Transforming the Lindblad Equation into a System of Linear Equations: Performance Optimization and Parallelization

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Abstract: Rapidly growing performance and memory capacity of modern supercomputers open new perspectives for numerical studies of open quantum systems. These systems are in contact with their environments and their modeling is typically based on Markovian kinetic equations, describing the evolution of the system density operators. Additional to the exponential growth of the system dimension $N$ with the number of the system’s parts, the computational complexity scales quadratically with $N$, since we have to deal now with super-operators represented by $N^2 \times N^2$ matrices (instead of standard $N \times N$ matrices of operators). In this paper we consider the so-called Lindblad equation, a popular tool to model dynamics of open systems in quantum optics and superconducting quantum physics. Using the generalized Gell-Mann matrices as a basis, we transform the original Lindblad equation into a system of ordinary differential equations (ODEs) with real coefficients. Earlier, we proposed an implementation of this idea with the complexity of computations scaling as $O(N^5 \log(N))$ for dense systems and $O(N^3 \log(N))$ for sparse systems. However, infeasible memory costs remained an obstacle on the way to large models. Here we present a new parallel algorithm based on cluster manipulations with large amount of data needed to transform the original Lindblad equation into an ODE system. We demonstrate that the algorithm allows us to integrate sparse systems of dimension $N = 200$ and dense systems of dimension $N = 2000$ by using up to 25 nodes with 64 GB RAM per node. We also managed to perform large-scale supercomputer sampling to study the spectral properties of an ensemble of random Lindbladians for $N = 200$, which is impossible without the distribution of memory costs among cluster nodes.

Keywords: Open Quantum Systems; Lindblad Equation; Supercomputing; Parallel Computing; MPI; Performance Analysis; Performance Optimization

1. Introduction

Supercomputer simulations of open quantum systems [1,2] are becoming increasingly important both for theoretical studies and technological applications [3]. From the computational point of view, numerical evaluation of a coherent quantum system, isolated from its environment and described with a time-independent Hamiltonian, reduces to the problem of finding eigenvalues of a Hermitian matrix of size $N \times N$. In the case of an open system, i.e., a system interacting with its environment, we have to deal with superoperators represented by matrices of size $N^2 \times N^2$ [3]. Numerical simulations of such systems require large memory resources and computation time, which calls for development of new algorithms utilizing modern supercomputer technologies [1,4–6].
In this paper, we consider the so-called "Lindblad equation" [3], which describes the evolution of the density operator of an open system. This equation is used as a theoretical tool to model dynamics of open systems in quantum optics, quantum nanomechanics and several other fields [7]. Quantum systems subjected to periodic modulation of their parameters are of particular interest, since modulations can significantly modify the dynamics and broaden the spectrum of attainable states [8]. Standard integration methods can be used to study systems of relatively small size [9]. There are specialized methods developed for large-scale problems [1], but each of these methods has a restricted application area. For example, specialized methods, such as the matrix product operators method [1], apply only to multicomponent (many-body) systems of 1-d chain topology under an additional condition of strong spatial localization of quantum correlations. When solving by the Monte Carlo wave function method, it is necessary to perform sampling of a large number of trajectories, which is very computationally intensive problem [5]. Integrations using the expansion in systems of orthogonal Faber or Newton polynomials [10] are time-consuming, while the prospects for applying these methods to systems with hundreds and thousands of states remain unclear.

In this paper we utilize the approach which transforms the original Lindblad equation into a system of linear ordinary differential equations (ODE) with real coefficients. This approach employs the set of generalized Gell-Mann matrices as the expansion basis [11]. Numerical propagation of the obtained ODE system guarantees the preservation of the normalization and Hermiticity of the density matrix. Such a transformation also provides possibility to use highly efficient methods to solve large ODE systems. Earlier, we proposed an implementation of this method optimized in terms of the complexity of computations and the amount of memory used [12]. The corresponding algorithm consists of two main stages: data preparation (calculation of expansion coefficients, which form the ODE system) and numerical integration of the obtained system of ODEs. The complexity of the transformation is \(O(N^5 \log(N))\) for dense systems and \(O(N^3 \log(N))\) for sparse systems [12]. The sequential implementation of the algorithm posed another problem that is infeasible memory requirements to solve large-scale systems. Due to the complexity of the algorithms, the solution of the new problem is not straightforward. In this paper, we propose a parallel version of the algorithm that distributes memory costs across cluster nodes thus allowing for a significant increase the model size – up to \(N = 2000\) for sparse systems and up to \(N = 200\) for dense systems.

