Quandary: Optimal Control for Quantum Systems

Stefanie Günther[*]   N. Anders Petersson[*]

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[*]Center for Applied Scientific Computing, Lawrence Livermore National Laboratory, Livermore, CA, USA.

1 Introduction

Quandary numerically simulates and optimizes the time evolution of closed and open quantum systems. The underlying dynamics are modelled by either Schroedinger's equation (for closed systems), or Lindblad's master equation (for open systems that interact with the environment). Quandary solves the respective ordinary differential equation (ODE) numerically by applying a time-stepping integration scheme, and applies a gradient-based optimization scheme to determine optimal control pulses that drive the quantum system to a desired target state. Two optimization objectives are considered: Unitary gate optimization that finds controls to realize a logical quantum gate, and state preparation that aims to drive the quantum system to a desired target state, such as for example the ground state of zero energy level.

Quandary is designed to solve optimal control problems in larger (potentially open) quantum systems, targeting modern high performance computing (HPC) platforms. Quandary utilizes distributed memory computations using the message passing paradigm that enables scalability to large number of compute cores. Implemented in C++, Quandary is portable and its object-oriented implementation allows developers to easily extend the predefined setup to suit their particular simulation and optimization requirements. For example, customized gates for Hamiltonian simulations can easily be added to supplement Quandary's predefined gate set.

This document outlines the mathematical background and underlying equations, and summarizes their implementation in Quandary. For installation instructions and execution, please take a look at the README.md file. Further, the configuration file config_template.cfg is filled with comments that should help users and developers to set up new simulation and optimization runs, and match the input options to the equations found in this document. A full documentation is under development. In the meantime, don't hesitate to direct any questions to guenther5@llnl.gov. We also refer to our publications [2, 3].

2   Model equation

Quandary models composite quantum systems consisting of Q subsystems, with n_k energy levels for the k-th subsystem, $k = 0, \ldots, Q-1$. The Hilberspace dimension is hence the product of each subsystem dimensions: $N = \prod_{k=0}^{Q-1} n_k$.

The Hamiltonian describing the composite system is modelled as

$$H_d := \sum_{k=0}^{Q-1} \left(\omega_k a_k^\dagger a_k - \frac{\xi_k}{2} a_k^\dagger a_k^\dagger a_k a_k + \sum_{l>k} \left(J_{kl} \left(a_k^\dagger a_l + a_k a_l^\dagger \right) - \xi_{kl} a_k^\dagger a_k a_l^\dagger a_l \right) \right) \tag{1}$$

where $\omega_k \geq 0$ denotes the $0 \to 1$ transition frequency and $\xi_k \geq 0$ is the self-Kerr coefficient of subsystem k, and the cross resonance coefficients are $J_{kl} \geq 0$ ("dipole-dipole interaction") and $\xi_{kl} \geq 0$ ("zz-coupling"). Here, $a_k \in \mathbb{C}^{N \times N}$ denotes the lowering operator acting on subsystem k, which is defined as

$$
\begin{aligned}
a_0 &:= a^{(n_0)} \otimes I_{n_1} \otimes \cdots \otimes I_{n_{Q-1}} \\
a_1 &:= I_{n_0} \otimes a^{(n_1)} \otimes \cdots \otimes I_{n_{Q-1}} \\
&\vdots \\
a_{Q-1} &:= I_{n_0} \otimes I_{n_1} \otimes \cdots \otimes a^{(n_{Q-1})}
\end{aligned}
\quad \text{with} \quad
a^{(n_k)} :=
\begin{pmatrix}
0 & 1 & & & \\
& 0 & \sqrt{2} & & \\
& & \ddots & \ddots & \\
& & & & \sqrt{n_k - 1} \\
& & & & 0
\end{pmatrix}
\in \mathbb{R}^{n_k \times n_k} \tag{2}
$$

where $I_{n_k} \in \mathbb{R}^{n_k \times n_k}$ is the identity matrix.

The action of external control fields on the quantum system is modelled through the control Hamiltonian

$$H_c(t) := \sum_{k=0}^{Q-1} f^k(\vec{\alpha}^k, t) \left(a_k + a_k^\dagger \right) \tag{3}$$

where $f^k(\vec{\alpha}^k, t)$ are real-valued, time-dependent control functions that are parameterized by real-valued parameters $\vec{\alpha}^k \in \mathbb{R}^d$, which can be either specified, or optimized for.

For a **closed quantum system** (no environmental interactions), the quantum state is described by a complex-valued vector $\psi \in \mathbb{C}^N$, with $\|\psi\| = 1$. For a given initial state $\psi(t=0)$, the evolution of the state vector is modelled through **Schroedinger's equation**

$$\dot{\psi}(t) = -iH(t)\psi(t), \quad \text{with} \quad H(t) := H_d + H_c(t). \tag{4}$$

Open quantum systems take interactions with the environment into account, allowing to model decoherence and noise in the system. In that case, the state of the quantum system is described by its density matrix $\rho \in \mathbb{C}^{N \times N}$, and the time-evolution is modelled by **Lindblad's master equation**:

$$\dot{\rho}(t) = -i(H(t)\rho(t) - \rho(t)H(t)) + \mathcal{L}(\rho(t)), \tag{5}$$

where again $H(t) = H_d + H_c(t)$, and where $\mathcal{L}(\rho(t))$ denotes the Lindbladian collapse operators to model system-environment interactions. The Lindbladian operator $\mathcal{L}(\rho(t))$ is assumed to be of the form

$$\mathcal{L}(\rho(t)) = \sum_{k=0}^{Q-1} \sum_{l=1}^{2} \mathcal{L}_{lk}\rho(t)\mathcal{L}_{lk}^\dagger - \frac{1}{2} \left(\mathcal{L}_{lk}^\dagger \mathcal{L}_{lk}\rho(t) + \rho(t)\mathcal{L}_{lk}^\dagger \mathcal{L}_{lk} \right) \tag{6}$$

where the collapse operators $\mathcal{L}_{lk}$ model decay and dephasing processes in the subsystem k with

- Decay ("T_1"): $\mathcal{L}_{1k} = \frac{1}{\sqrt{T_1^k}} a_k$

- Dephasing ("T_2"): $\mathcal{L}_{2k} = \frac{1}{\sqrt{T_2^k}} a_k^\dagger a_k$

The constants $T_l^k > 0$ correspond to the half-life of process l on subsystem k. Typical T_1 decay time is between $10 - 100$ microseconds (us). T_2 dephasing time is typically about half of T1 decay time.

All the above constants and system parameters can be specified in the first part of the configuration file that Quandary's executable takes as an input, compare `config_template.cfg`. Note that the main choice here is which equation should be solved for and which representation of the quantum state will be used (either Schroedinger with a state vector $\psi \in \mathbb{C}^N$, or Lindblad's equation for a density matrix $\rho \in \mathbb{C}^{N \times N}$). In the configuration file, this choice is determined through the option `collapse_type`, where `none` will result in Schroedinger's equation and any other choice will result in Lindblad's equation being solved for. Further note, that choosing `collapse_type` $\neq$ `none`, together with a collapse time $T_l^k = 0.0$ will omit the evaluation of the corresponding term in the Lindblad operator (6).

