

# Geometry-aware variational real-time quantum evolution

André J. Ferreira-Martins, Renato M. S. Farias, Giancarlo Camilo, Thiago O. Maciel, Allan Tosta, Tobias Haug, and Leandro Aolita

Quantum Research Center, Technology Innovation Institute, Abu Dhabi, UAE

Simulating the real-time dynamics of quantum systems is a key application of quantum computing [17], in fields such as quantum chemistry [21], material design [6], and quantum many-body physics [11]. Notably, real-time evolution is especially hard to simulate classically, thus offering a more straightforward route towards quantum advantage compared to ground-state problems. For example, the ground state of local one-dimensional Hamiltonians or even the FeMoco molecule [25] can be efficiently computed with classical methods, while no such classical algorithms are known for their corresponding quantum real-time evolution [22].

However, for noisy quantum computers [2], simulation methods such as Trotterization can be resource-intensive to implement as the circuit depth significantly increases with time [5]. *Variational quantum simulation* (VQS) [16,24] attempts to overcome this bottleneck by using a variational quantum circuit, controlled by  $m$  parameters, to simulate the time evolution. However, so far, VQS and all its variants suffer from at least one of the four following drawbacks: (i)  $\mathcal{O}(m^2)$  complexity due to estimation of the quantum geometric tensor; (ii) implementation of the Hadamard test for the imaginary gradient; (iii) NP-hardness of optimization of the variational ansatz [3]; (iv) Trotter step errors. VQS suffers from (i, ii); while variants such as *projected variational quantum dynamics* (p-VQD) [19,1] or variational fast forwarding [4], from (iii, iv); and Ref. [10] from (iii). These restrictions have hampered the study and experimental implementations of real-time evolution in noisy quantum computers [15].

Here, we propose the geometry-aware variational quantum simulator (GVQS) as the first near-term, real-time simulation method that avoids all four drawbacks. We achieve this by relying on a geometry-aware amplitude encoder [7, QTML 2024] and methods based on *exact geodesic transport* (EGT) [8, QTML 2025]. In particular, GVQS removes the restrictions of VQS by using an analytic quantum geometric tensor, removing (i), and making use of our special ansatz structure to directly estimate the imaginary gradient, removing (ii). As a further result, we significantly enhance the performance of p-VQD by integrating the EGT optimizer of Ref. [8]. We demonstrate GVQS on the fixed-particle-number, two-mode Bose-Hubbard Hamiltonian, observing superior performance over p-VQD. Our methods open up simulation of quantum evolution as a promising application of noisy quantum computers.

**Main idea.** In [7], we introduced  $n$ -qubit auxiliary-qubit-free data loaders for both real- and complex-valued amplitudes. There, the  $d$ -dimensional Hilbert (sub)space of interest is parametrized as a hypersphere  $\mathbb{S}^{d-1}$ , and the amplitudes are written in the hyperspherical coordinate system. Our recent follow-up [8] introduced the EGT optimizer for *real-valued* amplitudes based on the structure of the aforementioned manifold. The hypersphere is associated with a metric tensor  $\mathbf{g}(\boldsymbol{\theta})$  that is both diagonal and known analytically, defined as  $(\mathbf{g}(\boldsymbol{\theta}))_{\ell\ell} = \prod_{j=0}^{\ell-1} \sin^2(\theta_j)$  and the parameters update uses geodesic paths based on the analytical expression for the exponential map. This goes beyond first- and second-order update rules, such as the quantum natural gradient [23] and its second-order corrections [12]. A normalized complex vector can be represented as  $\mathbf{y} = (\text{Re } \mathbf{x}, \text{Im } \mathbf{x}) \in \mathbb{S}^{2d-1}$ . In this real embedding, we use hyperspherical coordinates  $\boldsymbol{\alpha} = (\alpha_0, \dots, \alpha_{2d-2})$ , for which the metric is diagonal and given by  $(\mathbf{g}(\boldsymbol{\alpha}))_{\ell\ell}$ , where  $\boldsymbol{\alpha}$  denotes the hyperspherical coordinates of the real embedding  $(\text{Re } \mathbf{x}, \text{Im } \mathbf{x}) \in \mathbb{S}^{2d-1}$ , and should not be confused with the encoder angles  $(\boldsymbol{\theta}, \boldsymbol{\varphi})$  of the modulus-phase circuit parametrization. The EGT-CG update is performed on this  $\mathbb{S}^{2d-1}$  manifold, and the updated complex amplitudes are then mapped back to the modulus-phase encoder parameters. Note that  $\mathbf{g}$  does not depend on the phase parameters  $\boldsymbol{\phi}$ . The exponential map and, consequently, the update rule defined in [8], are preserved w.r.t. to the case of real amplitudes.

