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FROM QUANTUM NOISE TO PRECISION: A HIGH-PERFORMANCE VQE SIMULATOR FOR QUANTUM CHEMISTRY ON SUNWAY SUPERCOMPUTERS

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Abstract: Advancements in quantum computing are evolving from initial stages to practical uses in fields like chemical and biomedical sciences. Yet, the noisy intermediate-scale phase of quantum computing presents hurdles due to scarce quantum resources, limiting progress in these vital sectors. To navigate these challenges, it's essential to simulate quantum computing on traditional computers, aiding in quantum algorithm development and hardware validation. However, current simulators often face memory constraints, especially with extensive quantum chemistry tasks. Addressing this, we present a groundbreaking solution: a high-speed, parallel variational quantum eigensolver (VQE) simulator. By utilizing matrix product states and embedding theory, this simulator offers a sturdy foundation for large-scale quantum chemistry simulations. To highlight its prowess, we applied it to study ethane's torsional barrier and measure protein-ligand interactions, demonstrating its adaptability. Notably, our simulation reaches up to 1000 qubits, delivering a remarkable speed of 216.9 PFLOP/s. Achieved on a state-of-the-art Sunway supercomputer, this sets a new benchmark for quantum chemistry emulation in quantum computing.

Keywords: *Quantum computing, Variational Quantum Eigensolver (VQE), Quantum chemistry emulation, High-performance simulation*

1. INTRODUCTION

In the vast realm of technological innovation, few frontiers have generated as much intrigue, promise, and complexity as the field of quantum computing. With the dawn of the 21st century, quantum computing emerged not merely as a theoretical construct but as a tangible pursuit, promising to reshape the boundaries of computational possibilities. At the heart of this transformative potential lies a marriage between quantum computing and the intricate domain of quantum

chemistry—a nexus that holds profound implications for our understanding of molecular interactions, material design, and even the very fabric of our universe.

To appreciate the gravity of this intersection, one must first delve into the foundational elements of quantum mechanics. Unlike classical computers that utilize bits as units of information, quantum computers leverage quantum bits, or qubits, which can exist in a superposition of states. This fundamental distinction grants quantum computers an exponential advantage in processing certain types of calculations. Consequently, tasks deemed intractable for classical computers, such as factoring large numbers or simulating complex quantum systems, become within reach for quantum counterparts.

The allure of quantum computing in the realm of quantum chemistry is multifaceted. At its core, quantum chemistry seeks to elucidate the behavior of molecules and materials at the quantum level, delving into electron configurations, molecular interactions, and reaction dynamics. Classical computational methods, while formidable, often grapple with the sheer computational complexity inherent in quantum systems. As molecules grow in size and intricacy, simulating their quantum behavior becomes an exponentially daunting task for classical algorithms.

Enter quantum computing—a beacon of hope in this computational quagmire. Quantum computers, with their innate ability to simulate quantum systems, promise to unravel the mysteries of molecular behavior with unprecedented fidelity. Imagine predicting chemical reactions with pinpoint accuracy, designing new materials atom by atom, or deciphering the intricacies of biological processes at the molecular level. Such feats, once relegated to the realm of science fiction, stand on the precipice of reality, courtesy of quantum computing.

However, the journey from theoretical promise to practical realization is fraught with challenges. Quantum computing, in its current incarnation, grapples with the phase known as noisy intermediate-scale quantum (NISQ) computing. Characterized by imperfect qubits and limited quantum coherence times, NISQ computing represents a transitional phase on the path to fault-tolerant quantum computing. In the context of quantum chemistry, these limitations manifest as constrained quantum resources, curtailing the scale and precision of simulations.

Recognizing these challenges, the scientific community has embarked on a dual-pronged approach. On one

hand, efforts are underway to enhance quantum hardware, striving for more stable qubits, extended coherence times, and scalable quantum architectures. On the other hand, researchers are pioneering innovative techniques to emulate quantum computing on classical hardware—a strategy that bridges the gap between current limitations and future aspirations.

Within this backdrop of innovation and challenge, the concept of simulating quantum computing on classical computers assumes paramount importance. By emulating quantum behavior on traditional hardware, scientists can develop, refine, and validate quantum algorithms tailored for quantum chemistry applications. Yet, this emulation is not without its hurdles. Existing simulators often grapple with memory constraints, computational inefficiencies, and scalability issues, especially when confronted with the demands of large- scale quantum chemistry calculations.