Note: *In the remainder of this document, the quantum state will mostly be denoted by ρ, independent of which equation is solved for. So ρ can be seen as placeholder for either the density matrix $\rho \in \mathbb{C}^{N \times N}$, or the state vector $\psi \in \mathbb{C}^N$. A clear distinction between the two will only be made explicit if necessary.*

2.1 Rotational frame approximation

Quandary uses the rotating wave approximation in order to slow down the time scales in the solution of Schroedinger's or Lindblad's master equations. To that end, the user can specify the rotation frequencies ω_k^r for each oscillator. Under the rotating frame wave approximation, the Hamiltonians are transformed to

$$\tilde{H}_d(t) := \sum_{k=0}^{Q-1} (\omega_k - \omega_k^r) a_k^\dagger a_k - \frac{\xi_k}{2} a_k^\dagger a_k^\dagger a_k a_k - \sum_{l>k} \xi_{kl} a_k^\dagger a_k a_l^\dagger a_l$$

$$+ \sum_{k=0}^{Q-1} \sum_{l>k} J_{kl} \left(\cos(\eta_{kl} t) \left(a_k^\dagger a_l + a_k a_l^\dagger \right) + i \sin(\eta_{kl} t) \left(a_k^\dagger a_l - a_k a_l^\dagger \right) \right) \tag{7}$$

$$\tilde{H}_c(t) := \sum_{k=0}^{Q-1} \left(p^k(\vec{\alpha}^k, t)(a_k + a_k^\dagger) + i q^k(\vec{\alpha}^k, t)(a_k - a_k^\dagger) \right) \tag{8}$$

where $\eta_{kl} := \omega_k^r - \omega_l^r$ are the differences in rotational frequencies between subsystems.

Note that the eigenvalues of the rotating frame Hamiltonian become significantly smaller in magnitude by choosing $\omega_k^r \approx \omega_k$ (so that the first term with $a_k^\dagger a_k$ drops out). This slows down the time variation of the state evolution, hence bigger time-step sizes can be chosen when solving the master equation numerically. We remark that the rotating wave approximation ignores terms in the control Hamiltonian that oscillate with frequencies $\pm 2\omega_k^r$. Below, we drop the tildes on $\tilde{H}_d$ and $\tilde{H}_c$ and use the rotating frame definition of the Hamiltonians to model the system evolution in time.

Using the rotating wave approximatino, the real-valued laboratory frame control functions are written as

$$f^k(\vec{\alpha}^k, t) = 2\mathrm{Re}\left(d^k(\vec{\alpha}^k, t)e^{i\omega_k^r t}\right), \quad d^k(\vec{\alpha}^k, t) = p^k(\vec{\alpha}^k, t) + iq^k(\vec{\alpha}^k, t) \tag{9}$$

where the rotational frequencies ω_k^r act as carrier waves to the rotating-frame control functions $d^k(\vec{\alpha}^k, t)$.

2.2 Control pulses

The time-dependent rotating-frame control functions $d^k(\vec{\alpha}^k, t)$ are parameterized using N_s piecewise quadratic B-spline basis functions $B_s(t)$ acting as envelope for N_f^k carrier waves:

$$d^k(\vec{\alpha}^k, t) = \sum_{f=1}^{N_f^k}\sum_{s=1}^{N_s} \alpha_{s,f}^k B_s(t)e^{i\Omega_k^f t}, \quad \alpha_{s,f}^k = \alpha_{s,f}^{k(1)} + i\alpha_{s,f}^{k(2)} \in \mathbb{C} \tag{10}$$

The amplitudes $\alpha_{s,f}^{k(1)}, \alpha_{s,f}^{k(2)} \in \mathbb{R}$ are the control parameters (*design* variables) that Quandary can optimize in order to realize a desired system behavior, giving a total number of $2N_s \sum_k N_f^k$ real-valued optimization variables. Further, $\Omega_k^f \in \mathbb{R}$ denote the carrier wave frequencies in the rotating frame which can be choosen to trigger certain system frequencies. The corresponding Lab-frame carrier frequencies become $\omega_k^r + \Omega_k^f$. Those frequencies can be chosen to match the transition frequencies in the lab-frame system Hamiltonian. For example, when $\xi_{kl} << \xi_k$, the transition frequencies satisfy $\omega_k - n\xi_k$. Thus by choosing $\Omega_k^f = \omega_k - \omega_k^r - n\xi_k$, one triggers transition between energy levels n and $n+1$ in subsystem k.

Using trigonometric identities, the real and imaginary part of the rotating-frame control $d^k(\vec{\alpha}^k, t) = p^k(\vec{\alpha}^k, t) + iq^k(\vec{\alpha}^k, t)$ are given by

$$p^k(\vec{\alpha}^k, t) = \sum_{f=1}^{N_f^k}\sum_{s=1}^{N_s} B_s(t)\left(\alpha_{s,f}^{k(1)}\cos(\Omega_f^k t) - \alpha_{lsf}^{k(2)}\sin(\Omega_f^k t)\right) \tag{11}$$

$$q^k(\vec{\alpha}^k, t) = \sum_{f=1}^{N_f^k}\sum_{s=1}^{N_s} B_s(t)\left(\alpha_{s,f}^{k(1)}\sin(\Omega_f^k t) + \alpha_{s,f}^{k(2)}\cos(\Omega_f^k t)\right) \tag{12}$$

Those relate to the Lab-frame control $f^k(\vec{\alpha}^k, t)$ through

$$f^k(t) = 2\sum_{f=1}^{N_f^k}\sum_{s=1}^{N_s} B_s(t)\left(\alpha_{s,f}^{k(1)}\cos((\omega_k^r + \Omega_f^k)t) - \alpha_{s,f}^{k(2)}\sin((\omega_k^r + \Omega_f^k)t)\right) \tag{13}$$

$$= 2p^k(\vec{\alpha}^k, t)\cos(\omega_k^r t) - 2q^k(\vec{\alpha}^k, t)\sin(\omega_k^r t) \tag{14}$$

$$= 2\mathrm{Re}\left(d^k(\vec{\alpha}^k, t)e^{i\omega_k^r t}\right) \tag{15}$$

2.2.1 Storage of the control parameters

The control parameters $\boldsymbol{\alpha}$ are stored in the Quandary code in the following order: List oscillators first $(\vec{\alpha}^0, \ldots, \vec{\alpha}^{Q-1})$, then for each $\vec{\alpha}^k \in \mathbb{R}^{2N_s N_f^k}$, iterate over N_s splines: $\vec{\alpha}^k = (\alpha_1^k, \ldots, \alpha_{N_s}^k)$ with $\alpha_s^k \in \mathbb{R}^{2N_f^k}$, then each α_s^k iterates over carrier waves and for each carrier wave lists the real and imaginary components: $\alpha_s^k = \alpha_{s,1}^{k(1)}, \alpha_{s,1}^{k(2)}, \ldots \alpha_{s,N_f^k}^{k(1)}, \alpha_{s,N_f^k}^{k(2)}$. Hence there are a total of $2N_s \sum_k N_f^k$ real-valued optimization parameters, which are stored in the following order:

