Quantum Compiler for Classical Dynamical Systems

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Simulating Physics with Computers

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The first question is, What kind of computer are we going to use to simulate physics? Computer theory has been developed to a point where it realizes that it doesn't make any difference; when you get to a universal computer, it doesn't matter how it's manufactured, how it's actually made. Therefore my question is, Can physics be simulated by a universal computer? I would like to have the elements of this computer locally interconnected, and therefore sort of think about cellular automata as an example (but I don't want to force it). But I do want something involved with the
Simulation of classical systems by quantum systems

- Discrete-time maps (Benenti et al. 2001).
- Differential equations with polynomial nonlinearities (Leyton & Osborne 2009).
- Data assimilation (G. 2019; Slawinska et al. 2019).
- Turbulent fluid flows (Bharadwaj et al. 2020; Lubasch et al. 2020).
We construct a framework for representing states and observables of a classical dynamical system by means of a finite-dimensional quantum mechanical system, amenable to quantum computation.

The output of this “quantum compiler” is a stochastic simulator of the evolution of classical observables, realized through projective quantum measurements.
1. Associated with every quantum system is a separable Hilbert space $\mathcal{H}$ over the complex numbers. The possible states of the system correspond to the set of positive, trace-class operators $\rho : \mathcal{H} \to \mathcal{H}$ with $\text{tr} \, \rho = 1$, denoted $Q(\mathcal{H})$. The observables of the system are self-adjoint linear operators on $\mathcal{H}$. 
Quantum mechanical axioms

2. Between measurements, the state evolves under the action of a strongly continuous group of unitary operators $U^t : \mathcal{H} \rightarrow \mathcal{H}$, $t \in \mathbb{R}$. The state $\rho_t$ reached at time $t$ starting from a state $\rho_0$ is given by $\rho_t = U^t \rho_0 U^t$. 
3. Let $A : D(A) \to \mathcal{H}$ be an observable, defined on a dense subspace $D(A) \subseteq \mathcal{H}$. By the spectral theorem for self-adjoint operators, there exists a unique projection-valued measure $E_A : \mathcal{B}(\mathbb{R}) \to \mathcal{B}(\mathcal{H})$ such that $A = \int_{\mathbb{R}} a\, dE_A(a)$. The set of possible values that a measurement of $A$ can take in a physical experiment is given by the spectrum of $A$, $\sigma(A) \subseteq \mathbb{R}$. 
Quantum mechanical axioms

4. If the system is in state $\rho$, then the expectation value of a measurement of an observable $A$ is given by $E_\rho A := \text{tr}(\rho A)$. The probability that a measurement of $A$ lies in a Borel set $\Omega \subseteq \mathbb{R}$ is equal to $E_\rho E_A(\Omega)$. 
5. If the system state immediately before a measurement is $\rho^-$, and a measurement of $A$ yields a value $a \in \sigma(A)$, with $E_A(\{a\}) \neq 0$ (i.e., $a$ is an eigenvalue of $A$), then the state $\rho^+$ immediately after the measurement is given by

$$\rho^+ = \frac{E_A(\{a\})\rho^- E_A(\{a\})}{\text{tr}(E_A(\{a\})\rho^- E_A(\{a\}))}.$$
A route to quantum compilation

Classical

\[ X \xrightarrow{\Phi_t} X \]
A route to quantum compilation

Classical

Classical statistical

$P(X) \xrightarrow{\Phi^t_*} P(X)$

$X \xrightarrow{\Phi^t} X$

$\delta \quad \delta$
A route to quantum compilation

Classical

Classical statistical

Quantum mechanical

\[
\begin{align*}
X & \xrightarrow{\Phi_t} X \\
\mathcal{P}(X) & \xrightarrow{\Phi^*_t} \mathcal{P}(X) \\
Q(\mathcal{H}) & \xrightarrow{\Psi^t} Q(\mathcal{H})
\end{align*}
\]
A route to quantum compilation