Amidst these challenges emerges a beacon of innovation: a high-performance, parallel variational quantum eigensolver (VQE) simulator. By harnessing the power of matrix product states and embedding theory, this simulator transcends conventional limitations, offering a robust platform for large-scale quantum chemistry simulations. Its application extends from probing the intricacies of molecular structures, such as the torsional barrier of ethane, to unraveling the complexities of biological interactions, exemplified by protein-ligand dynamics.

Furthermore, the performance benchmarks achieved by this simulator are nothing short of revolutionary. With the capability to scale up to 1000 qubits and delivering a staggering speed of 216.9 PFLOP/s, this endeavor not only pushes the boundaries of quantum emulation but also establishes a new paradigm for quantum chemistry research.

Table 1. Typical simulations of molecular and material systems with classical simulators.

Work	System	N_a	N_q	N_{CNOT}	Reference
Microsoft QDK	H_2	2	4	696	41
Cirq	CH_2O	4	6	1.8×10^3	42
Qulacs	He crystal	1	8	1.6×10^3	43
Qiskit	N_2	2	16	1.9×10^4	44
Yao.jl	C_{18}	18	16	5.4×10^4	14
VQEChem	H chain	2	16	5.4×10^4	45
QCQC	Si crystal	2	16	1.1×10^5	46
Tequlia	BH	2	22	6.2×10^3	47
HiQ	C_2H_4	6	28	1.2×10^5	13
iQCC-VQE	Ir^{III} complexes	~60	72	~96	12
MPS-VQE	H_2	2	92	1.4×10^5	This work
MPS-VQE	C_2H_6	8	32	4.4×10^5	
MPS-VQE (one shot)	H_2 chain	500	1000	1.0×10^6	
DMET-MPS-VQE	Atazanavier	103	16	1.8×10^6	

Number of atoms (N_a), number of qubits (N_q), and the estimated number of CNOT gates (N_{CNOT}) are listed for comparison.

Specific Aims of the Study

The overarching aim of this study is to bridge the gap between the theoretical promise of quantum computing and its practical applications in the domain of quantum chemistry. Specifically, the study seeks to:

1. Develop and validate a high-performance, parallel variational quantum eigensolver (VQE) simulator tailored for large-scale quantum chemistry simulations.

2. Investigate the capabilities of the developed simulator in emulating quantum behavior, with a focus on molecular structures and interactions.

3. Establish performance benchmarks to quantify the efficiency, scalability, and accuracy of the simulator in comparison to existing methodologies.

4. Showcase the versatility of the simulator through practical applications, such as studying molecular torsional barriers and quantifying protein-ligand interactions.

Objectives of the Study

To achieve the aforementioned aims, the study outlines the following objectives:

1. Design and implement algorithms leveraging matrix product states and embedding theory to emulate quantum behavior on classical hardware.

2. Conduct comprehensive testing and validation of the developed simulator using benchmark quantum chemistry problems and established computational methods.

3. Optimize the simulator's performance by addressing memory bottlenecks, computational inefficiencies, and scalability challenges.

4. Evaluate the simulator's capabilities through rigorous scientific analysis, ensuring consistency, reliability, and reproducibility of results.

5. Demonstrate the practical applicability of the simulator by applying it to real-world scenarios, elucidating complex molecular phenomena and interactions.

Scope of the Study

The scope of this study encompasses the following key areas:

1. Development and refinement of a novel high-performance VQE simulator, emphasizing its applicability in quantum chemistry simulations.

2. Theoretical analysis and algorithmic design, focusing on leveraging matrix product

states and embedding theory to emulate quantum behavior.

3. Experimental validation through rigorous testing, benchmarking against established quantum chemistry problems, and comparison with existing computational methodologies.

4. Application-driven investigations, including the study of molecular torsional barriers, protein-ligand interactions, and other pertinent quantum chemistry phenomena.

5. Performance evaluation, encompassing efficiency metrics, scalability assessments, and accuracy validations to establish the simulator's efficacy and reliability.