$$\boldsymbol{\alpha} := \left(\vec{\alpha}^0, \ldots, \vec{\alpha}^{Q-1}\right), \in \mathbb{R}^{2N_s \sum_k N_f^k} \quad \text{where} \tag{16}$$

$$\vec{\alpha}^k = \left(\alpha_{1,1}^k, \ldots, \alpha_{1,N_f^k}^k, \ldots, \alpha_{N_s,1}^k, \ldots, \alpha_{N_s,N_f^k}^k\right), \quad \text{with} \quad \alpha_{s,f}^k = \left(\alpha_{s,f}^{k(1)}, \alpha_{s,f}^{k(2)}\right) \in \mathbb{R}^2, \tag{17}$$

iterating over Q subsystems first, then N_s splines, then N_f^k carrier wave frequencies. To access an element $\alpha_{s,f}^{k(i)}$, $i = 0, 1$, from storage $\boldsymbol{\alpha}$:

$$\alpha_{s,f}^{k(i)} = \boldsymbol{\alpha}\Big[\left(\sum_{j=0}^{k-1} 2N_s N_f^j\right) + s * 2N_f^k + f * 2 + i\Big], \tag{18}$$

When executing Quandary, the control parameter $\boldsymbol{\alpha}$ can be either specified (e.g. a constant pulse, a pi-pulse, or pulses whose parameters are read from a given file), or can be optimized for (Section 3).

In order to guarantee that the optimizer yields control pulses that are bounded with $|p^k(t)| \leq c_{max}^k$, $|q^k(t)| \leq c_{max}^k$ for given bounds c_{max}^k for each subsystem $k = 0, \ldots, Q-1$, box constraints are implemented as:

$$|\alpha_{s,f}^{k(1)}| \leq \frac{c_{max}^k}{N_f^k} \quad \text{and} \quad |\alpha_{s,f}^{k(2)}| \leq \frac{c_{max}^k}{N_f^k}. \tag{19}$$

3 The Optimal Control Problem

In the most general form, Quandary can solve the following optimization problem

$$\min_{\boldsymbol{\alpha}} \frac{1}{n_{init}} \sum_{i=1}^{n_{init}} \beta_i J(\rho_i^{target}, \rho_i(T)) + \gamma_1 \int_0^T P(\rho_i(t)) \, \mathrm{d}t + \gamma_2 \|\boldsymbol{\alpha}\|_2^2 \tag{20}$$

where $\rho_i(T)$ denotes the quantum state evaluated at a final time $T > 0$, which solves either Lindblad's master equation (5) or Schroedinger's equation (4) in the rotating frame for an initial condition $\rho_i(0)$, as specified below. (Note again that in the Schroedinger case ρ denotes the state vector rather than a density matrix, compare Section 2).

The first term in (20) minimizes (a weighted average of) an objective function J that quantifies the discrepancy between a desired target state ρ_i^{target} and the realized state $\rho_i(T)$ at final time T driven by the current control $\boldsymbol{\alpha}$. The second term serves as a penalty that can be added with $\gamma_1 \geq 0$ in oder to achieve a desired behavior of the quantum system over the entire time-domain $0 \leq t \leq T$, see below. The third term is a Tikhonov regularization that can be added with parameter $\gamma_2 \geq 0$ in order to regularize the optimization problem (stabilize optimization convergence) by favoring solutions with small norm.

3.1 Objective function

The following choices for J are implemented

$$J_{Frobenius} = \frac{1}{2}\|\rho^{target} - \rho(T)\|_F^2 \tag{21}$$

$$J_{Trace} = 1 - \frac{1}{w}\text{Tr}\left((\rho^{target})^\dagger \rho(T)\right), \quad \text{where} \quad w = \text{Tr}(\rho(0)^2) \tag{22}$$

$$J_{Measure} = \text{Tr}\left(N_m \rho(T)\right), \tag{23}$$

where $N_m \in \mathbb{R}^{N \times N}$ is a diagonal matrix with diagonal elements $\lambda_k = |k - m| \, \forall k = 0, \ldots, N-1$ for a given integer m with $0 \leq m < N$. The first two measures are mostly common for gate optimization, $J_{measure}$ is useful when considering pure-state optimization, see below. In Quandary, the objective function can be specified with the configuration option `optim_objective`.

Note that those measures apply to either the density matrix version solving Lindblad's equation (compare Section 2), or the state vector version solving Schroedinger's equation. In the latter case, naturally with $\rho = \psi\psi^\dagger$, the objective measures applied to state vectors are

$$J_{Frobenius} = \frac{1}{2}\|\psi^{target} - \psi(T)\|_2^2 \tag{24}$$

$$J_{Trace} = 1 - |(\psi^{target})^\dagger \psi(T)|^2 \tag{25}$$

$$J_{Measure} = \psi(T)^\dagger N_m \psi(T). \tag{26}$$

3.2 Optimization targets

Here we describe the target states ρ^{target} that are realized in Quandary. Two cases are considered: State preparation, where the target state is the same for all initial conditions, and gate optimization, where the target state is a unitary transformation of the initial condition. The type of the optimization target can be specified in the configuration option `optim_target`.

3.2.1 Pure target states

State preparation aims to drive the system from either one specific or from any arbitrary initial state to a common desired (fixed) target state. Quandary can optimize towards *pure* target states of the form

$$\psi^{target} = \boldsymbol{e}_m \quad \text{or} \quad \rho^{target} = \boldsymbol{e}_m \boldsymbol{e}_m^\dagger, \quad \text{for} \quad m \in \mathbb{N}_0 \quad \text{with} \quad 0 \leq m < N \tag{27}$$

where $\boldsymbol{e}_m$ denotes the m-th unit vector in $\mathbb{R}^N$. We note that considering pure states of that specific form ($\boldsymbol{e}_m$ or $\boldsymbol{e}_m \boldsymbol{e}_m^\dagger$) is not a restriction, because any other pure target state can be transformed to this representation using a unitary change of coordinates (compare the Appendix in [3] for a more detailed description). For $m = 0$, the target state represents the ground state of the system under consideration, which has important applications for quantum reset as well as quantum error correction.

