, e.g. by C-NOT gates, are only possible for qubits which are connected by the bars in the panel. No error correction was performed.

We backed up this investigation by two runs on the Qiskit simulator with the same configuration. One is the ideal simulator that has been used already before. The other simulation was done on a noisy Qiskit simulator for which you can prescribe the probabilities of measurement errors, here $p_m = 0.05$, gate errors, here $p = 0.1$, and qubit resets, here $p_r = 0.03$. Values have been chosen such that they come close to those on the real devices. All environments are compared in Fig. 4(b). The data from the noisy Qiskit simulator and the real quantum device do partly deviate, but are found to follow the overall trend fairly well. This proves the concept of an QRRCM for a classical dynamical system on a NISQ device.

C. Stepwise reduction of reservoir entanglement and quantum advantage

Finally, we investigated if a simulation of the Lorenz-type model with the simpler quantum reservoir than from Fig. 4(a) is successful when the corresponding quantum circuit is decomposed into several $p$-qubit-blocks which are disentangled. If $p = n$ the circuit is fully entangled, for $p = 1$ the $n$-qubit quantum state is separable; see appendix B for the definitions of both possible multi-qubit quantum states. The decomposition is illustrated in Figs. 5(b,c). The rational behind this analysis, which we did with the ideal Qiskit simulator for $n = 8$, is that a $p$-blocked structure might be simulated efficiently on a classical computer loosing the quantum advantage [55].

In Fig. 5(a), we summarize the MSE in a diagram for circuits with $3 \leq n \leq 8$ and possible block size $2 \leq p \leq 8$. For example, $n = 4$ and $p = 3$ imply that a single qubit remains which is disentangled from the 3-qubit-block. In general, the number of blocks of size $p$ follows by $n_p = \lfloor n/p \rfloor$. All reservoirs were trained, the simulations were carried out for different 100 seeds of the quantum reservoir. The block diagram shows that the MSE decreases when block size is increased. We can conclude from this analysis that the entanglement of the
FIG. 5: Performance of the quantum reservoir computing model for different reservoir architectures. (a) Mean squared error on a logarithmic scale as a function of the total number of qubits and the size of the blocks of entangled qubits. The dark cells in the lower left stand for impossible decompositions. (b) Sketch of an example case. Fully entangled 4-qubit-quantum circuit which is the normal setting. (c) Two 2-qubit blocks ($p = 2$) build the 4-qubit-quantum circuit.

qubits in the reservoir is essential for the performance of the QRCM. This is different compared to the classical reservoir which is a sparse network for which 20% of the network nodes are actively only, but the number of perceptrons is by 2 to 3 order of magnitude larger in comparison to the number of qubits of the quantum reservoir.

In a final discussion of a prospective quantum advantage of the algorithm, we stress that the main computational effort of a single time step lies in the calculation of the leaking rate equation (12). This effort scales linearly with the number of reservoir states $N = 2^n$. In detail, one needs $3N$ operations to multiply each vector with the corresponding prefactor to add them subsequently. The dynamical part in its simplest form can be seen in the circuit scheme of Fig. 4(a). There, the 7 qubit circuit with $N = 128$ states needs 20 operations only, whereas a classical counterpart, cf. eq. (C5), would require more operations than states to produce a comparable dynamical counterpart. For a further more comprehensive analysis, it would be necessary to determine if the layer depth – 3 gate operations per qubit in our case – can be held constant for a larger number of qubits. This would result in a clear quantum advantage for the dynamical part of the reservoir update equation.

V. SUMMARY AND OUTLOOK

The main objective of our present work was to show the feasibility of a quantum reservoir computing model to predict and to reproduce the dynamical evolution of a classical, nonlinear thermal convection flow, on an actual quantum computer with up to 7 superconducting qubits. In a nutshell, quantum reservoir computing models are recurrent machine learning algorithms for which the reservoir state is built by a highly entangled tensor product quantum state that grows exponentially in dimension with the number of qubits.

Our work showed that a quantum reservoir has a qubit number that is by 2 to 3 orders smaller than that of the perceptrons in a classical one. On the one hand, we could thus take advantage of the data compression capabilities of quantum machine learning algorithms where the dimension of the data space grows exponentially with the number of qubits which is essential for the modeling of higher-dimensional nonlinear dynamical systems. On the other hand, it shows that a classical reservoir state which is caused by a sparsely occupied network matrix of dimension $\gtrsim 10^3$ can be substituted by a highly entangled quantum state that is caused by the application of unitary transformations. The qubit number was $n < 10$ in the present case.