Given a Hamiltonian  $H$ , its time evolution  $e^{-itH}$  can be implemented via VQS using the MacLachlan’s variational principle, which is equivalent to solving the differential equation  $\mathbf{M}\dot{\boldsymbol{\theta}} = \mathbf{V}$  [24, Eq.

(14)], where matrix  $\mathbf{M}$  is related to the quantum geometric tensor, vector  $\mathbf{V}$  to the imaginary part of the gradient, and  $\dot{\boldsymbol{\theta}} := \frac{d}{dt}\boldsymbol{\theta}$ . Most importantly, due to the orthonormality of the hyperspherical coordinate system in use,  $\mathbf{M}$  coincides with  $\mathbf{g}$ . Therefore,  $\mathbf{M}$  is analytically known and does not require experimental estimation, in contrast to standard VQS where its quantum estimation scales as  $O(m^2)$ . Moreover, even though VQS requires Hadamard tests in general, for GVQS the estimation of  $\mathbf{V}$  with our encoder [7] can be performed without a Hadamard test using a setup equivalent to the gradient estimation presented in [8, App. J].

As reference, we also consider the p-VQD algorithm [19,1] for which we also propose an improved optimization method. In p-VQD, the parameters  $\boldsymbol{\theta}_\tau$  are updated to time  $\tau + 1$  following the update rule  $\boldsymbol{\theta}_{\tau+1} = \boldsymbol{\theta}_\tau + \arg \min_{\delta\boldsymbol{\theta}} \left[ 1 - |\langle \psi(\boldsymbol{\theta}_\tau + \delta\boldsymbol{\theta}) | e^{-it'H} | \psi(\boldsymbol{\theta}_\tau) \rangle|^2 \right]$ . One could, for instance, implement  $e^{-it'H}$  as a single Trotter step and estimate the overlap on the r.h.s. of the above equation. This defines a new target state at each time step  $\tau$ , saving hardware resources on the total evolution until time  $t$  w.r.t. full Trotterization of  $e^{-it'H}$ . To implement time evolution via p-VQD, one needs to minimize the function in the update rule above. For that, we use the EGT optimized from our work in [8]. We also benchmark the performance against the Adam optimizer [14].

**Two-mode BH model.** We consider the two-mode Bose–Hubbard Hamiltonian [18]

$$H = -J(a_L^\dagger a_R + a_R^\dagger a_L) + \frac{U}{2} \{n_L(n_L - 1) + n_R(n_R - 1)\} + \frac{\Delta}{2}(n_L - n_R), \quad (1)$$

where  $a_{L,R}^\dagger$  ( $a_{L,R}$ ) are the left- and right-mode annihilation (creation) operators,  $n_{L,R} := a_{L,R}^\dagger a_{L,R}$  are the left- and right-mode number operators,  $J$  is the tunnel coupling between the two modes,  $U$  is the onsite interaction, and  $\Delta$  is the left-right bias. We fix the particle number  $N := n_L + n_R$  such that the dynamics is restricted to the  $(N + 1)$ -dimensional subspace spanned by the Fock states  $\{|n, N - n\rangle\}_{n \in [N]}$ , where  $n$  is the occupation of the left mode. The two-mode BH Hamiltonian is a minimal model for coherent tunneling between two weakly coupled condensates, including Josephson oscillations, and exhibits nontrivial dynamics for observables such as population imbalance, coherence, and number fluctuations [20]. Moreover, its behavior is controlled by the interaction ratio, often written as  $\Lambda = \frac{UN}{2J}$ ; by the bias  $\Delta$ ; and by the initial imbalance and phase. Large interactions and biased junctions generate strongly nonlinear dynamics and enhanced number fluctuations, making the model a useful benchmark. More broadly, real-time Bose–Hubbard dynamics is a demanding classical target: in extended and higher-dimensional settings, even tensor-network cross-validation becomes challenging, motivating tensor-network benchmarks for two-dimensional Bose–Hubbard quenches [13].