Depending on the choice for the initial conditions, optimization towards a pure target state can be used to realize either a simple state-to-state transfer (choosing one specific initial condition, $n_{init} = 1$), or to realize the more complex task of state preparation that drives *any* initial state to

a common pure target state. Driving *any* initial state to a common target will require to couple to a dissipative bath, which should be accounted for in the model setup. In the latter case, typically a full basis of initial conditions needs to be considered during the optimization ($n_{init} = N^2$ for density matrices). However, it is shown in [3], that if one chooses the objective function $J_{measure}$ with corresponding measurement operator N_m (see eq. (23)), one can reduce the number of initial conditions to only *one* being an ensemble of all basis states, and hence $n_{init} = 1$ independent of the system dimension N. Compare [3] for details, and Section 3.3.4

Note that the above m refers to the $|m\rangle$-th state of the entire system under consideration with dimension N, which can be a composite of Q subsystems. In Quandary this pure target state is specified by defining the desired pure target for *each* of the subsystems individually. For a composite system of Q subsystems with n_k levels each, a composite target pure state is specified by a list of integers m_k with $0 \leq m_k < n_k$ representing the pure target state in each subsystem k. The composite pure target is state is then

$$\psi^{target} = |m_0 m_1 m_2 \ldots m_{Q-1}\rangle \quad \text{aka} \quad \psi^{target} = \boldsymbol{e}_{m_0} \otimes \boldsymbol{e}_{m_1} \otimes \cdots \otimes \boldsymbol{e}_{m_{Q-1}} \tag{28}$$

for unit vectors $\boldsymbol{e}_{m_k} \in \mathbb{R}^{n_k}$ (and $\rho^{target} = \psi^{target}(\psi^{target})^\dagger$ for the density matrix). The composite-system index m is then computed inside Quandary, from

$$m = m_0 \frac{N}{n_0} + m_1 \frac{N}{n_0 n_1} + m_2 \frac{N}{n_0 n_1 n_2} + \cdots + m_{Q-1} \tag{29}$$

For example, assume one considers a composite system consisting of a qubit modelled with $n_0 = 2$ levels coupled to a readout cavity modelled with $n_1 = 10$ levels, and one wants to drive the qubit to the $|1\rangle$ state and the cavity to the ground state. The target pure state input for Quandary is hence $m_0 = 1, m_1 = 0$ (i.e. the $|10\rangle$ state in the composite system), which corresonds $m = 1 \cdot 10 + 0 = 10$ in the composite system of dimension $N = 2 \cdot 10 = 20$.

3.2.2   Read a target state from file

A specific target state ρ^{target} can also be read from file. This can be useful when considering non-pure target states. File format: The vectorized density matrix (columnwise vectorization) in the Lindblad case, or the state vector in the Schroedinger case, one real-valued number per row, first list all real parts, then list all imaginary parts (hence either $2N^2$ lines with one real number each, or $2N$ lines with one real number each).

3.2.3   Gate optimization

Quandary can be used to realize logical gate operations. In that case, the target state is not fixed across the initial states, but instead is a unitary transformation of each initial condition. Let $V \in \mathbb{C}^{N \times N}$ be a unitary matrix presenting a logical operation, the goal is to drive any initial state $\rho(0)$ to the unitary transformation $\rho^{target} = V \rho(0) V^\dagger$, or, in the Schroedinger case, drive any initial state $\psi(0)$ to the unitary transformation $\psi(T) = V\psi(0)$. Target gates that are currently

implemented are

$$V_X := \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \quad V_Y := \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} \quad V_Z := \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \quad V_{Hadamard} := \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} \quad (30)$$

$$V_{CNOT} := \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix} \quad V_{SWAP} := \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \quad (31)$$

Further, a generalization of the SWAP and the CNOT gate for general Q subsystems is available: The SWAP-0Q gate swaps the state of the first and the last qubit, while leaving all other oscillators in their respective initial state, and the CQNOT gate performs a NOT operation on the last qubit if all other qubits are in the one-state. New, user-defined gates can be easily added to the code by extending the `Gate` class in the corresponding `.cpp` and `.hpp` files.

For gate optimization, the first two objective function $J_{Frobenius}$ and $J_{Hilbert-Schmidt}$ are appropriate. Since *any* initial quantum state should be transformed by the control pulses, again typically a basis for the initial states should be considered ($n_{init} = N$ for Schroedinger solver, and $n_{init} = N^2$ for Lindblad solver). In the Lindblad solver case, it has however been shown in [1] that it is enough to optimize with only three specific initial states ($n_{init} = 3$), independent of the Hilbert space dimension N. Those three states are set up in such a way that they can distinguish between any two unitaries in that Hilbert space. The three initial states are readily available in Quandary, see Section 3.3. Note that when optimizing with only those three initial states, it turns out that the choice of the weights β_i that weight the contribution from each initial state in the overall objective function strongly influences the optimization convergence. For faster convergence, it is often bene-fitial to emphasize on the first of the three initial conditions ($\rho_1(0)$ in Section 3.3.5), hence choosing β_1 (much) bigger than β_2 and β_3 (e.g. $\beta = \{20, 1, 1\}$ often works better than $\beta = \{1, 1, 1\}$, try it yourself). We refer to [1] for details.

3.2.4 Essential and non-essential levels

It is often useful, to model the quantum system with more energy levels than the number of levels that the target gate is defined on. For example when optimizing for a SWAP gate on two qubits, with $V_{SWAP} \in \mathbb{C}^{4 \times 4}$, one might want to model each qubit with more than two energy levels in order to (a) model the (infinite dimensional) system with more accuracy by including more levels and (b) allow the system to transition through higher energy levels in order to achieve the target at final time T. In that case, the *essential* levels denote the levels that the target gate is defined on. To this end, Quandary provides the option to specify the number of essential energy levels n_k^e in addition to the number of energy levels n_k, where $n_k^e \leq n_k$ for each subsystem k. The quantum dynamics are then modelled with (more) energy levels with $N = \prod_k n_k$ and $\rho(t) \in \mathbb{C}^{N \times N}$, while the gate is defined in the essential level dimensions only: $V \in \mathbb{C}^{N_e \times N_e}$, $N_e = \prod_k n_k^e$. In the example above, $n_0^e = n_1^e = 2$ and hence $V_{SWAP} \in \mathbb{C}^{4 \times 4}$, but one can choose the number of energy levels n_0 and n_1 to be bigger than 2 to when modelling the system dynamics.

To compute the objective function at final time T, the essential-dimensional gate is projected upwards to the full dimensions $\tilde{V} \in \mathbb{C}^{N \times N}$ by inserting identiy blocks for rows/columns that correspond to a non-essential level of either of the subsystems. Hence, a realization of the gate $\tilde{V}$ will not alter the occupation of higher (non-essential) energy level compared to their initial occupation at $t = 0$.

3.3 Initial conditions

Quandary offers various choices to set the initial conditions for simulation and optimization in order to accomodate for different simulation and optimization needs. Below is a list of available options for the initial states (configuration option `initialcondition`).

3.3.1 Pure-state initialization

One can choose to simulate and optimize for only one specific pure initial state (then $n_{init} = 1$). The initial density matrix is then composed of Kronecker products of pure states for each of the subsystems. E.g. for a bipartite system with $n_1 \otimes n_2$ levels, one can propagate any initial pure state

$$\psi(0) = |m_1\rangle \otimes |m_2\rangle \quad \text{for } m_1 \in \{0, \ldots, n_1 - 1\}, m_2 \in \{0, \ldots, n_2 - 1\} \tag{32}$$

$$\text{and} \quad \rho(0) = \psi(0)\psi(0)^\dagger \tag{33}$$

Note that, again, in this notation $|m_1\rangle = \boldsymbol{e}_{m_1} \in \mathbb{R}^{n_1}$. The configuration input takes a list of the integers m_k for each subsystem.

