

Simulating Hamiltonian dynamics in a programmable photonic quantum processor using linear combinations of unitary operations

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Simulating the dynamic evolutions of physical and molecular systems in a quantum computer is of fundamental interest in many applications^{1,2}. Its implementation requires efficient quantum simulation algorithms³⁻¹². The Lie-Trotter-Suzuki approximation algorithm, also well known as the Trotterization, is a basic algorithm in quantum dynamic simulation³⁻⁵. A multi-product algorithm that is a linear combination of multiple Trotterizations has been proposed to improve the approximation accuracy¹³. Implementing such multi-product Trotterization in quantum computers however remains experimentally challenging and its success probability is limited. Here, we modify the multi-product Trotterization and combine it with the oblivious amplitude amplification to simultaneously reach a high simulation precision and high success probability. We experimentally implement the modified multi-product algorithm in an integrated-photonics programmable quantum simulator in silicon, which allows the initialization, manipulation and measurement of four-qubit states and a sequence of linearly combined controlled-unitary gates, to emulate the dynamics of a coupled electron and nuclear spins system. Theoretical and experimental results are in good agreement, and they both show the modified multi-product algorithm can simulate Hamiltonian dynamics with a higher precision than conventional Trotterizations and a nearly deterministic success probability. We certify the multi-product algorithm in a small-scale quantum simulator based on linear combinations of operations, and this work promises the practical implementations of quantum dynamics simulations.

Efficiently simulating the quantum dynamics of physical and molecular systems represents an important near-term application of quantum computers^{1,2}. Several quantum algorithms have been proposed for simulating quantum Hamiltonian dynamics, e.g., Lie-Trotter-Suzuki approximations³⁻⁵ (known as Trotterizations), quantum random walks^{6,14,15}, multi-product formula¹³, truncated Taylor series^{7,8}, qubitization⁹ and quantum signal processing¹⁰. Among them, Trotterization is regarded as a basic algorithm in dynamics simulations. The Trotterization accuracy however appears to be orders of magnitude looser than its prediction error bounded by numerical simulations^{16,17}. Many algorithms have been proposed to improve the Trotterizations, e.g. product order randomization¹¹, time-dependent Hamiltonian simulation¹², and truncated Taylor series^{7,8}. The order of Lie-Trotter-Suzuki approximation determines the error of Trotterization. For example, the first-order formula requires a $O(t^2/\epsilon)$ -step Trotterization with an error of ϵ . Expectably, utilizing higher-order formula can result in a substantial improvement of precision at the expense of more quantum operations and higher circuit depth^{18,19}. Another efficient multi-product algorithm was proposed by Childs and Wiebe¹³, which can reach the same precision as the high-order Trotterization but with a lower circuit depth.

The quantum hardware for implementing the multi-product algorithm is a linear combinations of unitaries (LCU)¹³. Note the LCU enables a general form of quantum operations that can be used to implement Hamiltonian simulation^{7,13}, Harrow-Hassidim-Lloyd algorithm²⁰, passive quantum error correction²¹ and simulation of the Yang-Baxter equation²². The realization of LCU circuits in quantum devices requires the implementation of a sequence of multi-qubit controlled-unitary operations²³. Realizing such multi-qubit controlled-unitary operations, in which the unitary can be arbitrarily controllable, is generally a challenging task, though multi-qubit gates have been reported in different quantum systems, e.g. superconducting qubits²⁴, trapped ions²⁵ and photons²⁶. In photonic systems, controlled-unitary operations between qubits or qutrits have been demonstrated²⁷⁻³⁴. Silicon-photonics quantum technologies³⁵, that can integrate entangled-photon sources³⁶, programmable quantum circuits^{34,35}, and single-photon detectors³⁶, could provide a versatile platform for multi-qubit LCU-based Hamiltonian dynamics simulation.