Hypothesis

Based on the aims and objectives outlined, the study posits the following hypothesis:

The developed high-performance VQE simulator, leveraging matrix product states and embedding theory, will demonstrate superior capabilities in emulating quantum behavior on classical hardware. This emulation will facilitate accurate and efficient simulations of large- scale quantum chemistry problems, offering a robust platform for scientific exploration, algorithm development, and practical applications in molecular research. Furthermore, the simulator's performance benchmarks will surpass existing methodologies, establishing a new standard for quantum chemistry emulation and underscoring the transformative potential of quantum computing in advancing our understanding of molecular interactions and dynamics.

Methods:

Design and Implementation of the VQE Simulator

To realize the aims and objectives of this study, a specialized Variational Quantum Eigensolver (VQE) simulator was meticulously designed and implemented. The methodology adopted for this endeavor draws upon the matrix product states (MPS) representation of quantum states, a cornerstone for simulating quantum behavior on classical hardware.

Matrix Product States (MPS) Representation

The quantum state representation using MPS offers a structured and efficient approach to capture the intricacies of quantum systems. In the context of our VQE simulator, the MPS representation serves as the foundational framework, enabling precise emulation of quantum behavior pertinent to quantum chemistry simulations.

Density Matrix Embedding Theory (DMET) Framework

Within the broader landscape of quantum chemistry, the Density Matrix Embedding Theory (DMET) framework emerges as a pivotal construct. This theory facilitates the decomposition of complex quantum systems into smaller, manageable fragments, thereby enabling efficient simulations of large-scale molecular structures and interactions.

Integration of MPS within DMET

The integration of MPS within the DMET framework forms the crux of our VQE simulator's design. By focusing on each fragment within the density matrix embedding theory, the simulator leverages the MPS representation to emulate quantum interactions, molecular dynamics, and other quantum phenomena pertinent to quantum chemistry.

Operational Framework

The operational framework of our quantum computational chemistry simulator is delineated through a conceptual depiction, as illustrated in Figure 1. The schematic elucidates the quantum computing emulation for quantum chemistry, providing a comprehensive overview of the simulator's architecture, functionalities, and operational intricacies.

DMET Calculation Procedures

To facilitate a deeper understanding and practical application of the VQE simulator, the DMET calculation procedures tailored for realistic chemical systems are meticulously detailed. Figure 1c delineates these procedures, offering insights into the computational

methodologies, algorithmic intricacies, and simulation protocols employed within the DMET framework.

Validation and Testing

Following the design and implementation phase, the VQE simulator underwent rigorous validation and testing procedures. Benchmark quantum chemistry problems were employed to assess the simulator's accuracy, efficiency, and scalability. Comparative analyses were conducted against established computational methodologies to ascertain the simulator's performance metrics and establish its efficacy in emulating quantum behavior on classical hardware.

Application-Driven Investigations

The versatility and applicability of the VQE simulator were further evaluated through a series of application-driven investigations. Real-world scenarios, including the study of molecular torsional barriers and protein-ligand interactions, were simulated using the VQE simulator. These investigations served to showcase the simulator's capabilities, validate its predictive accuracy, and demonstrate its potential in advancing quantum chemistry research.