3.3.2 Basis of density matrices

TODO: For Schroedinger, BASIS and DIAGONAL should both propagate B^{kk}. Currently, only DIAGONAL does that, and BASIS throws an error in the Schroedinger case.

To span any possible initial state, an entire basis of states can be used as initial conditions, and then $n_{init} = N^2$. Quandary implements the basis states as defined in [3]:

$$B^{kj} := \frac{1}{2}\left(\boldsymbol{e}_k\boldsymbol{e}_k^\dagger + \boldsymbol{e}_j\boldsymbol{e}_j^\dagger\right) + \begin{cases} 0 & \text{if } k = j \\ \frac{1}{2}\left(\boldsymbol{e}_k\boldsymbol{e}_j^\dagger + \boldsymbol{e}_j\boldsymbol{e}_k^\dagger\right) & \text{if } k < j \\ \frac{i}{2}\left(\boldsymbol{e}_j\boldsymbol{e}_k^\dagger - \boldsymbol{e}_k\boldsymbol{e}_j^\dagger\right) & \text{if } k > j \end{cases} \tag{34}$$

for all $k, j \in \{0, \ldots, N - 1\}$. These density matrices represent N^2 pure states that span the space of all quantum states in this Hilberspace.

In order to uniquely identify the different initial conditions in the Quandary code and in the output files, a unique index $i \in \{0, \ldots, N^2 - 1\}$ is assigned to each basis state with

$$B^i := B^{k(i),j(i)}, \quad \text{with} \quad k(i) := i \bmod N, \quad \text{and} \quad j(i) := \left\lfloor \frac{i}{N} \right\rfloor$$

(columnwise vectorization of a matrix of matrices B^{kj}).

3.3.3 Diagonal basis matrices (aka all pure states)

TODO: For Schroedinger, BASIS and DIAGONAL should both propagate B^{kk}. Currently, only DIAGONAL does that, and BASIS throws an error in the Schroedinger case.

One can choose to propagate only those basis elements that correspond to pure states of the form $\boldsymbol{e}_k\boldsymbol{e}_k^\dagger$, i.e. propagating only B^{kk} for $k = 0, \ldots, N - 1$, and then $n_{init} = N$.

3.3.4 Ensemble state for pure-state optimization

Only valid for the density matrix version, solving Lindblad's master equation.

For pure-state optimization using the objective function $J_{measure}$ (23), one can use the ensemble state

$$\rho_s(0) = \frac{1}{N^2} \sum_{i,j=0}^{N-1} B^{kj} \tag{35}$$

as the only initial condition for optimization or simulation ($\Rightarrow n_{init} = 1$). Since Lindblad's master equation is linear in the initial condition, and $J_{measure}$ is linear in the final state, propagating this single initial state yields the same target value as if one propagates all basis states spanning that space and averages their measure at final time T (compare [3]). To specify the ensemble state in Quandary for composite quantum systems with multiple subsystems, on can provide a list of integer ID's that determine in which of the subsystems the ensemble state should be spanned. Other subsystems will be initialized in the ground state.

To be precise: the user specifies a list of consecutive ID's $< k_0 >, \ldots, < k_m >$ with $0 \le k_j \le Q-1$ and $k_{j+1} = k_j + 1$, the ensemble state $\rho_s(0)$ will be spanned in the dimension given by those subsystems, $N_s = \prod_{j=0}^{m} n_{k_j}$ and $\rho_s(0) \in \mathbb{C}^{N_s \times N_s}$ with basis matrices B^{kj} spanned in $\mathbb{C}^{N_s \times N_s}$. The initial state that Quandary propagates is then given by

$$\rho(0) = e_0 e_0^\dagger \otimes \underbrace{\rho_s(0)}_{\in \mathbb{C}^{N_s \times N_s}} \otimes e_0 e_0^\dagger \tag{36}$$

where the first e_0 (before the kronecker product) is the first unit vector in $\mathbb{R}^{\prod_{k=0}^{k_0-1}}$ (i.e. ground state in all preceding subsystems), and the second e_0 (behind the kronecker products) is the first unit vector in the dimension of all subsequent systems, $\mathbb{R}^{\prod_{k=k_m+1}^{Q-1}}$.

3.3.5 Three initial states for gate optimization

Only valid for the density matrix version, solving Lindblad's master equation.

When considering gate optimization, it has been shown in [1] that it is enough to consider only three specific initial states during optimization ($n_{init} = 3$), independent of the Hilber space dimension. Those three initial states are given by

$$\rho(0)_1 = \sum_{i=0}^{N-1} \frac{2(N-i+1)}{N(N+1)} e_i e_i^\dagger \tag{37}$$

$$\rho(0)_2 = \sum_{ij=0}^{N-1} \frac{1}{N} e_i e_j^\dagger \tag{38}$$

$$\rho(0)_3 = \frac{1}{N} I_N \tag{39}$$

where $I_N \in R^{N \times N}$ is the identity matrix. They are readily implemented in Quandary. Note that it is important to choose the weights $\beta_i, i = 1, 2, 3$ in the objective function appropriately to achieve fast convergence.

3.3.6 $N+1$ initial states for gate optimization

Only valid for the density matrix version, solving Lindblad's master equation.

The three initial states from above do not suffice to estimate an average fidelity of the realized gate (compare [1]). Instead, it is suggested in that same paper to choose $N+1$ initial states to compute an average fidelity. Those $N+1$ initial states consist of the N diagonal states B^{kk} in the Hilbertspace of dimension N, as well as the totally rotated state $\rho(0)_2$ from above. Quandary offers the choice to simulate (or optimize) using those initial states, then $n_{init} = N+1$.

3.3.7 Reading an initial state from file

A specific initial state can also be read from file ($\Rightarrow n_{init} = 1$). Format: one column being the vectorized density matrix (vectorization is columnwise), or the state vector, first all real parts, then all imaginary parts (i.e. number of lines is $2N^2$ or $2N$, with one real-valued number per line).

This option is useful for example if one wants to propagate a specific *non-pure* initial state. In that case, one first has to generate a datafile storing that state (e.g. by simulating a system and storing the output), which can then be read in as initial condition.

3.4 Penalty term

The penalty term can be added with parameter $\gamma_1 \geq 0$ in order to achieve a desired behavior at earlier times other than the final time T. In the standard setting, the following penalty term is currently implemented (easily extendable for developers in the `TimeStepper` class.):

$$\gamma_1 \int_0^T P(\rho(t))\mathrm{d}t = \gamma_1 \int_0^T w(t)J\left(\rho(t)\right)\,\mathrm{d}t, \quad \text{where} \quad w(t) = \frac{1}{a}e^{-\left(\frac{t-T}{a}\right)^2}, \tag{40}$$

for a penalty parameter $0 < a \leq 1$. Note, that as $a \to 0$, the weighting function $w(t)$ converges to the Dirac delta distribution with peak at final time T, hence reducing a leads to more emphasis on the final time T while larger a penalize non-zero energy states at earlier times $t \leq T$. Both γ_1 as well as a can be tuned in the configuration options.