The paper is organized as follows. In Section 2 we introduce test-bed models and outline the algorithm. Section 3 presents the parallel implementation of the algorithm. Section 4 reports results of the numerical experiments. The results are summarized in Section 5.

2. Model and Method

Model a method are described in details in [12]; here we only introduce definitions, equations and formulas necessary for the parallel algorithm description.

Evolution of an open quantum system is modeled by the Markovian master equation in the Gorini-Kossakowski-Sudarshan-Lindblad (GKSL) form [13–15]:

\[
\frac{d\rho}{dt} = -i[H, \rho] + \frac{1}{2} \sum_{p=1}^{P} \gamma_p ([L_p \rho, L_p^\dagger] + [L_p^\dagger \rho, L_p]),
\]

(1)

where \(\rho \in \mathbb{C}^{N \times N}\) is a system’s density operator, \(H(t) \in \mathbb{C}^{N \times N}\) – a time-dependent Hamiltonian, \(\{L_p \in \mathbb{C}^{N \times N}, p = 1, \ldots, P\}\) – set of quantum dissipative operators with coefficients \(\gamma_p \in \mathbb{R}^+\). Any matrix \(L\) can be decomposed as \(L = L_1 + iL_2\), where \(L_1, L_2\) are Hermitian matrices. Therefore, we can consider only the case when all \(L_p\) in (1) are Hermitian matrices. To simplify the notation, we assume that \(P = 1\) (a single dissipative operator).
Consider the following set of \( M = N^2 - 1 \) Hermitian matrices \( \{F_i\} = \{S^{(j,k)}, J^{(j,k)}, D^l\} \):

- \( (N \ast (N - 1)) / 2 \) symmetric \( S^{(j,k)} = \frac{1}{\sqrt{2}}(e_j e_k^T + e_k e_j^T) \), \( 1 \leq j < k \leq N \);
- \( (N \ast (N - 1)) / 2 \) antisymmetric \( J^{(j,k)} = \frac{1}{\sqrt{2}}(e_j e_k^T - e_k e_j^T) \), \( 1 \leq j < k \leq N \);
- \( N - 1 \) diagonal \( D^l = \frac{i}{\sqrt{t(l+1)}}(\sum_{k=1}^l (e_k e_k^T - e_{l+1} e_{l+1}^T)) \), \( 1 \leq l \leq N - 1 \).

Any Hermitian matrix can be expanded with real coefficients over the basis \( \{F_i\} \) complemented with the identity matrix \( E \):

\[
A = a_0 E + \sum_{j=1}^{M} a_j F_j, a_0 = \frac{\text{Tr}(A)}{N}, a_j = \text{Tr}(F_j A), a_j \in R,
\]

Without loss of generality we can assume \( H \) and \( L \) to be traceless. Expansion of the density operator \( \rho(t) = \frac{E}{N} + \sum_{i=1}^{M} \psi_i(t) F_i \) contains the “Bloch vector” [16,17]: \( \vec{v} = (v_1, ..., v_M) \) which consists of real-valued elements. After all expansions equation (1) transforms into (3) which can be rewritten as a system of real-valued linear differential equations (4).

\[
\sum_{i=1}^{M} \frac{dv_i}{dt} F_i = -i \sum_{i,j} h_{ij} \psi_i [F_j, F_i] + \gamma / 2 \sum_{i,j,k} l_{ijk} \psi_i ([F_j, F_i^+ F_k^+]) \tag{3}
\]

\[
\frac{dv(t)}{dt} = (Q(t) + R)v(t) + K, \tag{4}
\]

where the matrices \( Q(t) \), \( R \) and the vector \( K \) are calculated by formulas (5)–(9).

\[
f_{mn} = -i \text{Tr}(F_s [F_m, F_n]), d_{mn} = \text{Tr}(F_s F_m F_n), m,n,s = 1, \ldots, M \tag{5}
\]

\[
z_{mn} = f_{mn} + i d_{mn}, m,n,s = 1, \ldots, M \tag{6}
\]

\[
q_{sn} = \sum_{m=1}^{M} h_{mn} f_{mn}, s,n = 1, \ldots, M \tag{7}
\]

\[
k_s = \frac{i}{N} \sum_{m,n=1}^{M} l_{mn} f_{mn}, s = 1, \ldots, M \tag{8}
\]

\[
r_{sn} = \frac{-\gamma}{2} \sum_{j,k,l=1}^{M} l_{jlk}(z_{jlin} f_{ks} + \overline{z_{jlin}} f_{sli}), s,n = 1, \ldots, M \tag{9}
\]

The solution vector \( \vec{v}(t) \) of system (4) is easily converted to the density operator \( \rho(t) \) of the original system (1).