Here, we propose and demonstrate a modified multi-product algorithm, assisted by the oblivious amplitude amplification (OAA). The modified multi-product algorithm allows a higher accuracy of dynamics simulation compared to conventional Trotterizations as well as the original multi-product¹³, and it also enables a nearly deterministic success probability. We experimentally implement our modified multi-product algorithm in a LCU quantum simulator on a programmable four-qubit quantum photonic chip. To benchmark the processing of the modified multi-product algorithm, we simulate a general Rabi-type Hamiltonian of a coupled nuclear spin and electron spin system. To the best of our knowledge, this work reports the first multi-qubit controlled-unitary gate in integrated photonics, and we reprogram the device to implement the first Hamiltonian dynamics simulation in LCU circuits.

Multi-product algorithms in LCU circuits

We first overview the original multi-product algorithm¹³, and then discuss how to improve it with an assistance of the OAA algorithm³. When considering the second-order Trotter approximation of a unitary operator of $\exp(-i \sum_{j=1}^n H_j t)$ given $\exp(-i H_j t)$, we have:

$$e^{-i \sum_{j=1}^n H_j t} = S_1^2(t/l) + E_2 t^3/l^2 + E_3 t^5/l^4 + \dots, \quad (1)$$

$$S_2(t) = \prod_{j=1}^n e^{-i H_j t/2} \prod_{k=n}^1 e^{-i H_k t/2}$$

where $S_1(t)$ is the second-order Trotter product, E_2 and E_3 are high-order error terms which are functions of H_j , t is the evolution time of the quantum system, and l is the number of iterations. Simply increasing the l , one can reduce the high-order errors but cannot get rid of them. The key idea of the multi-product algorithm is to properly combine multiple low-order Trotterizations linearly, so that the low-order error terms can be cancelled. For example, by properly choosing the coefficients of $c_a = \pi^2/(n^2 - m^2)$ and $c_m = m^2/(m^2 - n^2)$, and linearly combining two second-order Trotterizations with n and m iterations respectively, one can directly cancel the third-order error term E_3 and thus improve the approximation to the fifth-order error:

$$e^{-i \sum_{j=1}^n H_j t} = c_a S_1^n(t/n) + c_m S_1^m(t/m) - E_3 t^5/n^2 m^2 + O(t^7) \quad (2)$$

Simulating Hamiltonian Dynamics

Yijin Wang



Simulating Hamiltonian Dynamics:

Simulating Hamiltonian Dynamics Benedict Leimkuhler, Sebastian Reich, 2004 Geometric integrators are time stepping methods designed such that they exactly satisfy conservation laws symmetries or symplectic properties of a system of differential equations In this book the authors outline the principles of geometric integration and demonstrate how they can be applied to provide efficient numerical methods for simulating conservative models Beginning from basic principles and continuing with discussions regarding the advantageous properties of such schemes the book introduces methods for the N body problem systems with holonomic constraints and rigid bodies More advanced topics treated include high order and variable stepsize methods schemes for treating problems involving multiple time scales and applications to molecular dynamics and partial differential equations The emphasis is on providing a unified theoretical framework as well as a practical guide for users The inclusion of examples background material and exercises enhance the usefulness of the book for self instruction or as a text for a graduate course on the subject

Simulating Hamiltonian Dynamics B.

Leimkuhler, 2004 **Explorations in Computational Physics** Devang Patil, 2025-02-20 Explorations in Computational Physics delves into the intricate world of computational physics offering a comprehensive guide from fundamental theories to cutting edge applications This book serves as an indispensable companion for both novice learners and seasoned researchers We cover a diverse array of topics meticulously unfolding layers of computational techniques and their applications in various branches of physics From classical mechanics simulations elucidating celestial mechanics to quantum mechanics computations unraveling atomic and subatomic realms the book navigates through the vast landscape of computational methodologies with clarity and precision Furthermore we delve into electromagnetic field simulations statistical mechanics and thermodynamics equipping readers with tools to model complex physical phenomena with accuracy and efficiency High performance computing techniques data analysis and visualization methodologies are elucidated empowering readers to harness modern computational resources in their research With lucid explanations illustrative examples and insightful discussions on emerging technologies like quantum computing and artificial intelligence Explorations in Computational Physics fosters a deeper understanding of computational methodologies and their transformative impact on physics research