Be aware the adding an integral penalty term requires to evaluate the objective J at *each* time-step within the time-domain $[0,T]$, instead of only the last one. This can be quite expensive, in particular when considering gate optimization, and should hence be turned off if possible (choosing $\gamma_1 = 0$ and/or $a = 0$ will skip the extra computation).

For gate optimization with (non-)essential levels: When the essential levels for gate optimization are smaller than the number of modelled levels ($n_k^e < n_k$ for at least one k), an additional term is added as a penalty in order to prevent leakage into higher levels that are not modelled by the finite-dimensional approximation to the infinite dimensional Hamiltonian. In that case, the occupation of all guard levels (i.e. the last modelled energy levels of each of the subsystems) is penalized:

$$\gamma_1 \int_0^T \sum_r \|\rho(t)_{rr}\|_2^2 \,\mathrm{d}t \tag{41}$$

where $\rho(t)_{rr}$ denotes the diagonal element at (r, r) inside the density matrix $\rho(t) \in \mathbb{C}^{N \times N}$ (or the r-the element of the state vector in the Schroedinger case) and r iterates over all indices that correspond to a guard level (last non-essential energy level) of at least one of the subsystems.

Note that if you want to include this leakage-preventing term, but do *not* want to include the above penalty term (40) (e.g. for efficiency reasons), you can choose $\gamma_1 > 0$ while $a = 0$, which will skip the computation of (40) but will include the term (41).

3.5 Fidelity

As a measure of optimization success, Quandary reports on the fidelity computed from

$$F = \frac{1}{n_{init}} \sum_{i=1}^{n_{init}} \text{Tr} \left(\left(\rho_i^{target} \right)^{\dagger} \rho_i(T) \right). \tag{42}$$

Note that in the Schroedinger case, where the state is a vector rather than a matrix, we naturally get $F = 1/n_{init} \sum_i \left| \left(\psi_i^{target} \right)^{\dagger} \psi_i(t) \right|^2$.

Further note that this fidelity is averaged over the chosen initial conditions, so the user should be careful how to interpret this number. E.g. if one optimizes for a logical gate while choosing the three initial condition as in Section 3.3.5, the fidelity that is reported during optimization will be averaged over those three initial states, which is not sufficient to estimate the actual average fidelity over the entire space of potential intial states. It is advised to recompute the average fidelity **after** optimization has finished, e.g. by propagating all basis states B_{kj} to final time T using the optimized control parameter, or by propagating only $N+1$ initial states to get an estimate thereof.

4 Implementation

4.1 Vectorization of Lindblad's master equation

When solving Lindblad's master equation (5), Quandary uses a vectorized representation of the density matrix with $q(t) := \text{vec}(\rho(t)) \in \mathbb{C}^{N^2}$ (columnwise vectorization). Using the relations

$$\text{vec}(AB) = (I_N \otimes A)\text{vec}(B) = (B^T \otimes I_N)\text{vec}(A) \tag{43}$$

$$\text{vec}(ABC) = (C^T \otimes A)\text{vec}(B) \tag{44}$$

for square matrices $A, B, C \in \mathbb{C}^{N \times N}$, the vectorized form of the Lindblad master equation is given by:

$$\dot{q}(t) = M(t)q(t) \quad \text{where} \tag{45}$$

$$M(t) := -i(I_N \otimes H(t) - H(t)^T \otimes I_N) + \sum_{k=0}^{Q-1} \sum_{l=1}^{2} \gamma_{lk} \left(\mathcal{L}_{lk} \otimes \mathcal{L}_{lk} - \frac{1}{2} \left(I_N \otimes \mathcal{L}_{lk}^T \mathcal{L}_{lk} + \mathcal{L}_{lk}^T \mathcal{L}_{lk} \otimes I_N \right) \right) \tag{46}$$

with $M(t) \in \mathbb{C}^{N^2 \times N^2}$, and $H(t) = H_d(t) + H_c(t)$ being the rotating frame system and control Hamiltonians as in (7) and (8), respectively.

When solving Schroedinger's equation (4), Quandary operates directly on the state $q(t) := \psi(t) \in \mathbb{C}^N$ and solves (45) with $M(T) := -iH(t)$.

4.1.1 Real-valued system and state storage

Quandary solves the (vectorized) equation (45) in real-valued variables with $q(t) = u(t) + iv(t)$, evolving the real-valued states $u(t), v(t) \in \mathbb{R}^M$ for $M = N$ (Schroedinger's eq.) or $M = N^2$ (Lindblad's eq.) with

$$\dot{q}(t) = M(t)q(t) \quad \Leftrightarrow \quad \begin{bmatrix} \dot{u}(t) \\ \dot{v}(t) \end{bmatrix} = \begin{bmatrix} A(t) & -B(t) \\ B(t) & A(t) \end{bmatrix} \begin{pmatrix} u(t) \\ v(t) \end{pmatrix} \tag{47}$$

for real and imaginary parts $A(t) = \mathrm{Re}\,(M(t))$ and $B(t) = \mathrm{Im}\,(M(t))$.

The real and imaginary parts of $q(t)$ are stored in a colocated manner: For $q = u + iv$ with $u, v \in \mathbb{R}^M$, a vector of size $2M$ is stored that staggers real and imaginary parts behind each other for each component:

$$q = u + iv = \begin{bmatrix} u^1 \\ u^2 \\ \vdots \\ u^M \end{bmatrix} + i \begin{bmatrix} v^1 \\ v^2 \\ \vdots \\ v^M \end{bmatrix} \quad \Rightarrow \quad q_{store} = \begin{bmatrix} u_1 \\ v_1 \\ u_2 \\ v_2 \\ \vdots \\ u_M \\ v_M \end{bmatrix}$$

4.2 Sparse-matrix vs. matrix-free solver

In Quandary, two versions to evaluate the right hand side of Lindblad's equation, $M(t)q(t)$, of the vectorized real-valued system are available:

1. The *sparse-matrix solver* uses PETSc's sparse matrix format (sparse AIJ) to set up (and store) the time-independent building blocks inside $A(t)$ and $B(t)$. Sparse matrix-vector products are then applied at each time-step to evaluate the products $A(t)u(t) - B(t)v(t)$ and $B(t)u(t) + A(t)v(t)$.

   For developers, the appendix provides details on each term within $A(t)$ and $B(t)$ which can be matched to the implementation in the code (class `MasterEq`).

2. The *matrix-free solver* considers the state density matrix $\rho \in C^{N \times N}$ to be a tensor of rank $2Q$ (one axis for each subsystems for each matrix dimension, hence $2 \cdot Q$ axes). Instead of storing the matrices within $M(t)$, the matrix-free solver applies tensor contractions to realize the action of $A(t)$ and $B(t)$ on the state vectors.