We consider two test-bed models. The first model describes \( N - 1 \) indistinguishable interacting bosons, which are hopping between the sites of a periodically modulated dimer. The model is described with a time-periodic Hamiltonian

\[
H(t) = -J(b_1^\dagger b_2 + b_1 b_2^\dagger) + \frac{2U}{N-1} \sum_{j=1}^{2} n_j (n_j - 1) + \epsilon(t)(n_2 - n_1), \tag{10}
\]

where \( b_j \) and \( b_j^\dagger \) are the annihilation and creation operators of an atom at site \( j \), while \( n_j = b_j^\dagger b_j \) is the operator of number of particle on \( j \)-th site, \( J \) is the tunneling amplitude, \( \frac{2U}{N-1} \) is the interaction strength
(normalized by a number of bosons), and $\varepsilon(t)$ represents the modulation of the local potential. $\varepsilon(t)$ is chosen as $\varepsilon(t) = \varepsilon(t + T) = E + A\Theta(t)$, where $E$ is the stationary energy offset between the sites and $A$ is the dynamic offset.

The dissipation is represented by a "sparse" dissipative operator

$$L = \frac{\gamma}{N-1}(b_1^* + b_2^*)(b_2 + b_1).$$

(11)

This dissipative coupling tries to "synchronize" the dynamics on the sites by constantly recycling antisymmetric out-phase mode into symmetric in-phase one. Numerical experiments were performed with the following parameter values: $J = -1.0$, $U = 2.2$, $E = -1.0$, $A = -1.5$, $\Theta(t) = \text{sgn}(t - \pi)$, $T = 2\pi$, $\gamma = 0.1$, $N = 100, \ldots, 2000$.

From the "matrix" point of view, both operators, Hamiltonian and dissipator, are represented by sparse matrices. Therefore, we call this model "sparse".

The second model is described with a time-independent Hamiltonian $H$ as a member of the Gaussian orthogonal ensemble and dissipative operator $L$ which is a member of the Ginibre ensemble [18]. Another words, $L$ it is a complex $N \times N$ matrix with entries being complex random variables distributed according to normal law, of zero mean and variance equals one. We term this model as "dense".

3. Parallel Algorithm

In our recent paper [12], we presented a detailed description of the sparse and dense data structures and sequential algorithm for performing the expansion described in Section 2 and the subsequent propagation. We also provided estimates of time complexity and required memory. Below we briefly overview the algorithm and describe its parallel modification.

1. Initialization (sequential; performed on every node of a cluster). At the first step we load initial data from configuration files, allocate and initialize necessary data structures and perform some precomputing. It takes $O(N^2)$ time and $O(N^2)$ memory only and, therefore, can be done sequentially on every computational node.

2. Data Preparation (parallelized via MPI). The second step (fig. 1) implements the key idea of our approach. During this step only values needed for the ODE solution are calculated. This improves the software performance in several orders of magnitude compared to a naive implementation [12]. This step requires $O(N^5\log(N))$ operations and $O(N^4)$ memory for dense matrices $H$ and $L$, and $O(N^3\log(N))$ operations and $O(N^3)$ memory for sparse matrices. Unfortunately, this approach leads to infeasible memory requirements in a sequential mode when exploring models of large dimension. Thus, on a single node with 64 GB RAM we can study models with dense matrices of size up to $N = 150$ and sparse matrices $H$ and $L$ of size $N = 1000$. Below we show how to overcome this problem by using the new parallel data preparation algorithm which distributes data and operations over cluster nodes.

2.1. Compute the expansion coefficients $h_j, l_j$ for matrices $H$ and $L$. Each element of the vectors $h_j$ and $l_j$ corresponds to the product of one of the matrix $\{F_i\}$ and the matrix $H$ and $L$, respectively. Based on specific sparsity structure of the matrices $\{F_i\}$, the coefficients can be computed in one pass over nonzero elements of the $H$ and $L$ matrices. This step is performed on each MPI-process.