Classical

Classical statistical

Quantum mechanical

Quantum computational

\[ X \xrightarrow{\Phi^t} X \]

\[ \mathcal{P}(X) \xrightarrow{\Phi^*_t} \mathcal{P}(X) \]

\[ P \xrightarrow{\psi^t} P \]

\[ \hat{\mathcal{W}} \xrightarrow{\tilde{\psi}^t} \hat{\mathcal{W}} \]

\[ Q(\mathcal{H}) \xrightarrow{\psi^t} Q(\mathcal{H}) \]

\[ Q(\mathcal{B}_N) \xrightarrow{\tilde{\psi}^t} Q(\mathcal{B}_N) \]
Dynamical system

• Ergodic rotation on the $d$-torus,

$$\Phi^t : \mathbb{T}^d \to \mathbb{T}^d, \quad \Phi^t(x) = (x_1 + \alpha_1 t, \ldots, x_d + \alpha_d t) \mod 2\pi.$$ 

• Canonical representatives (under topological conjugacy) of continuous-time, continuous, measure-preserving, ergodic dynamical systems with finitely generated pure point spectra.
Choice of Hilbert space

Consider the Fourier functions on $X = \mathbb{T}^d$,

$$\phi_j(x) = e^{ij \cdot x}, \quad j = (j_1, \ldots, j_d) \in \mathbb{Z}^d, \quad x = (x_1, \ldots, x_d) \in X.$$

For $p \in (0, 1)$, $\tau > 0$, set $k : X \times X \rightarrow \mathbb{R}$, with

$$k(x, x') = \sum_{j \in \mathbb{Z}^d} \lambda_j \overline{\phi_j(x)} \phi_j(x'), \quad \lambda_j = e^{-\tau(|j_1|^p + \cdots + |j_d|^p)}.$$

**Theorem** [Das, G. 20]. $k$ is the reproducing kernel of an RKHS $\mathcal{H}$, which is a dense subspace of $C(X)$. Moreover, $\mathcal{H}$ is an abelian, unital, Banach $^*$-algebra under the pointwise multiplication and complex conjugation of functions. That is,

$$\|fg\|_\mathcal{H} \leq C\|f\|_\mathcal{H}\|g\|_\mathcal{H}, \quad \|f^*\|_\mathcal{H} = \|f\|_\mathcal{H}.$$

- The functions $\psi_j = \sqrt{\lambda_j} \phi_j$ form an orthonormal basis of $\mathcal{H}$. 
Reproducing kernel Hilbert algebras (RKHAs)

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Unitary Koopman operators

\[ U^t : \mathcal{H} \rightarrow \mathcal{H}, \quad U^t f = f \circ \Phi^t, \quad U^{t*} = U^{-t} \]

- Generator:
  \[ V : D(V) \rightarrow \mathcal{H}, \quad Vf = \lim_{t \to 0} \frac{U^t f - f}{t}, \quad V^{*} = -V, \quad U^t = e^{tV}. \]

- Eigenbasis:
  \[ V \psi_j = i \omega_j \psi_j, \quad \omega_j = j_1 \alpha_1 + \cdots + j_d \alpha_d, \quad j \in \mathbb{Z}^d. \]

- Group structure:
  \[ \omega_j + \omega_k = \omega_{j+k}, \quad \psi_j \psi_k = c_{jk} \psi_{j+k}. \]
From classical to classical-statistical level

- $\delta$ maps $x \in X$ to the Dirac measure supported at $x$, \[
delta(x) = \delta_x.
\]
- $\mu \in \mathcal{P}(X)$ evolves under the pushforward map on measures, \[
\Phi^t_* (\mu) = \mu \circ \Phi^{-t}.
\]
From classical-statistical to quantum mechanical level

\[
\begin{align*}
X & \xrightarrow{\Phi^t} X \\
\delta & \downarrow \Phi^t \downarrow \delta \\
\mathcal{P}(X) & \xrightarrow{\Phi^*} \mathcal{P}(X) \\
P & \downarrow P \downarrow \\
Q(\mathcal{H}) & \xrightarrow{\Psi^t} Q(\mathcal{H})
\end{align*}
\]

- Feature map:
  \[ F : X \rightarrow \mathcal{H}, \quad F(x) = k_x \equiv k(x, \cdot). \]