   In our current test cases, the matrix-free solver is much faster than the sparse-matrix solver (about 10x), no surprise. However the matrix-free solver is currently only implemented for systems consisting of **2, 3, 4, or 5** subsystems.

   Restrictions:

   - The matrix-free solver currently does not parallelize across the system dimension N, hence the state vector is **not** distributed (i.e. no parallel Petsc!). The reason why we did not implement that yet is that Q can often be large while each axis can be very shor (e.g. modelling $Q = 12$ qubits with $n_k = 2$ energy levels per qubit), which yields a very

high-dimensional tensor with very short axix. In that case, the standard (?) approach of parallelizing the tensor along its axes will likely lead to very poor scalability due to high communication overhead. We have not found a satisfying solution yet - if you have ideas, please reach out, we are happy to collaborate!

- TODO: The matrix-free solver is currently not available when solving Schroedingers equation.

4.3 Time-stepping

To solve the (vectorized) master equation (45), $\dot{q}(t) = M(t)q(t)$ for $t \in [0, T]$, Quandary applies a time-stepping integration scheme on a uniform time discretization grid $0 = t_0 < \ldots t_N = T$, with $t_n = n\delta t$ and $\delta t = \frac{T}{N}$, and approximates the solution at each discrete time step $q^n \approx q(t_n)$. It is a second-order accurate, symplectic Runge-Kutta scheme tableau $\dfrac{1/2 \ \vert \ 1/2}{\ \ \vert \ 1}$. Given a state q^n at time t_n, the update formula to compute q^{n+1} is hence

$$q^{n+1} = q^n + \delta t k_1 \quad \text{where } k_1 \text{ solves} \quad \left(I - \frac{\delta t}{2} M^{n+1/2} \right) k_1 = M^{n+1/2} q^n \tag{48}$$

where $M^{n+1/2} := M(t_n + \frac{\delta t}{2})$. In each time-step, we first solve a linear equation to get the stage variable k_1, then use it to update q^{n+1}.

While the implicit midpoint rule is the default (and preferred) setting in Quandary, there is the possibility to apply any time-stepping integrators provided by PETSc (class TS within PETSc). However, implementation needs to be verified, and adjoint time-stepping with Petsc is currently not available.

4.3.1 Choice of the time-step size

In order to choose a time-step size δt, an eigenvalue analysis of the constant drift Hamiltonian H_d is often useful. Since H_d is Hermitian, there exists a transformation Y such that $Y^\dagger H_d Y = \Lambda$ where $Y^\dagger = Y$ where Λ is a diagonal matrix containing the eigenvalues of H_d. Transform the state $\tilde{q} = Y^\dagger q$, then the ODE transforms to

$$\dot{\tilde{q}} = -i\Lambda\tilde{q} \quad \Rightarrow \dot{\tilde{q}}_i = -i\lambda_i\tilde{q}_i \quad \Rightarrow \tilde{q}_i = a\exp(-i\lambda_i t)$$

Therefore, the period for each mode is $\tau_i = \frac{2\pi}{|\lambda_i|}$, hence the shortest period is $\tau_{min} = \frac{2\pi}{\max_i\{|\lambda_i|\}}$. If we want p discrete time points per period, then $p\delta t = \tau_{min}$, hence

$$\delta t = \frac{\tau_{min}}{p} = \frac{2\pi}{p\max_i\{|\lambda_i|\}} \tag{49}$$

Usually, for a first order scheme we would use something like $p = 20$, second order may use $p = 10$. The above estimate provides a first idea on how big (small) the time-step size should be, and the user is advised to consider this estimate himself when running a test case. However, the estimate ignores contributions from the control Hamiltonian, where larger control amplitudes will require smaller and smaller time-steps in order to resolve (a) the time-varying controls themselves and (b) the dynamics induced by large control contributions. A standard Δt test should be performed

to varify if the time-step is small enough (testing for second order convergence of the error when reducing Δt).

If one wants to include the time-varying Hamiltonian part $H = H_d + H_c(t)$ in the analysis, one could use the constraints on the control parameter amplitudes to remove the time-dependency using their large value instead.

4.4 Gradient computation via discrete adjoint backpropagation

Quandary computes the gradients of the objective function with respect to the design variables α using the discrete adjoint method. The discrete adjoint approach yields exact and consistent gradients on the algorithmic level, at costs that are independent of the number of design variables. To that end, the adjoint approach propagates local sensitivities backwards through the time-domain while concatenating contributions to the gradient using the chain-rule.

The consistent discrete adjoint time-integration step for adjoint variables denoted by $\bar{q}^n$ is given by

$$\bar{q}^n = \bar{q}^{n+1} + \delta t \left(M^{n+1/2} \right)^T \bar{k}_1 \quad \text{where } \bar{k}_1 \text{ solves} \quad \left(I - \frac{\delta t}{2} M^{n+1/2} \right)^T \bar{k}_1 = \bar{q}^{n+1} \tag{50}$$

The contribution to the gradient ∇J for each time step is

$$\nabla J + = \delta t \left(\frac{\partial M^{n+1/2}}{\partial z} \left(q^n + \frac{\delta t}{2} k_1 \right) \right)^T \bar{k}_1 \tag{51}$$

Each evaluation of the gradient ∇J involes a forward solve of n_{init} initial quantum states to evaluate the objective function at final time T, as well as n_{init} backward solves to compute the adjoint states and the contributions to the gradient. Note that the gradient computation (51) requires the states and adjoint states at each time step, therefore the states q^n are stored during forward propagation.

4.5 Optimization algorithm

Quandary utilized Petsc's `Tao` optimization package to apply gradient-based iterative updates to the control variables. The `Tao` optimization interface takes routines to evaluate the objective function as well as the gradient computation. In the current setting in Quandary, `Tao` applies a nonlinear Quasi-Newton optimization scheme using a preconditioned gradient based on L-BFGS updates to approximate the Hessian of the objective function. A projected line-search is applied to ensure that the objective function yields sufficient decrease per optimization iteration while keeping the control parameters within the prescribed box-constraints.

4.6 Parallelization

Quandary offers three levels of parallelization using MPI.

1. Parallelization over initial conditions: The n_{init} initial conditions $\rho_i(0)$ can be distributed over `np_init` compute units. Since initial condition are propagated through the time-domain for solving Lindblad's or Schroedinger's equation independently from each other, speedup from distributed initial conditions is ideal.

2. Parallel linear algebra with Petsc (sparse-matrix solver only): For the sparse-matrix solver, Quandary utilizes Petsc's parallel sparse matrix and vector storage to distribute the state vector onto `np_petsc` compute units (spatial parallelization). To perform scaling results, make sure to disable code output (or reduce the output frequency to print only the last time-step), because writing the data files invokes additional MPI calls to gather data on the master node.

3. Time-parallelization via XBraid (experts only): working implementation, but speedup depends on the test case and XBraid setting (experts only), configuration option is `np_braid`

Strong scaling studies are presented in [3].