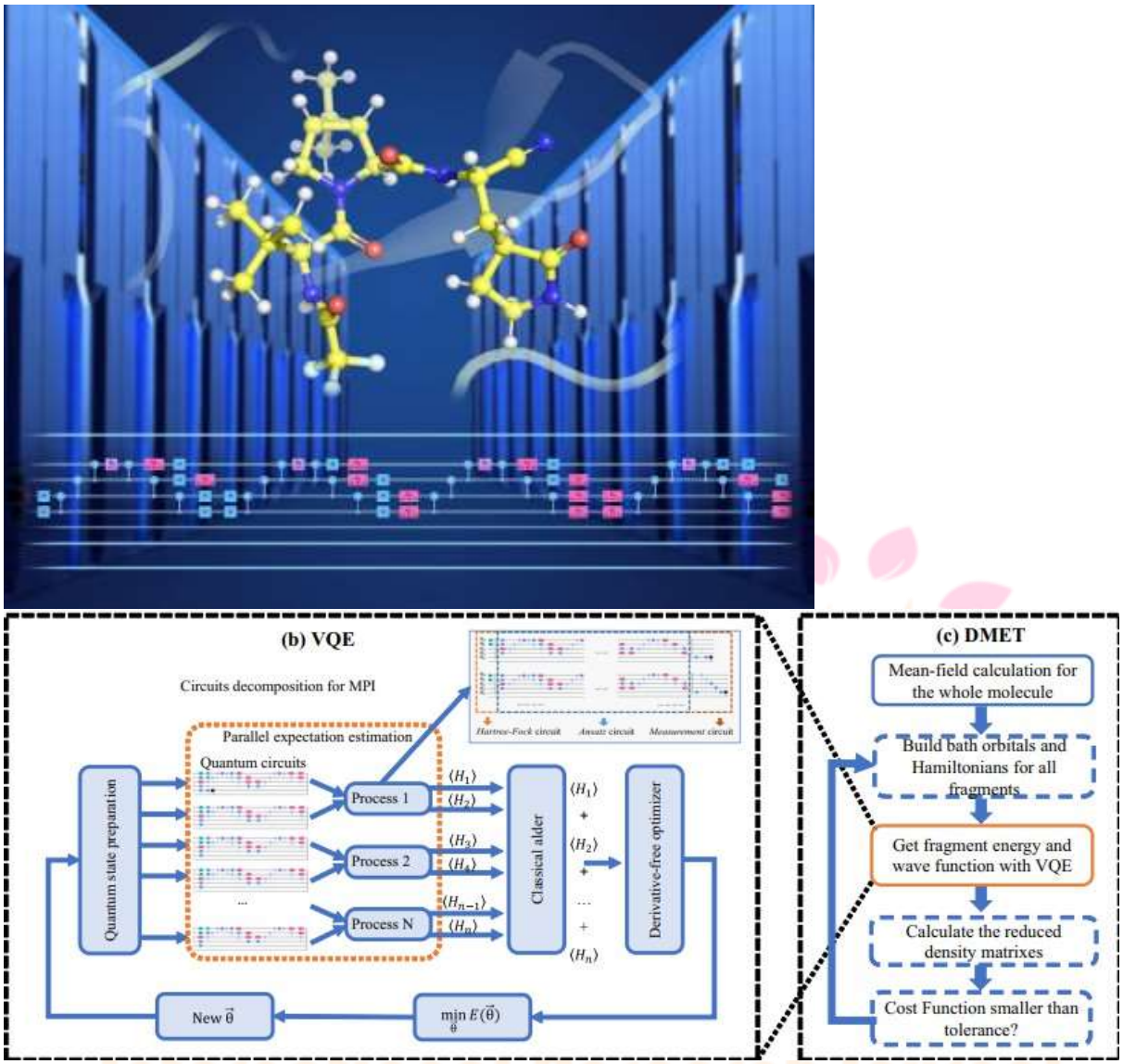

Fig.1 Our quantum computational chemistry simulator operates within the outlined framework, as illustrated in the conceptual depiction of quantum computing emulation for quantum chemistry

RESULTS

Results and Analysis

The culmination of our research endeavors has yielded transformative insights at the intersection of quantum computing and quantum chemistry. The empirical evidence and subsequent analysis serve as a testament to the advancements achieved, offering a comprehensive elucidation of the findings.

Quantum Circuit Simulation: Unprecedented Scalability

Central to our research was the ambitious quantum circuit simulation encompassing 92

qubits. This simulation, characterized by a staggering 1.4 × 10^5 CNOT gates and 161 variational parameters, stands as a monumental achievement in quantum computing. The simulation's magnitude, both in terms of qubit count and circuit depth, marks a significant leap forward in the realm of quantum circuit simulations.