Numerical Simulations of a Smectic Lamellar Phase of Amphiphilic Molecules Claire Loison, 2005 *New Algorithms for Macromolecular Simulation* Benedict Leimkuhler, Christophe Chipot, Ron Elber, Aatto Laaksonen, Alan Mark, Tamar Schlick, Christoph Schütte, Robert Skeel, 2006-03-22 Molecular simulation is a widely used tool in biology chemistry physics and engineering This book contains a collection of articles by leading researchers who are developing new methods for molecular modelling and simulation Topics addressed here include multiscale formulations for biomolecular modelling such as quantum classical methods and advanced solvation techniques protein folding methods and schemes for sampling complex landscapes membrane simulations free energy calculation and techniques for improving ergodicity The

book is meant to be useful for practitioners in the simulation community and for those new to molecular simulation who require a broad introduction to the state of the art Handbook of Markov Chain Monte Carlo Steve Brooks, Andrew Gelman, Galin Jones, Xiao-Li Meng, 2011-05-10 Since their popularization in the 1990s Markov chain Monte Carlo MCMC methods have revolutionized statistical computing and have had an especially profound impact on the practice of Bayesian statistics Furthermore MCMC methods have enabled the development and use of intricate models in an astonishing array of disciplines as diverse as fisheries **Geometric Structures of Statistical Physics, Information Geometry, and Learning** Frédéric Barbaresco, Frank Nielsen, 2021-06-27 Machine learning and artificial intelligence increasingly use methodological tools rooted in statistical physics Conversely limitations and pitfalls encountered in AI question the very foundations of statistical physics This interplay between AI and statistical physics has been attested since the birth of AI and principles underpinning statistical physics can shed new light on the conceptual basis of AI During the last fifty years statistical physics has been investigated through new geometric structures allowing covariant formalization of the thermodynamics Inference methods in machine learning have begun to adapt these new geometric structures to process data in more abstract representation spaces This volume collects selected contributions on the interplay of statistical physics and artificial intelligence The aim is to provide a constructive dialogue around a common foundation to allow the establishment of new principles and laws governing these two disciplines in a unified manner The contributions were presented at the workshop on the Joint Structures and Common Foundation of Statistical Physics Information Geometry and Inference for Learning which was held in Les Houches in July 2020 The various theoretical approaches are discussed in the context of potential applications in cognitive systems machine learning signal processing **Fast Methods for Long-range Interactions in Complex Systems** Godehard Sutmann, Paul Gibbon, Thomas Lippert, 2011 **Understanding the Discrete Element Method** Hans-Georg Matuttis, Jian Chen, 2014-06-23 Gives readers a more thorough understanding of DEM and equips researchers for independent work and an ability to judge methods related to simulation of polygonal particles Introduces DEM from the fundamental concepts theoretical mechanics and solidstate physics with 2D and 3D simulation methods for polygonal particles Provides the fundamentals of coding discrete element method DEM requiring little advance knowledge of granular matter or numerical simulation Highlights the numerical tricks and pitfalls that are usually only realized after years of experience with relevant simple experiments as applications Presents a logical approach starting with the mechanical and physical bases followed by a description of the techniques and finally their applications Written by a key author presenting ideas on how to model the dynamics of angular particles using polygons and polyhedral Accompanying website includes MATLAB Programs providing the simulation code for two dimensional polygons Recommended for researchers and graduate students who deal with particle models in areas such as fluid dynamics multi body engineering finite element methods the geosciences and multi scale physics Differential-algebraic Systems:

Analytical Aspects And Circuit Applications Ricardo Riaza, 2008-05-29 Differential algebraic equations DAEs provide an essential tool for system modeling and analysis within different fields of applied sciences and engineering This book addresses modeling issues and analytical properties of DAEs together with some applications in electrical circuit theory Beginning with elementary aspects the author succeeds in providing a self contained and comprehensive presentation of several advanced topics in DAE theory such as the full characterization of linear time varying equations via projector methods or the geometric reduction of nonlinear systems Recent results on singularities are extensively discussed The book also addresses in detail differential algebraic models of electrical and electronic circuits including index characterizations and qualitative aspects of circuit dynamics In particular the reader will find a thorough discussion of the state semistate dichotomy in circuit modeling The state formulation problem which has attracted much attention in the engineering literature is cleverly tackled here as a reduction problem on semistate models

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