The study can be extended into several directions. It is clear that the present thermal convection flow model is still very low-dimensional and thus far away from convective turbulence. Our efforts should be considered as one first step to model real fluid flows on a quantum computer, a possible route beside other directions, such as quantum embeddings of nonlinear dynamical systems by the Koopman operator framework [60] or variational quantum algorithms for the direct solution of the equations of motion [61], see also ref. [66] for further directions such as lattice Boltzmann methods. Extensions to
higher-dimensional models are currently still limited by the technological capabilities of quantum computers. As the technological progress in this field is very rapidly, it can be expected that Galerkin models with significantly more modes will be modeled on upcoming devices with chips with a higher noise-resilience and lower error rates at the gates. The model that we applied here can be systematically extended towards turbulent convection, as discussed in detail in refs. [43, 62]. A QRCM with \( n \sim 10 \) might thus be able to run a two-dimensional turbulent convection flow usable as a subgrid-scale superparametrization in a global circulation model [63]. A further possible route of research is to compose the quantum reservoir from first principles, e.g. in the form of a multilayer tensorial network that potentially improve the performance of quantum algorithms on NISQ devices [64].

Acknowledgments

This work is supported by the project no. P2018-02-001 “DeepTurz – Deep Learning in and of Turbulence” of the Carl Zeiss Foundation and the Deutsche Forschungsgemeinschaft under grant no. DFG-SPP 1881. We acknowledge the use of IBM Quantum services for this work. The views expressed are those of the authors, and do not reflect the official policy or position of IBM or the IBM Quantum team. In this paper we used ibmq_ehningen and ibmq_perth, which are run with the IBM Quantum Falcon Processor.

Appendix A: Lorenz-type model of dimension 8

In this appendix, we provide details of the derivation of reduced Lorenz-type models for thermally driven convection flows. The Lorenz-type models are obtained from eqns. (6) and (7) by means of the following finite expansions. The Lorenz-type models are obtained from reduced Lorentz-type models for thermally driven convection, as discussed in detail in refs. [43, 62]. The model that we applied here takes place at a critical Rayleigh number \( Ra_c \) and \( Ra \), which initiates fluid motion due to a sufficiently large temperature difference between the bottom and the top, respectively. We acknowledge the use of IBM Quantum services for this work. The views expressed are those of the authors, and do not reflect the official policy or position of IBM or the IBM Quantum team. In this paper we used ibmq_ehningen and ibmq_perth, which are run with the IBM Quantum Falcon Processor.

The resulting system of nonlinear coupled ordinary differential equations is given by

\[
\frac{dA_1}{d\tau} = \sigma \left( B_1 - A_1 \right) - \frac{3B_2^2 + \alpha^2}{\sqrt{2(\alpha^2 + \beta^2)}} A_2 A_3 + \frac{3\alpha^2 - 15\beta^2}{\sqrt{2(\alpha^2 + \beta^2)}} A_3 A_4, \quad (A6)
\]

\[
\frac{dA_2}{d\tau} = -\frac{\sigma b}{4} A_2 - \frac{3}{2\sqrt{2}} A_1 A_3, \quad (A7)
\]

\[
\frac{dA_3}{d\tau} = -\sigma \frac{\alpha^2 + 4\beta^2}{\alpha^2 + \beta^2} A_3 - \frac{\sigma}{\sqrt{2(4\beta^2 + \alpha^2)}} B_3 + \frac{\alpha^2}{\sqrt{2(\alpha^2 + \beta^2)}} A_1 A_2 + \frac{24\beta^2 - 3\alpha^2}{\sqrt{2(4\beta^2 + \alpha^2)}} A_1 A_4, \quad (A8)
\]

\[
\frac{dA_4}{d\tau} = -\frac{9\sigma b}{4} A_4 - \frac{1}{2\sqrt{2}} A_1 A_3, \quad (A9)
\]

\[
\frac{dB_1}{d\tau} = -B_1 + r A_1 + A_1 B_2 + \frac{1}{2} A_2 B_3 + \frac{3}{2} A_4 B_3, \quad (A10)
\]

\[
\frac{dB_2}{d\tau} = -b B_2 - A_1 B_1, \quad (A11)
\]

\[
\frac{dB_3}{d\tau} = -\frac{\alpha^2 + 4\beta^2}{\alpha^2 + \beta^2} B_3 - A_2 B_3 + \sqrt{2} A_3 + 3A_4 B_1 \quad - 2\sqrt{2} A_3 B_4, \quad (A12)
\]

\[
\frac{dB_4}{d\tau} = -4b B_4 + \frac{3\sqrt{2}}{4} A_3 B_3, \quad (A13)
\]

with \( b = 4\beta^2/(\alpha^2 + \beta^2) \), \( Ra_c = (\alpha^2 + \beta^2)^3/\alpha^2 \), and the rescaled time \( \tau = (\alpha^2 + \beta^2)t \). The Lorenz 63 model [39] is recaptured for \( A_2 = A_3 = A_4 = 0 \) and \( B_3 = B_4 = 0 \).