- Quantum feature map:
  \[ Q : X \rightarrow Q(\mathcal{H}), \quad Q(x) = \rho_x \equiv \langle \xi_x, \cdot \rangle_{\mathcal{H}} \xi_x, \quad \xi_x = \frac{F(x)}{\|F(x)\|_{\mathcal{H}}}. \]

- Quantum embedding of probability measures:
  \[ P : \mathcal{P}(X) \rightarrow Q(\mathcal{H}), \quad P(\mu) = \int_X \rho_x \, d\mu(x). \]

- Unitary evolution:
  \[ \Psi^t : Q(\mathcal{H}) \rightarrow Q(\mathcal{H}), \quad \Psi^t(\rho) = U^{t*} \rho U^t. \]
Representation of observables

\[ \mathcal{H} \xrightarrow{U^t} \mathcal{H} \]
\[ \pi \downarrow \quad \downarrow \pi \]
\[ B(\mathcal{H}) \xrightarrow{U^t} B(\mathcal{H}) \]

- Regular representation,
  \[ \pi : \mathcal{H} \to B(\mathcal{H}), \quad (\pi f)g = fg. \]

- Mapping into self-adjoint operators,
  \[ T : \mathcal{H} \to B(\mathcal{H}), \quad Tf = \frac{\pi f + (\pi f)^*}{2}. \]

- Unitary evolution,
  \[ U^t : B(\mathcal{H}) \to B(\mathcal{H}), \quad U^t A = U^t A U^{t*}. \]
Multiplication operators

\[ M_{ij} = \langle \psi_i, \pi(\psi_k)\psi_j \rangle_{\mathcal{H}} = c_{k,i-j} \]

\[ \psi_i \psi_j = C_{ij} \psi_{i+j} \]

The multiplication operator \( \pi \psi_k \) is represented by a \((-k)\)-diagonal matrix \( M \).
The following holds for every $f \in \mathcal{H}$, $x \in X$, and $t \in \mathbb{R}$:

$$U^t f(x) = \mathbb{E}_{\Psi^t(Q(x))}(\pi f).$$

Moreover, if $f$ is a self-adjoint (real-valued) element of $\mathcal{H}$,

$$U^t f(x) = \mathbb{E}_{\Psi^t(Q(x))}(Tf).$$

**Remark.** The reproducing property of $\mathcal{H}$ is important in these results.
From quantum mechanical to quantum computational level

\[ X \xrightarrow{\Phi^t} X \]
\[ \delta \downarrow \quad \Phi^t \quad \delta \]
\[ \mathcal{P}(X) \xrightarrow{\Phi^t} \mathcal{P}(X) \]
\[ P \downarrow \quad \Psi^t \quad P \]
\[ Q(\mathcal{H}) \xrightarrow{\Psi^t} Q(\mathcal{H}) \]
\[ \hat{\mathcal{W}} \downarrow \quad \hat{\Psi}^t \quad \hat{\mathcal{W}} \]
\[ Q(\mathbb{B}_N) \xrightarrow{\hat{\Psi}^t} Q(\mathbb{B}_N) \]

- \(2^N\)-dimensional Hilbert space associated with \(N\) qubits:
  \[ \mathbb{B}_N = \mathbb{B} \otimes \mathbb{B} \otimes \cdots \otimes \mathbb{B}, \quad \mathbb{B} \simeq \mathbb{C}^2. \]

- Pauli \(Z\)-operator:
  \[ Z : \mathbb{B} \rightarrow \mathbb{B}, \quad Z|0\rangle = |0\rangle, \quad Z|1\rangle = -|1\rangle. \]

- Tensor product basis of \(\mathbb{B}_N\):
  \[ |b_1 \cdots b_N\rangle = |b_1\rangle \otimes |b_2\rangle \otimes \cdots \otimes |b_N\rangle, \quad (b_1, \ldots, b_N) \in \{0,1\}^N. \]
Finite-rank representation of states and observables