The fixed- $N$  sector admits a compressed binary representation: we map  $|n, N - n\rangle$  to  $|\text{bin}(n)\rangle$ , so the physical Hilbert space of dimension  $N + 1$  is embedded into  $n = \lceil \log_2(N + 1) \rceil$  qubits; for example, the  $N = 31$  example studied below requires only  $n = 5$  qubits. The observables are chosen to test both the physical dynamics and numerical accuracy. We track the normalized population imbalance  $z(t) = 2 \langle J_z \rangle / N$  (where  $J_z = \frac{1}{2}(n_L - n_R)$ ), the normalized coherence regarding the hopping quadrature  $C_x(t) = 2 \langle J_x \rangle / N$  (where  $J_x = \frac{1}{2}(a_L^\dagger a_R + a_R^\dagger a_L)$ ), number fluctuations  $\text{Var}(J_z)$ , the energy  $\langle H \rangle$ , and relative errors with respect to exact sparse evolution. The first three quantities probe the dynamics directly, while the energy and relative observable errors expose conservation properties and accumulated numerical error.

**Numerical results.** We benchmark all methods against sparse exact dynamics in the compact-binary physical subspace; at this stage, simulations of all quantum methods are noiseless and performed at infinite precision. Figure 1 shows the  $N = 31$  two-mode BH Hamiltonian initialized in a coherent imbalanced state with  $z_0 = 0.5$ , evolved up to  $t = 20$  with  $\Delta t = 0.05$ . The comparison includes exact dynamics, p-VQD with EGT-CG or Adam projection using the Pauli-product-formula target, and McLachlan GVQS with Runge–Kutta 4 (RK4), using 10 uniform sub-steps for each output interval, or with a geometric implicit midpoint integrator on the GVQS manifold with energy projection (EPIM) [9]. VQS remains the most accurate family for the observables shown. EPIM achieves the overall smallest relative errors while providing explicit energy control. However, it requires more  $\mathbf{V}$  evaluations than RK4. For short-time raw accuracy, RK4 may look attractive, but for long-time GVQS