2.2. Compute the coefficients $f_{mnss}, d_{mnss}, z_{mnss}$ by formulas (5)-(6). Due to the sparsity structure of the matrices $\{F_i\}$, most of the coefficients $f_{mnss}, d_{mnss}, z_{mnss}$ are equal to zero. In this algorithm, nonzero coefficients of the tensors are calculated directly at the moment when they are required in the calculations (steps 2.3-2.5 of the algorithm). All three tensors are not simultaneously stored in memory.
\[
H(t) = -f(b_1^2 + b_1 b_2) + \frac{2U}{(N-1)} \sum_{j=1}^{N} n_j (n_j - 1) + \varepsilon(t) (n_2 - n_1)
\]
\[
L = \frac{N}{N-1} (b_1 + b_2) (b_2 + b_3)
\]

2.3. **Compute the coefficients** \( q_{sm} \) **by formula** (7). During this and two further steps, distribution of operations with the tensor \( F \) between MPI processes by the index \( s \) is performed. Each process calculates a set of nonzero terms \( h_n \times f_{mns} \) and the corresponding panel of the matrix \( Q \). Then all the panels are collected into resulting matrix by the master process. Note that a uniform distribution of ranges of index values \( s \) between processes can lead to a large imbalance in a number of operations and memory.
requirements. To overcome this problem we employ a two-stage load balancing scheme. First, we compute the number of non-zero entries in the rows of resulting matrix. Then, we distribute rows between cluster nodes providing approximately the same number of elements at every node.

2.4. **Compute the coefficients** $k_s$ **by formula** (8). Calculation of the vector $K$ uses the same balanced distribution of operations with tensor $F$ between MPI processes. Each process computes non-zero terms $l_n \times f_{nm}$ and calculates a block of vector $K$. All processes send results to the master process, which assembles them into a single vector.

2.5. **Compute the coefficients** $r_{mn}$ **by formula** (9). This step calculates the matrix $R$ using the distribution of operations on the tensor $Z$ between MPI processes. Each process calculates groups of columns of the matrix $R$. To do this, it computes only nonzero terms $l_m \times f_{nm}$, $l_m \times z_{nm}$ and fills corresponding group of columns of $R$. Upon completion, all processes transfer data to the master process. This stage is the most expensive in terms of memory, therefore we implemented a multistage procedure.

This procedure slightly slows down the calculation, but reduces maximum memory consumption. Thus, the tensor $f_{nm}$ can be computed in several stages by filtering on the third coordinate. Using this fact, each process calculates its portion of the columns of the matrix $R$ gradually, block by block. As a result, a process computes its portion of the data, reducing memory consumption when storing its part of the tensor $f_{nm}$. 

2.6. **Compute the initial value** $v(0)$. This step takes $O(N^2)$ time and $O(N^2)$ memory and can be done on every computational node.

3. **ODE integration (parallelized via MPI + OpenMP + SIMD)**. During this step we integrate the linear real-valued ODE system (4) over time. While the Data Preparation step is very memory consuming, this step is time consuming. Scalable parallelization of this step is a challenging problem because of multiple data dependencies. Fortunately, it does not take huge amount of memory and therefore can be run on smaller number of computational nodes than the Data Preparation step. If the matrices $Q$ and $R$ are sparse, we employ the graph partitioning library ParMetis to minimize further MPI communications. Then we employ the forth-order Runge-Kutta method, one step of which takes $O(N^4)$ time for dense matrices $H$ and $L$ and $O(N^3)$ time for sparse matrices. The method requires $O(N^2)$ additional memory for storing intermediate results. Computations are parallelized via MPI on $K$ cluster nodes as follows. Matrices $Q$ and $R$ are split to $K$ groups of rows (panels) so that each portion of data stores approximately equal number of non-zero values. Then, each MPI process performs steps of the Runge-Kutta method for corresponding panels. The most computationally intensive linear algebra operations are performed by high-performance parallel vectorized BLAS routines from Intel MKL utilizing all computational cores and vector units.

4. **Numerical Results**

Numerical experiments were performed on the supercomputers Lobachevsky (University of Nizhni Novgorod), Lomonosov (Moscow State University) and MVS-10P (Joint Supercomputer Center of RAS). The performance results are collected on the following cluster nodes: 2 × Intel Xeon E5 2660 (8 cores, 2.2 GHz), 64 GB of RAM. The code was built using the Intel Parallel Studio XE 17 software package.