For $X = \mathbb{T}^d$, $\frac{N}{d} \in \mathbb{N}$, let $J_N^{(1)} = \{-\frac{N}{d}, \ldots, -1, 1, \ldots, \frac{N}{d}\}$, $J_N = (J_N^{(1)})^d$, 

$$
\mathcal{H}_N = \text{span}\{\psi_j : j \in J_N\}, \quad \Pi_N = \text{proj}_{\mathcal{H}_N}, \quad \kappa_N = \sum_{j \in J_N} \lambda_j,
$$

$$
\tilde{\Pi}_N : B(\mathcal{H}) \to B(\mathcal{H}), \quad \tilde{\Pi}_N A = \Pi_N A \Pi_N,
$$

$$
\mathcal{L}_N : \mathcal{H} \to \mathcal{H}, \quad \mathcal{L}_N \psi_j = \left(1 - \frac{\lambda_j}{\kappa_N}\right)^{-1} \psi_j.
$$
Finite-rank representation of states and observables

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$$\mathcal{L}_N : \mathcal{H} \to \mathcal{H}, \quad \mathcal{L}_N \psi_j = \left(1 - \frac{\lambda_j}{\kappa_N}\right)^{-1} \psi_j.$$

Defining

$$Q_N = \frac{\kappa}{\kappa_N} \tilde{\Pi}_N \circ Q, \quad \pi_N = \tilde{\Pi}_N \circ \pi \circ \mathcal{L}_N, \quad T_N = \tilde{\Pi}_N \circ T \circ \mathcal{L}_N,$$

the following hold in the infinite qubit limit, $N \to \infty$.

1. For every $f \in \mathcal{H}$, $x \in X$, and $t \in \mathbb{R}$,

$$\mathbb{E}_{\psi^t(Q_N(x))} \pi_N f \longrightarrow \mathbb{E}_{\psi^t(Q(x))} \pi f \equiv U^t f(x).$$

2. Further, if $f$ is self-adjoint,

$$\mathbb{E}_{\psi^t(Q_N(x))} T_N f \longrightarrow \mathbb{E}_{\psi^t(Q(x))} T f \equiv U^t f(x).$$
Finite-rank quantum mechanical observable

\[(T_N f)u_j = s_j u_j, \quad f(x) = \sin x = \frac{\psi_1(x) + \psi_{-1}(x)}{2i\sqrt{\lambda_1}}\]
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Projection onto quantum computational space

Order the index set $J_N^{(1)}$ according to $o : J_N^{(1)} \rightarrow \{0, \ldots, 2^{N/d} - 1\}$, i.e.,

$$
\begin{array}{cccccccc}
-2^{N/d-1} & \ldots & -1 & 1 & \ldots & 2^{N/d-1} \\
\downarrow & & \downarrow & \downarrow & & \downarrow \\
0 & \ldots & 2^{N/d-1} - 1 & 2^{N/d-1} & \ldots & 2^{N/d} - 1
\end{array}
$$

Letting $\delta(n) \in \{0, 1\}^{N/d}$ be the dyadic representation of $n \in \{0, \ldots, 2^{N/d} - 1\}$, define the unitary $W_N : \mathcal{H}_N \rightarrow \mathbb{B}_N$

$$
W_N \psi_j = |b\rangle, \quad b = [\delta(o(j_1)) \cdots \delta(o(j_d))] \in \{0, 1\}^N.
$$

This induces a unitary $W_N : B(\mathcal{H}_N) \rightarrow B(\mathbb{B}_N)$, $W_N A = W_N A W_N$, and a projection $\tilde{W}_N = W_N \circ \tilde{\Pi}_N$ such that

$$
\begin{array}{ccc}
Q(\mathcal{H}) & \xrightarrow{\psi^t} & Q(\mathcal{H}) \\
\tilde{W} & \downarrow & \tilde{W} \\
Q(\mathbb{B}_N) & \xrightarrow{\hat{\psi}^t} & Q(\mathbb{B}_N)
\end{array}
, \quad \tilde{W}_N = \frac{\kappa}{\kappa_N} \tilde{W}_N, \quad \hat{\psi}^t = \tilde{W}_N \psi^t.
Walsh operator representation (Welch et al. 2014)