A primary linear instability of the convection flow, which initiates fluid motion due to a sufficiently large temperature difference between the bottom and the top, takes place at a critical Rayleigh number \( Ra_c = 27\pi^4/4 \) when free-slip boundary conditions hold at the top and bottom [65]. The 1st parameter \( \sigma \) is the Prandtl num-

The 2nd parameter \( r \) in the Lorenz-type models is then defined as \( r = Ra/Ra_c > 1 \). The 3rd parameter \( b \) is
connected to the aspect ratio $\Gamma$ of the fluid volume that is considered. In detail,

$$b = \frac{4\Gamma^2}{4 + \Gamma^2}. \quad (A14)$$

If $b = 8/3$ then the aspect ratio is $\Gamma = \text{length/height} = 2\sqrt{2}$ which corresponds to the critical wavelength of plane wave perturbations of the quiescent equilibrium of the convection flow. In other words, at this wavelength the thermal convection flow becomes linearly unstable first.

**Appendix B: Qubits and tensor product spaces**

In this appendix, we summarize in brief some basic definitions of quantum computing. For more details we refer to the textbook of Nielsen and Chuang [19] or a review by Bharadwaj and Sreenivasan [66]. While a single classical bit can take two discrete values, namely $\{0, 1\}$ only, a single quantum bit (in short qubit) is a superposition of two basis states in the vector space $\mathbb{C}^2$ which can take any state on the surface of a (Bloch) sphere

$$|q_1\rangle = c_1|0\rangle + c_2|1\rangle = c_1 \begin{pmatrix} 1 \\ 0 \end{pmatrix} + c_2 \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \quad (B1)$$

with $c_1, c_2 \in \mathbb{C}$. Vectors $|0\rangle$ and $|1\rangle$ are the basis vectors in Dirac notation [19]. A two-qubit state is the tensor product of two single-qubit vectors,

$$|q_2\rangle = |q_1\rangle \otimes |q_1\rangle. \quad (B2)$$

The basis of this tensor product space is given by 4 vectors: $|j_1\rangle = |0\rangle \otimes |0\rangle$, $|j_2\rangle = |0\rangle \otimes |1\rangle$, $|j_3\rangle = |1\rangle \otimes |0\rangle$, and $|j_4\rangle = |1\rangle \otimes |1\rangle$. An $n$-qubit quantum state, which is given by

$$|\psi\rangle = \sum_{j_1,...,j_n} \psi_{j_1,...,j_n} |j_1\rangle \otimes \cdots \otimes |j_n\rangle, \quad (B3)$$

is called separable if the coefficients satisfy

$$\psi_{j_1,...,j_n} = \prod_{i=1}^n a_{j_i}, \quad (B4)$$

such that

$$|\psi\rangle = \sum_{j_1,...,j_n} a_{j_1} |j_1\rangle \otimes \cdots \otimes a_{j_n} |j_n\rangle. \quad (B5)$$

Otherwise, the quantum state is entangled.

**Appendix C: Classical reservoir computing model**

In this appendix, we provide details about the reservoir computing approach, a recurrent supervised machine learning algorithm. The training of the RCM proceeds as follows. The dynamical system state at time $t$, which is denoted more compactly as

$$x^t = \{A_1, ..., A_N, B_1, ..., B_M\} \in \mathbb{R}^{N_{in}}, \quad (C1)$$

is mapped to the reservoir state $\psi^t$ via the randomly initialized input weight matrix $W_{in} \in \mathbb{R}^{N_{res} \times N_{in}}$. Here, $N_{res} \gg N_{in}$ is the reservoir dimension. The reservoir state is updated as follows [20, 28, 35]

$$\psi^{t+1} = (1 - \varepsilon)\psi^t + \varepsilon \tanh \left[ W_{in} x^t + W^{r} \psi^t \right]. \quad (C2)$$

