Fast Matrix Methods for Quantum Control Algorithms

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Introduction

Fast and parallelized matrix methods have been developed and exploited for addressing the challenge of calculating quantum dynamics. As an interface to far-reaching applications, quantum control theory is a powerful framework for devising algorithms to steer quantum devices with optimal figures of merit. Controlling quantum systems experimentally is central to many branches of quantum technology including nanotechnology, quantum information processing and spectroscopy. However, to find such steerings is a (classically!) computationally demanding task, as the matrix dimensions and resource requirements grow exponentially with the size of the quantum system.

From a numerical linear algebra point of view, quantum control algorithms make heavy use of both matrix exponential calculations and computation of sequences of matrix products. Hence, the main task within the project was the improvement of these numerical tasks by massive parallelization.

Results

The project has achieved progress allowing to use high-end parallel clusters: this includes tailored preconditioning and parallelisation of matrix multiplication, matrix exponentials by Chebyshev series --- all these using matrix symmetries of the quantum system Hamiltonians. Thus a fully parallelised C++ version of the quantum control algorithm GRAPE was used [1], where 128 CPU nodes of the HLRB-II cluster brought a speed-up by more than a factor of 500 as compared to the runtime on a single node.

The main concept to parallelize the GRAPE-code was to distribute the M control matrices uniformly to all available processors, to compute the individual matrix exponentials sequentially on the responsible processors and to find an appropriate parallelization scheme for the forward and backward propagation, i.e. the computation of all M interior matrix-matrix products.

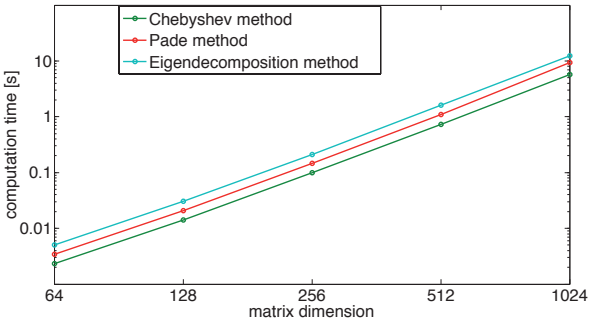

Figure 1: Runtime for the computation of one matrix exponential for different matrix sizes.

Matrix exponentials: In the first stage of the code, the matrix exponentials were calculated via the eigendecomposition of the Hamiltonians. We could improve this task by using Chebyshev-series methods, which allow to exploit the sparsity structure of the control Hamiltonians [1,2]. Figure 1 depicts the benefit of using the polynomial Chebyshev approach.

Prefix problem: Previously, the parallelization for the prefix problem was based on a coarse-grain tree-like approach. Using a 3D fine-grain approach where the individual matrix multiplications are parallelized, could help to obtain another speed-up by factor of 2-3 [2,3] as well as better scalability on the parallel cluster, see Figure 2.

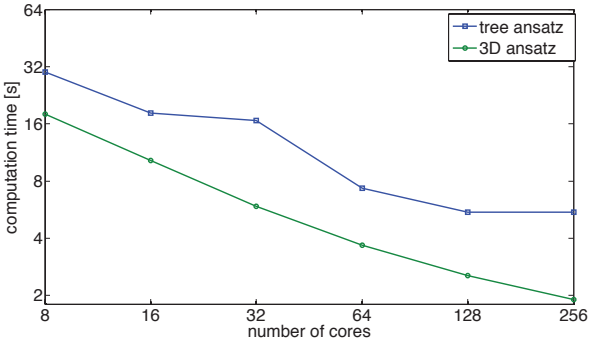

Figure 2: Comparison of runtimes for the matrix-multiplication prefix problem, executed on different numbers of available cores.

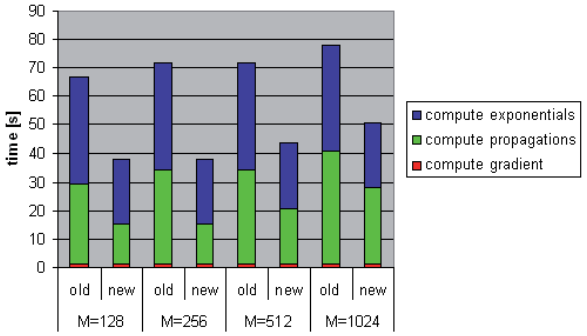

Figure 3: Runtime for one iteration of the GRAPE algorithm. Comparison of the old version and the current version for different problem instances in a 10-qubit system.

The presented enhancements in the computation of both matrix exponentials and matrix-multiplication prefix problem lead to an acceleration of the runtime for one iteration in the entire GRAPE algorithm. Fig. 3 provides a comparison of the runtimes of one GRAPE iteration required by the previous and the current version. Although the number of processers has been chosen to be M/2, which is the optimal choice for the tree-like approach, we obtain an acceleration of factor 2. For any other number of available processors we would expect even better runtime results.

More recently, we have expanded the original quantum control algorithm GRAPE [4] by incorporating more efficient second-order methods (BFGS) as well as by allowing for hybrid combinations between concurrent and sequential update of the control amplitudes [5]. In order to address the typical standard problems of numerical quantum control, the GRAPE algorithm has also been made available as a broadly applicable (fully modular) MATLAB package under the name DYNAMO [5].

However, matrix numerical methods over the entire Hilbert state space of quantum systems soon reach a limit due to the exponential growth of the state space, e.g. for n two-level systems, the state space is 2^n-dimensional. Therefore, in quantum mechanics, a general most challenging problem arises: what is the exact smallest eigenvalue (i.e. ground-state energy) of a matrix (representing the Hamiltonian) which is so large in dimension that it cannot even be stored on a computer but is just given in parameter form?

To this end, physicists developed concepts like Matrix Product States (MPS) for linear one-dimensional topologies or Projected Entangled Pair States for two-dimensional problems. In [6] we have addressed these problems in a unified way to show how computations, such as tensor contractions, can be performed efficiently while being versatile with respect to the coupling topology. The computation of ground states and ground-state energies is usually based on a variational ansatz for the Rayleigh-quotient minimization in the relevant representation format. Hence, the calculation of inner products of two vectors given in some representation format such as MPS is one of the key subroutines in simulation programs. As shown in [6], the costs for one individual contraction have complexity $O(nD^5)$ for periodic boundary conditions (PBC) and complexity $O(nD^3)$ for open boundary conditions (OBC). Table 1 illustrates the computation time for one individual contraction of two 100-qubit MPS tensors of different ranks D (the so-called bond dimension).

	D=20	D=40	D=60	D=80	D=100
OBC	0.072	0.150	0.238	0.310	0.380
PBC	1.4	33.0	233.7	886.5	3142.6

Table 1: Runtime [in seconds] for the computation of one contraction in the simulation of a n=100-qubit system with open boundary conditions (OBC) and periodic boundary conditions (PBC).

On-Going Research / Outlook

Moreover, by exploiting matrix symmetries in typical quantum mechanical Hamiltonians, another factor of two in parameter space can be saved [7] when using our unified versatile tensor contraction modules [6], which shall be parallelized in a follow-up project. We anticipate that these modules will be most useful in two of the major challenges in current numerical quantum physics, (i) the calculation of ground-state energies of Hamiltonians with 2D coupling topologies and (ii) in quantum simulation, where the entire time evolution of many-body systems has to be calculated such that the bond dimension D is kept tractably low by tensor-contraction methods. The latter will be key for extending the calculation of quantum many-body dynamics to optimal control of large-scale systems, where typically thousands of trajectories have to be calculated, see [1,2,4,5].

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