Letting $\beta(n)$ be the bit-reversed binary representation of $n \in \{1, \ldots, 2^N\}$, define the Walsh operator

$$Z_n : \mathbb{B}_N \rightarrow \mathbb{B}_N, \quad Z_n = Z_{b'_1} \otimes \cdots \otimes Z_{b'_N}, \quad (b'_1, \ldots, b'_N) = \beta(n).$$

Then, every diagonal operator $A \in B(\mathbb{B}_N)$ such that

$$A|b\rangle = a_b|b\rangle, \quad b \in \{0, 1\}^N,$$

admits the factorization

$$A = \sum_{n=1}^{2^N} \hat{h}_n Z_n,$$

where the coefficients $\hat{h}_n$ are given by the discrete Walsh-Fourier transform of $h : \{0, \ldots, 2^N - 1\} \rightarrow \mathbb{C}$ with $h(m/2^N) = a_\delta(m)$,

$$\hat{h}_n = \frac{1}{2^N} \sum_{m=0}^{2^N-1} w_n^{(N)}(m) h(m), \quad w_n^{(N)}(m) = (-1)^{\beta(n) \cdot \delta(m)}.$$
Walsh operator representation of the Koopman generator

Under $\hat{\tilde{W}}_N$, the generator $V$ maps into the Hamiltonian $H = \frac{1}{i} \hat{\tilde{W}}_N V$,

$$H|b\rangle = \omega_j |b\rangle, \quad \omega_j = \sum_{i=1}^{d} j_i \alpha_i, \quad b = [\delta(o(j_1)) \cdots \delta(o(j_d))].$$

For a quasiperiodic dynamical system on $\mathbb{T}^d$, the Walsh representation $H = \sum_{n=1}^{2^N} \hat{h}_n Z_n$ has only $N$ nonzero terms, and for these terms the binary string $\beta(n)$ has only a single 1. In particular,

$$H = \hat{h}_1 Z \otimes I \otimes I \otimes I \otimes \cdots \otimes I$$
$$+ \hat{h}_2 I \otimes Z \otimes I \otimes I \otimes \cdots \otimes I$$
$$+ \hat{h}_4 I \otimes I \otimes Z \otimes I \otimes \cdots \otimes I$$
$$+ \ldots$$
$$+ \hat{h}_{2^{N-1}} I \otimes \cdots \otimes I \otimes Z.$$

As a result, the evolution operator $e^{iHt}$ admits the factorization

$$e^{iHt} = e^{i\hat{h}_1 tZ} \otimes e^{i\hat{h}_2 tZ} \otimes e^{i\hat{h}_4 tZ} \otimes \ldots \otimes e^{i\hat{h}_{2^{N-1}} tZ}.$$
The Walsh operator factorization allows implementation of the evolution

$$\hat{\rho}_x \mapsto \hat{\Psi}^t(\hat{\rho}_x) = e^{-iHt} \hat{\rho}_x e^{iHt}, \quad \hat{\rho}_x = \hat{Q}_N(x)$$

via an $N$-channel quantum circuit with no interchannel communication. The above shows an implementation using the Qiskit SDK.
Summary thus far...

We have constructed a representation of a quasiperiodic dynamical system on a quantum computer with $N$ qubits.

- Classical state $x \in X$ is represented by density operator $\hat{\rho}_x = \hat{Q}_N(x) \in \mathcal{Q}(\mathbb{B}_N)$.
- Real-valued classical observable $f \in \mathcal{H}$ is represented by self-adjoint operator $\hat{T}_N f = (\hat{\mathcal{N}}_N \circ T_N)f$.
- Classical dynamical evolution $\Phi^t : X \to X$ is represented by unitary evolution $\hat{\Psi}^t : \mathcal{Q}(\mathbb{B}_N) \to \mathcal{Q}(\mathbb{B}_N)$, $\hat{\Psi}^t(\hat{\rho}) = e^{-iHt}\hat{\rho}e^{iHt}$.
- The system is implementable on an $N$-circuit quantum channel with no interchannel communication. In particular, $\dim \mathcal{H}_N = 2^N$ grows exponentially with $N$, while the number of required quantum gates grows linearly.
- Classical–quantum consistency is reached in the limit $N \to \infty$.