This update rule comprises external forcing by the inputs $x^t$ as well as a self-interaction with the reservoir state $\psi^t$. The two terms on the right hand side of (C2) are combined by the leaking rate $\varepsilon$. The hyperbolic tangent ($\tanh (\cdot)$) is the nonlinear activation function of each reservoir node. The randomly initialized matrix $W^r$ represents the reservoir, a sparse random network of neurons [67]. Thus the leaking rate $\varepsilon \in (0, 1]$ moderates the linear and nonlinear contributions. The updated reservoir state $\psi^{t+1}$ is mapped via the output matrix $W_{out} \in \mathbb{R}^{N_{out} \times N_{res}}$ to form the reservoir output $x^{t+1} \in \mathbb{R}^{N_{out}}$

$$x^{t+1} = W^{out} \psi^{t+1}. \quad (C3)$$

The elements of $W^{out}$ have to be computed. Therefore, a set of $T$ training data instances $\{x^{t+1}_{in}, x^{t+1}_{tg}\}$, where $t = -T, -T + 1, ..., -1$, needs to be prepared. The target output $x^{t+1}_{tg}$ (also denoted as ground truth (GT)) represents the desired output that the RCM should produce for the given input $x^t$. The resulting data pairs are assembled into a mean squared cost function $C(W^{out})$ with a Tikhonov regularization term which is given by

$$C(W^{out}) = \frac{1}{T} \sum_{t=-T}^{-1} |x^t - x^{t+1}_{tg}|^2 + \gamma \text{Tr} \left( W^{out} W^{outT} \right),$$

and has to be minimized corresponding to $W^{out*} = \arg \min C(W^{out})$. Superscript $T$ denotes the transposed. The regularization parameter $\gamma > 0$ avoids overfitting [13]. The optimized output matrix is given by

$$W^{out*} = U_{tg} R^T \left( R R^T + \beta \mathbb{I} \right)^{-1} \quad (C4)$$

where $\mathbb{I}$ is the identity matrix and $U_{tg}$, $R$ are matrices where the $t$-th column is the target output $x^{t+1}_{tg}$ and reservoir state $\psi^t$. The optimization of the output weights thus becomes computationally inexpensive. The hyper-parameters of the classical RCM are $N_{res}, \varepsilon, \gamma$, the reservoir density $D$, and the spectral radius $\rho(W^r)$.

Once the output weights are optimized and the hyper-parameters are tuned the RCM can run in the prediction mode. Equation (C2) changes to

$$\psi^{t+1} = (1 - \varepsilon)\psi^t + \varepsilon \tanh \left[ W^{in} W^{out*} \psi^t + W^{r} \psi^t \right]. \quad (C5)$$

Now the RCM can work independently of training input. The prediction for the dynamical system follows by $x^{t+1} = W^{out*} \psi^{t+1}$.
tiotemporal chaotic dynamics with recurrent neural networks: a comparative study of reservoir computing and backpropagation algorithms. Neur. Netw., 126:191–217, 2020.

35. S. Pandey and J. Schumacher. Reservoir computing model of two-dimensional turbulent convection. Phys. Rev. Fluids, 5:113506, 2020.

36. F. Heyder and J. Schumacher. Echo state network for two-dimensional turbulent moist Rayleigh-Bénard convection. Phys. Rev. E, 103:053107, 2021.

37. S. Pandey, P. Teutsch, P. Mäder, and J. Schumacher. Direct data-driven forecast of local turbulent heat flux in Rayleigh-Bénard convection. Phys. Fluids, 34:in press, 2022.

38. V. Valori, R. Kräuter, and J. Schumacher. Extreme vorticity events in turbulent Rayleigh-Bénard convection from stereoscopic measurements and reservoir computing. arXiv:2112.05442, 2021.

39. E. N. Lorenz. Deterministic nonperiodic flow. J. Atmos. Sci., 20:130–141, 1963.

40. L. N. Howard and R. Krishnamurti. Large-scale flow in turbulent convection: A mathematical model. J. Fluid. Mech., 170:385–410, 1986.

41. J.-L. Thiffeault and W. Horton. Energy-conserving truncations for convection with shear flow. Phys. Fluids, 8:1715–1719, 1996.

42. A. Gluhovsky, C. Tong, and E. Agee. Selection of modes in convective low-order models. J. Atmos. Sci., 59:1383–1393, 2002.