The correctness of the results was verified by comparison with the results of simulations presented in the paper [12]. Later in this section we examine the time and memory costs when integrating sparse and dense models. Note that Data preparation and ODE integration using the Runge-Kutta method are completely separable steps. Therefore, when analyzing performance we consider them as independent programs that transfer information by saving ODE coefficients to a file.

**The Data Preparation step.** First, we consider the Data Preparation step and examine how increasing the dimension of the problem and the number of cluster nodes affect memory consumption. For the sparse model, we empirically found that it is advisable to perform 20 filtering stages when calculating the matrix
Peak memory consumption when solving problems of size from $N = 100$ to $N = 2000$ is shown in fig. 2. Experiments show that when solving model of large dimension ($N = 1600$) the memory requirements per node are reduced from 54.5 GB using 5 nodes to 16.5 GB using 25 nodes (scaling efficiency is 66.5%). Additionally, we were able to perform calculations for $N = 2000$, which required 31 GB of memory at each of 25 nodes of the cluster. Computation time is significant but not critical for the Data Preparation step for the sparse problem. Nevertheless, we note that when using 5 cluster nodes computation time is reduced approximately by half compared to a single node and then decreases slightly.

Figure 2. Memory consumption per one node of the Data Preparation step for the sparse model.

For the dense model, we managed to meet memory requirements on five nodes of the cluster upon transformation to the new basis of the problem of size $N = 200$. On fig. 3, left we show how memory costs per node are reduced by increasing the number of nodes from 1 to 25. Note, unlike the case of the sparse model, the time spent on data preparation decreases almost linearly (fig. 3, right), which is an additional advantage of the algorithm.

Figure 3. Memory consumption per one node (left) and Computation time (right) of the Data Preparation step for the dense model.
The ODE Integration step. Next, we consider the ODE Integration step. In contrast to the Data Preparation step, where we concentrated on satisfying memory constraints, parallelization of this step is performed in order to reduce the computation time. Below we show the dependence of computation time and the number of cluster nodes used for the sparse (fig. 4, left) and dense (fig. 4, right) models. First, we load previously prepared data and run the ODE integration step for the sparse model of size \( N = 1600 \). The results show that it is enough to use only four nodes of the cluster. Further increase in the number of nodes does not reduce computation time due to MPI communications. When solving other sparse large-scale models, similar behavior is observed. Secondly, we load precomputed data and run the ODE integration step for the dense model of size \( N = 150 \). We found that an increase in the number of cluster nodes used rather quickly leads to an increase in the communications time, so it is enough to use 2 nodes to solve a dense problem of the considered size.

![Figure 4](image.png)

Figure 4. Computation time of the ODE integration step for the sparse (left) and dense (right) models. Numerical integration was performed for one period of modulation \( T \), 20000 steps per period were used.

5. Conclusion

We presented a parallel version of the algorithm to investigate open quantum systems by first transforming them into a new basis and then integrating the obtained real-valued ODE system forward in time. The parallelization is implemented for two key steps that are data preparation for the transformation of the original equation into the ODE system and integration of the obtained ODE system using the fourth-order Runge-Kutta scheme. The main purpose of the first step parallelization is to reduce memory consumption on the supercomputer nodes. We demonstrated that the achieved efficiency is enough to double the size of the sparse model compared to the sequential algorithm. In the case of dense model, the run time of the data preparation step decreases linearly with increase of the number of cluster nodes. Parallelization of the ODE integration step allows us to reduce the computation time for both the sparse and dense models. Our cluster implementation allows us to investigate sparse models of dimension \( N = 2000 \) and dense models of dimension \( N = 200 \) on a cluster of 25 nodes with 64 GB RAM on each.

The developed parallel version of the code allowed us to start studying the properties of spectral statistics of "quantum attractors" i.e. asymptotic density matrices, which are fixed points of the ensemble of random Linbladians. Statistical sampling over an ensemble of random Lindbladians is an embarrassingly parallel problem. However, the calculation of each sample in the case of dense models of dimension \( N \) requires huge, often infeasible memory costs, which requires the efficient distribution of these costs among cluster nodes. We overcame this problem with a two-level parallelization scheme. At the first level, we use trivial parallelization, in which each sample is calculated by a small group of nodes. At the second level,
every group of nodes uses all available computing cores and memory to work with one sample. Although
the speedup at the second level is not ideal, parallelization solves the main problem, allowing us to fit into
the limitations on memory size. The proposed parallel algorithm opens up new perspectives in the study
of large-scale quantum systems.

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