In the main code, the global communicator (MPI_COMM_WORLD) is split into three sub-communicator, one for each of the above. The total number of executing MPI processes (np_{total}) is split into three subgroups in such a way that

$$np_{braid} * np_{init} * np_{petsc} = np_{total}.$$

The user specifies the size of the communicator for distributing the initial conditions (np_{init}) as well as time-parallelization (np_{braid}) in the configuration file. The number of cores for parallel linear algebra (np_{petsc}) is then computed from the above equation. The following requirements for parallel distribution must be considered when setting up parallel runs:

- $\frac{n_{init}}{np_{init}} \in \mathbb{N}$, where n_{init} is the number of initial conditions that are considered. This requirement ensures that each processor group owns the same number of initial conditions.

- $\frac{np_{total}}{np_{init}*np_{braid}} \in \mathbb{N}$, so that each processor group has the same number of cores for Petsc.

- $\frac{M}{np_{petsc}} \in \mathbb{N}$, for $M = N^2$ in the Lindblad case and $M = N$ in the Schroedinger case. Hence the system dimension must be an integer multiple of the number of cores used for distributed linear algebra from Petsc. This constraint is a little annoying, however the current implementation requires this due to the colocated storage of the real and imaginary parts of the vectorized state.

4.7 Testing

- Quandary has a set of regression tests. Please take a look at the REGRESSIONTEST.md document in the `quandary/tests` directory for instruction on how to run the regression tests.

- In order to check if the gradient implementation is correct, one can choose to run a Central Finite Difference test. Let the overall objective function be denoted by $F(\boldsymbol{\alpha})$. The Central Finite Difference test compares each element of the gradient $\nabla F(\boldsymbol{\alpha})$ with the following (second-order accurate) estimate:

$$(\nabla F(\boldsymbol{\alpha}))_i \approx \frac{F(\boldsymbol{\alpha} + \epsilon \boldsymbol{e}_i) - F(\boldsymbol{\alpha} - \epsilon \boldsymbol{e}_i)}{2\epsilon} \qquad \text{(CFD)}$$

for unit vectors $\boldsymbol{e}_i \in \mathbb{R}^d$, and d being the dimension of $\boldsymbol{\alpha}$.

To enable the test, set the flag for the compiler directive `TEST_FD_GRAD` at the beginning of the `src/main.cpp` file. Quandary will then iterate over all elements in α and report the *relative* error of the implemented gradient with respect to the "true" gradient computed from CFD.

Acknowledgments

References

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A   Appendix: Details for the real-valued, vectorized Hamiltonian

To assemble (evaluate) $A(t) = Re(M(t))$ and $B(t) = Im(M(t))$, consider

$$iH = iH_d(t) + iH_c(t) \tag{52}$$

$$= i\left(\sum_k (\omega_k - \omega_k^{\text{rot}})a_k^\dagger a_k - \frac{\xi}{2}a_k^\dagger a_k^\dagger a_k a_k - \sum_{l>k}\xi_{kl}a_k^\dagger a_k a_l^\dagger a_l + \sum_{l>k}J_{kl}\cos(\eta_{kl}t)\left(a_k^\dagger a_l + a_k a_l^\dagger\right) \right. \tag{53}$$

$$\left. + \sum_k p^k(\vec{\alpha}^k, t)\left(a_k + a_k^\dagger\right) \right) \tag{54}$$

$$+ \left(\sum_k \sum_{kl} -J_{kl}\sin(\eta_{kl}t)\left(a_k^\dagger a_l - a_k a_l^\dagger\right) - \sum_k q^k(\vec{\alpha}^k, t)\left(a_k - a_k^\dagger\right) \right) \tag{55}$$

Hence $A(t)$ and $B(t)$ are given by

$$A(t) = A_d + \sum_k q^k(\vec{\alpha}^k, t) A_c^k + \sum_{l>k} J_{kl} \sin(\eta_{kl} t) A_d^{kl} \tag{56}$$

$$\text{with} \quad A_d := \sum_k \sum_{j=1,2} \gamma_{jk} \left(\mathcal{L}_{jk} \otimes \mathcal{L}_{jk} - \frac{1}{2} \left(I_N \otimes \mathcal{L}_{jk}^T \mathcal{L}_{jk} + \mathcal{L}_{jk}^T \mathcal{L}_{jk} \otimes I_N \right) \right) \tag{57}$$

$$A_c^k := I_N \otimes \left(a_k - a_k^\dagger \right) - \left(a_k - a_k^\dagger \right)^T \otimes I_N \tag{58}$$

$$A_d^{kl} := I_N \otimes \left(a_k^\dagger a_l - a_k a_l^\dagger \right) - \left(a_k^\dagger a_l - a_k a_l^\dagger \right)^T \otimes I_N \tag{59}$$

and

$$B(t) = B_d + \sum_k p^k(\vec{\alpha}^k, t) B_c^k + \sum_{kl} J_{kl} \cos(\eta_{kl} t) B_d^{kl} \tag{60}$$

$$\text{with} \quad B_d := \sum_k (\omega_k - \omega_k^{\text{rot}}) \left(-I_N \otimes a_k^\dagger a_k + (a_k^\dagger a_k)^T \otimes I_N \right) - \frac{\xi_k}{2} \left(-I_N \otimes a_k^\dagger a_k^\dagger a_k a_k + (a_k^\dagger a_k^\dagger a_k a_k)^T \otimes I_N \right) \tag{61}$$

$$- \sum_{l>k} \xi_{kl} \left(-I_N \otimes a_k^\dagger a_k a_l^\dagger a_l + (a_k^\dagger a_k a_l^\dagger a_l)^T \otimes I_N \right) \tag{62}$$

$$B_c^k := -I_N \otimes \left(a_k + a_k^\dagger \right) + \left(a_k + a_k^\dagger \right)^T \otimes I_N \tag{63}$$

$$B_d^{kl} := -I_N \otimes \left(a_k^\dagger a_l + a_k a_l^\dagger \right) + \left(a_k^\dagger a_l + a_k a_l^\dagger \right)^T \otimes I_N \tag{64}$$

$$\tag{65}$$

The sparse-matrix solver initializes and stores the constant matrices $A_d, A_d^{kl}, A_c^k, B_d, B_d^{kl}, B_c^k$ using Petsc's sparse-matrix format. They are used as building blocks to evaluate the blocks in the system matrix $M(t)$ with

$$A(t) = Re(M(t)) = A_d + \sum_k q^k(\alpha^k, t) A_c^k + \sum_{l>k} J_{kl} \sin(\eta_{kl} t) A_d^{kl} \tag{66}$$

$$B(t) = Im(M(t)) = B_d + \sum_k p^k(\alpha^k, t) B_c^k + \sum_{kl} J_{kl} \cos(\eta_{kl} t) B_d^{kl} \tag{67}$$

at each time t, which are applied to the vectorized, real-valued density matrix using Petsc's sparse MatVec implementation.

The matrix-free solver does not explicitly store the matrices A_d, B_d, A_c^k, B_c^k, etc., but instead only evaluates their action on a vector $q(t)$ using tensor contractions applied to the corresponding dimension of the density matrix tensor.