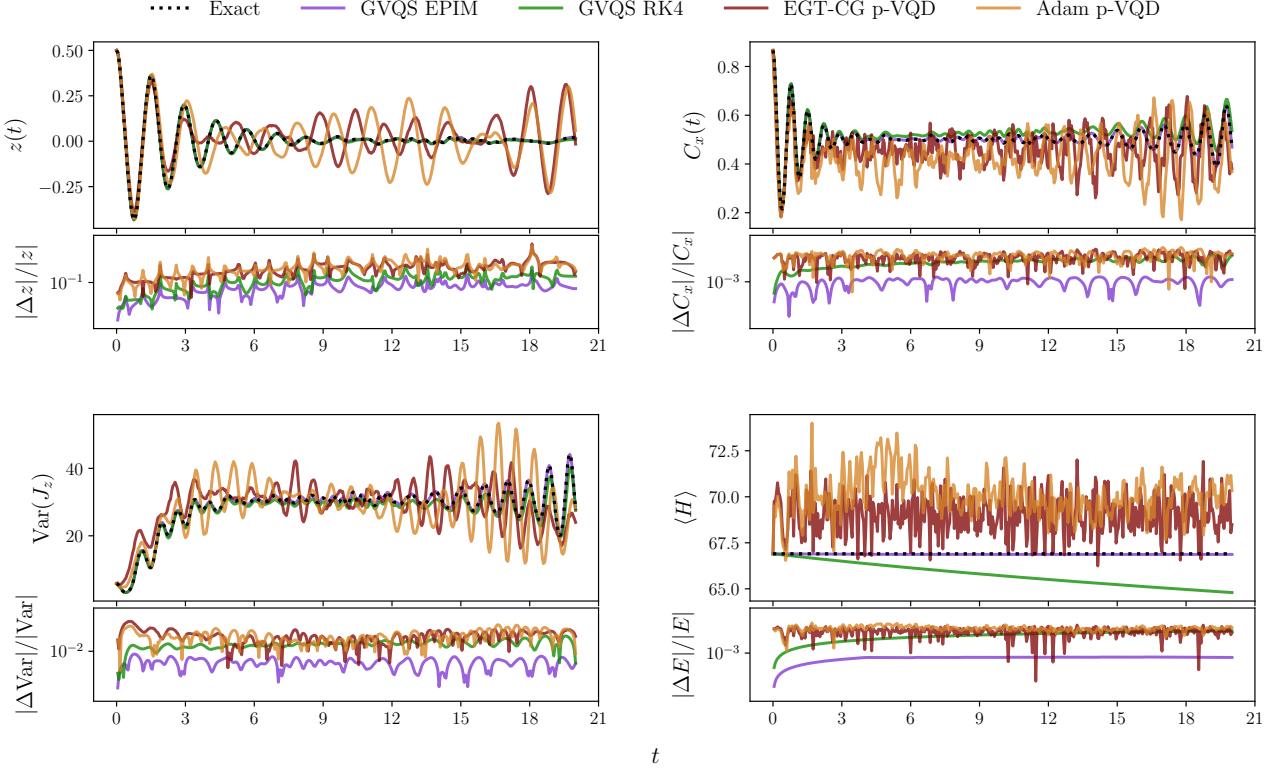


**Figure 1. Compact-binary two-mode Bose-Hubbard real-time benchmark for  $N = 31$ .** Dynamics are shown for the coherent imbalanced initial state with  $z_0 = 0.5$ ,  $J = 1$ ,  $\Lambda = 5$ ,  $\Delta = 0$ , and time step  $\Delta t = 0.05$ . The fixed- $N$  sector has dimension  $N + 1 = 32$  and is represented with the compact binary register using 5 qubits. Dotted black curves represent the exact statevector dynamics. We compare the hardware-target p-VQD, using a first-order Pauli-product-formula approximation to  $U_t$  and optimized either with EGT-CG or Adam, against the GVQS method using either RK4 or EPIM. For p-VQD, EGT-CG uses at most 20 inner epochs per time step, while Adam uses at most 200 epochs with a learning rate of  $10^{-2}$ . For GVQS, RK4 uses 10 sub-steps per output interval, whereas EPIM adaptively integrates the McLachlan flow with tolerance  $3 \times 10^{-3}$  and energy monitoring/projection. The upper panels show the population imbalance  $z(t) = 2 \langle J_z \rangle / N$ , transverse coherence  $C_x(t) = 2 \langle J_x \rangle / N$ , number fluctuation  $\text{Var}(J_z)$ , and energy  $\langle H \rangle$ . The lower panels show relative errors with respect to exact evolution, omitting the  $t = 0$  point.

dynamics with energy monitoring and chart geometry, the implicit midpoint family seems to be the more structurally appropriate integrator (see [9]). In p-VQD, the hardware-friendly target construction introduces product-formula error, and the final accuracy also depends on projection quality. EGT-CG reaches substantially smaller projection losses than Adam with far fewer inner epochs, demonstrating the value of geometry-aware projection even when the target evolution itself is approximate.

**Quantum resources and discussion.** In Fig. 1, EPIM used 40984 total  $\mathbf{V}$  evaluations, corresponding to 102.46 evaluations per output interval and 2.14 evaluations per accepted step. RK4 used 32000 total  $\mathbf{V}$  evaluations: 80 per output interval, and 8 per effective sub-step. Thus, EPIM required about  $1.28\times$  as many  $\mathbf{V}$  evaluations as RK4, despite using fewer evaluations per accepted internal step. On the other hand, for the hardware-like  $U_t$  target, EGT-CG p-VQD used 22000 loss evaluations and 2800 total epochs, whereas Adam p-VQD used 80400 loss evaluations and 80000 total epochs. Therefore, EGT-CG required about  $3.65\times$  fewer loss evaluations and about  $28.6\times$  fewer epochs than Adam. It also reached a smaller maximum projection loss,  $9.09 \times 10^{-11}$  versus  $2.18 \times 10^{-2}$  for Adam, which did not converge within the epoch budget. Overall, the complex hyperspherical parametrization gives two complementary advantages: geometry-aware low-iteration projection for p-VQD and low-overhead analytic metric handling for GVQS. The long-time EPIM result further shows that energy-preserving geometry, adaptive-step control, and projection cadence must be tuned together with the target accuracy to achieve optimal resource efficiency.

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