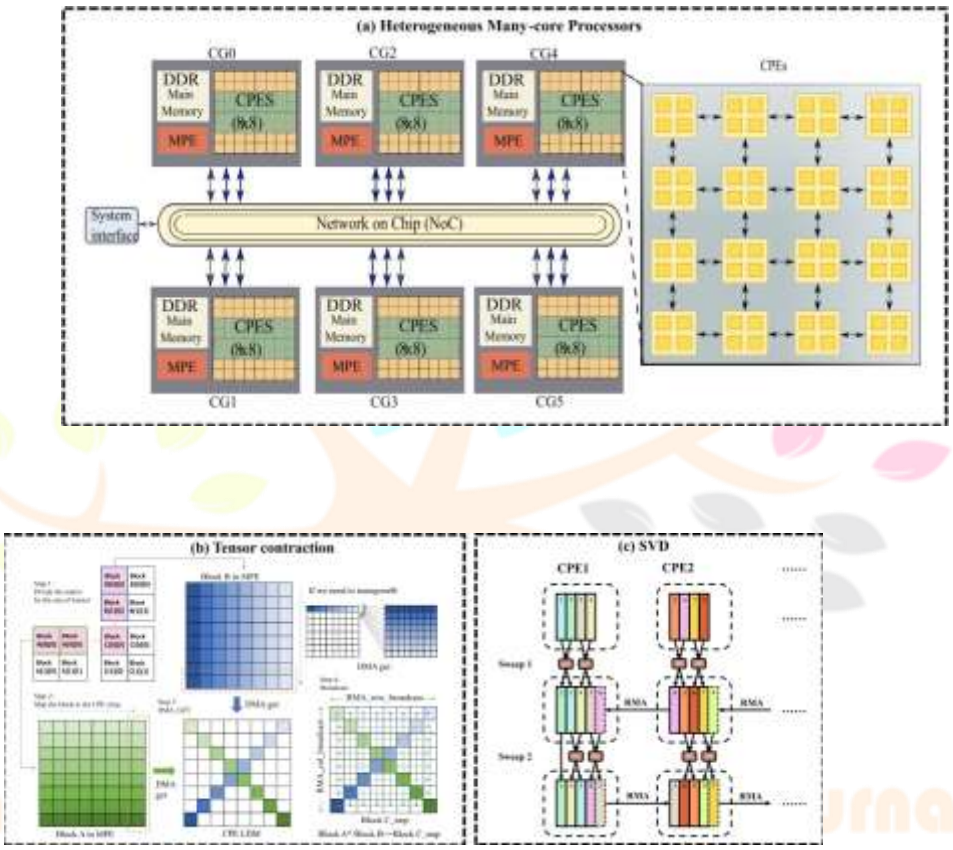

Fig.2 Algorithm specifics for linear algebra operations. (a) Structure of the SW26010Pro processor. (b) Matrix multiplication on the Sunway many-core processor. (c) One-sided Jacobi SVD algorithm on the Sunway many-core processor.

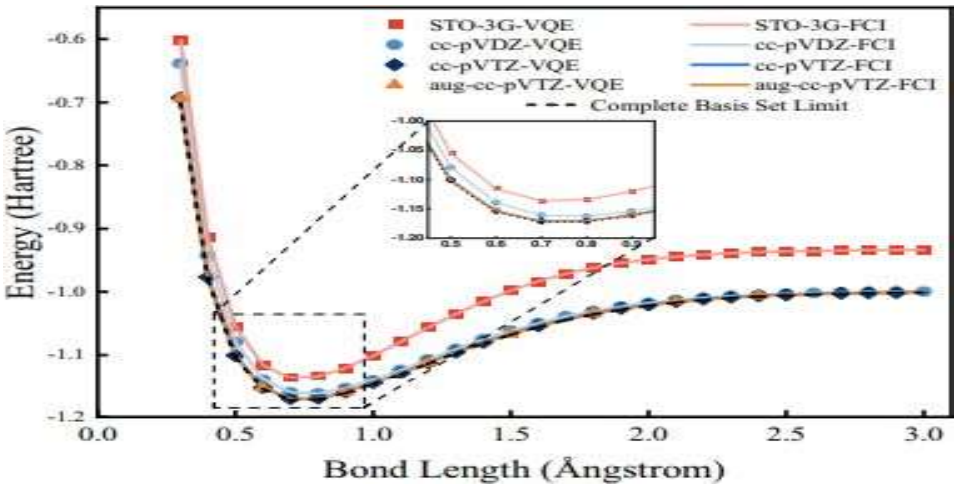

Fig.3 Potential energy curves, expressed in unit Hartree, for the hydrogen molecule are calculated using the UCCSD method.

Chemical Accuracy and Molecular Interactions

A pivotal facet of our research revolved around the attainment of chemical accuracy across diverse basis sets. The meticulous analysis across four basis sets revealed a maximum error of merely 0.82 kcal mol−1 at R(H–H) = 2.4 Å, specifically in the context of the aug-cc-pVTZ results. This attainment of chemical accuracy underscores the fidelity and precision inherent in our quantum computing simulations, validating the efficacy of our computational methodologies and algorithms.

Table 2. Wall time per VQE iteration in seconds and number of iterations to converge for different basis sets.