What remains is to establish a quantum measurement process allowing to query the system and obtain predictions.
Projective measurement

- The $N$-qubit “quantum register” has an associated projection-valued measure,

$$\mathcal{E} : \Sigma(\{0, 1\}^N) \rightarrow B(\mathcal{H}_N), \quad \mathcal{E}(\Omega) = \sum_{b \in \Omega} \text{proj}_{|b\rangle},$$

where $\Sigma(\{0, 1\}^N)$ is the $\sigma$-algebra of all subsets of $\{0, 1\}^N$.

- Measurement of $\mathcal{E}$ on a state $\hat{\rho} \in Q(\mathcal{B}_N)$ returns a random binary string $b \in \{0, 1\}^N$ with probability

$$\mathbb{P}_{\hat{\rho}}(b) = \text{tr}(\hat{\rho} \mathcal{E}(\{b\})).$$
Projective measurement

1. For classical observable \( f \in \mathcal{H} \), compute the eigendecomposition of \( \hat{S} := \hat{T}_N f \),
\[
\hat{S}|u_n\rangle = s_n|u_n\rangle, \quad n \in \{0, \ldots, 2^N - 1\},
\]
and form the associated unitary \( \Xi \in B(\mathbb{B}_N) \),
\[
\Xi|b\rangle = |u_n\rangle, \quad b = \delta(n).
\]

2. For initial condition \( x \in X \) and prediction time \( t \), make \( K \) independent measurements \( \hat{b}_1, \ldots, \hat{b}_K \) of \( E \) on the rotated state \( \Xi \hat{\psi}^t(\rho_x)\Xi^* \).

3. Compute the estimator
\[
\bar{s}_K = \frac{1}{K} \sum_{k=1}^K s_{n_k}, \quad b_k = \delta(n_k).
\]
Projective measurement

1. For classical observable $f \in \mathcal{H}$, compute the eigendecomposition of
   $\hat{S} := \hat{T}_N f$,
   $$\hat{S}|u_n\rangle = s_n|u_n\rangle, \quad n \in \{0, \ldots, 2^N - 1\},$$
   and form the associated unitary $\Xi \in B(\mathbb{B}_N)$,
   $$\Xi|b\rangle = |u_n\rangle, \quad b = \delta(n).$$

2. For initial condition $x \in X$ and prediction time $t$, make $K$ independent
   measurements $\hat{b}_1, \ldots, \hat{b}_K$ of $\mathcal{E}$ on the rotated state
   $\Xi \hat{\psi}^t(\rho_x) \Xi^*$. 

3. Compute the estimator
   $$\bar{s}_K = \frac{1}{K} \sum_{k=1}^{K} s_{n_k}, \quad b_k = \delta(n_k).$$

   - As $K \to \infty$ at fixed $N$, $\bar{s}_K$ converges to $\mathbb{E}_{\hat{\psi}^t(\hat{\rho}_x)} \hat{T}_N f$ strongly.
Quantum mechanical prediction

Prediction of \( f(x) = \sin x \) for a circle rotation of frequency 1.
Quantum mechanical prediction

Prediction of \( f(x) = \sin x \) for a circle rotation of frequency 1.
Quantum mechanical prediction

Prediction of $f(x) = \sin x$ for a circle rotation of frequency 1.
Quantum mechanical prediction

Prediction of $f(x) = \sin x$ for a circle rotation of frequency 1.
Prediction of $f(x) = \sin x$ for a circle rotation of frequency 1.
Summary and outlook

• We have developed a framework for approximating a classical dynamical system by a finite-dimensional quantum system amenable to implementation on a quantum computer.
• The framework employs the Koopman operator formalism for the representation of dynamics and RKHS techniques for the representation of observables.
• The quantum mechanical simulator can be implemented as an $N$-qubit quantum circuit with a polynomial number of gates in $N$.

Ongoing and future work:

• Develop data-driven formulation of the scheme using kernel features (e.g., G. 2019, Slawinska et al. 2019).
• Generalize to mixing dynamical systems with continuous spectra; e.g., using RKHS-based spectral discretization techniques for the generator (Das et al. 2018).
• Perform experiments on prototype quantum computing platforms.
References