43. S. Moon, B.-S. Han, J. Park, M. S. Seo, and J.-J. Baik. Periodicity and chaos of higher-order Lorenz systems. Int. J. Bifurc. Chaos, 27:1750176, 2017.

44. E. L. Koschmieder. Bénard cells and Taylor vortices. Cambridge University Press, Cambridge, UK, 1993.

45. F. Chillà and J. Schumacher. New perspectives in turbulent Rayleigh-Bénard convection. Eur. Phys. J. E, 35(7):58, 2012.

46. M. Lukoševičius and A. Uselis. Efficient implementations of echo state network cross-validation. Cogn. Comput., pages 1–15, 2021.

47. Qiskit Version 0.24.1, 2021.

48. K. Fujii and K. Nakajima. Harnessing disordered-ensemble quantum dynamics for machine learning. Phys. Rev. Applied, 8:024030, 2017.

49. K. Nakajima, K. Fujii, M. Negoro, K. Mitarai, and M. Kitagawa. Boosting computational power through spatial multiplexing in quantum reservoir computing. Phys. Rev. Applied, 11:034021, 2019.

50. A. Kutvonen, K. Fujii, and T. Sagawa. Optimizing a quantum reservoir computer for time series prediction. Sci. Rep., 10:14687, 2020.

51. L. C. G. Govia, G. J. Ribeill, G. E. Rowlands, H. K. Krovi, and T. A. Ohki. Quantum reservoir computing with a single nonlinear oscillator. Phys. Rev. Research, 3:013077, 2021.

52. J. Chen, H. I. Nurdin, and N. Yamamoto. Temporal information processing on noisy quantum computers. Phys. Rev. Applied, 14:024065, 2020.

53. S. Dasgupta, K. E. Hamilton, and A. Banerjee. Designing a NISQ reservoir with maximal memory capacity for volatility forecasting. arXiv:2004.08240, pages 1–12, 2020.

54. D. Marković and J. Grollier. Quantum neuromorphic computing. Appl. Phys. Lett., 117:150501, 2020.

55. R. Josza and N. Linden. On the role of entanglement in quantum-computational speed-up. Proc. R. Soc. Lond. A, 459:2011–2032, 2003.

56. B. J. Geurts, D. D. Holm, and E. Luesink. Lyapunov exponents in two stochastic Lorenz 63 systems. J. Stat. Phys., 179:1343–1365, 2020.

57. L. C. G. Govia, G. J. Ribeill, G. E. Rowlands, and T. A. Ohki. Nonlinear input transformations are ubiquitous in quantum reservoir computing. Neur. Comp. Eng., 2:xx, 2022.

58. M. Imbush and K. Yoshimura. Reservoir computing beyond memory-nonlinearity trade-off. Sci. Rep., 7:10199, 2017.

59. Julien Clinton Sprott and Julien C Sprott. Chaos and time-series analysis, volume 69. Oxford University Press Oxford, 2003.

60. D. Giannakis, A. Ourmazd, P. Pfeffer, J. Schumacher, and J. Slawinska. Embedding classical dynamics in a quantum computer. Phys. Rev. A, xx:in press, 2022.

61. N. Gourianov, M. Lubasch, S. Dolgov, Q. Y. van den Berg, H. Babae, P. Givi, M. Kiffner, and D. Jaksch. A quantum-inspired approach to exploit turbulence structures. Nat. Comput. Sci., 2:30–37, 2022.

62. Park J., S. Moon, J. M.. Seo, and J.-J. Baik. Systematic comparison between the generalized Lorenz equations and DNS in two-dimensional Rayleigh-Bénard convection. Chaos, 31:073119, 2021.

63. W. Grabowski and P. Smolarkiewicz. CRCP: a Cloud Resolving Convection Parametrization for modeling the tropical convecting atmosphere. Physica D, 133:171–178, 1999.

64. F. Barratt, J. Dborin, M. Bal, V. Stojevic, F. Pollmann, and A. G. Green. Parallel quantum simulation of large systems on small nisq computers. npj Quant. Inf., 7:79, 2021.

65. S. Chandrasekhar. Hydrodynamic and hydromagnetic stability. Claredon Press, Oxford, 2016.

66. S. S. Bharadwaj and K. R. Sreenivasan. Quantum computation of fluid dynamics. Indian Academy of Sciences Conference Series, 3:77–96, 2020.

67. H. Jaeger. A tutorial on training recurrent neural networks, covering BPPT, RTRL, EKF and the "echo state network" approach. GMD-Forschungszentrum Informationstechnik Technical Report, 2002.