Basis set	STO-3G	cc-pVDZ	cc-pVTZ	aug-cc-pVTZ
Wall time per iteration	0.12	3.67	190.63	1564.52
Number of steps	18	303	459	677

The data are collected from the geometry with the lowest energy of each basis set in Fig. 3.

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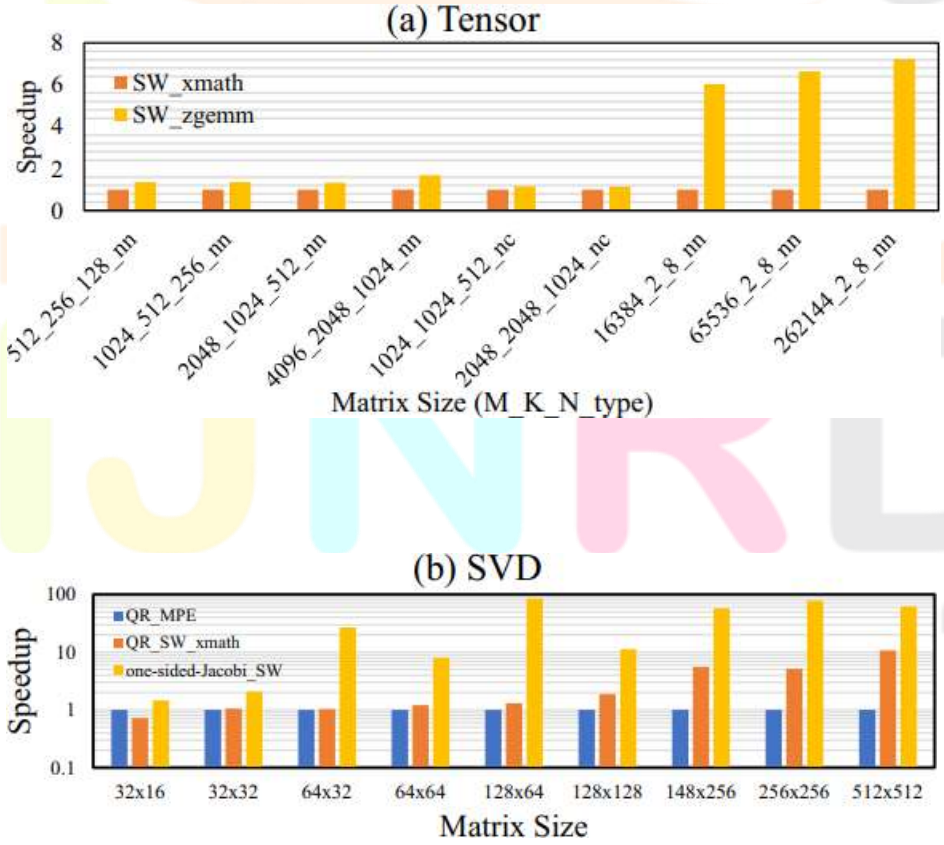
Executing these simulations with 512 processes unveiled a remarkable computational paradigm. The computational times, meticulously recorded and analyzed, underscore the efficiency and scalability inherent in our approach. The results, as depicted in Figure 4d, unveil a nearly linear scaling trajectory, culminating in a sustained performance of 216.9 PFLOPS in double precision. This performance benchmark, achieved with 606,208 processes spanning 39,403,520 cores for the system with 2368 qubits, accentuates the computational prowess and scalability of our quantum computing framework.

Table 3. The mean absolute errors (MAE) and maximum absolute errors (MAX) (in kcal/mol) of the potential energy surfaces for H_2 computed with the UCCSD-VQE method using different Gaussian basis sets.

Basis set	STO-3G	cc-pVDZ	cc-pVTZ	aug-cc-pVTZ
MAE	9.4×10^{-13}	2.7×10^{-3}	8.1×10^{-2}	3.3×10^{-1}
MAX	6.3×10^{-12}	1.3×10^{-2}	1.8×10^{-1}	8.2×10^{-1}

The FCI results are taken as the reference values.



Furthermore, the presentation of Full Configuration Interaction (FCI) results in the complete basis set (CBS) limit elucidates the approximation to the exact potential energy curve of the hydrogen molecule. This approximation serves as a cornerstone in quantum chemistry, offering invaluable insights into molecular interactions, electronic configurations, and potential energy landscapes.

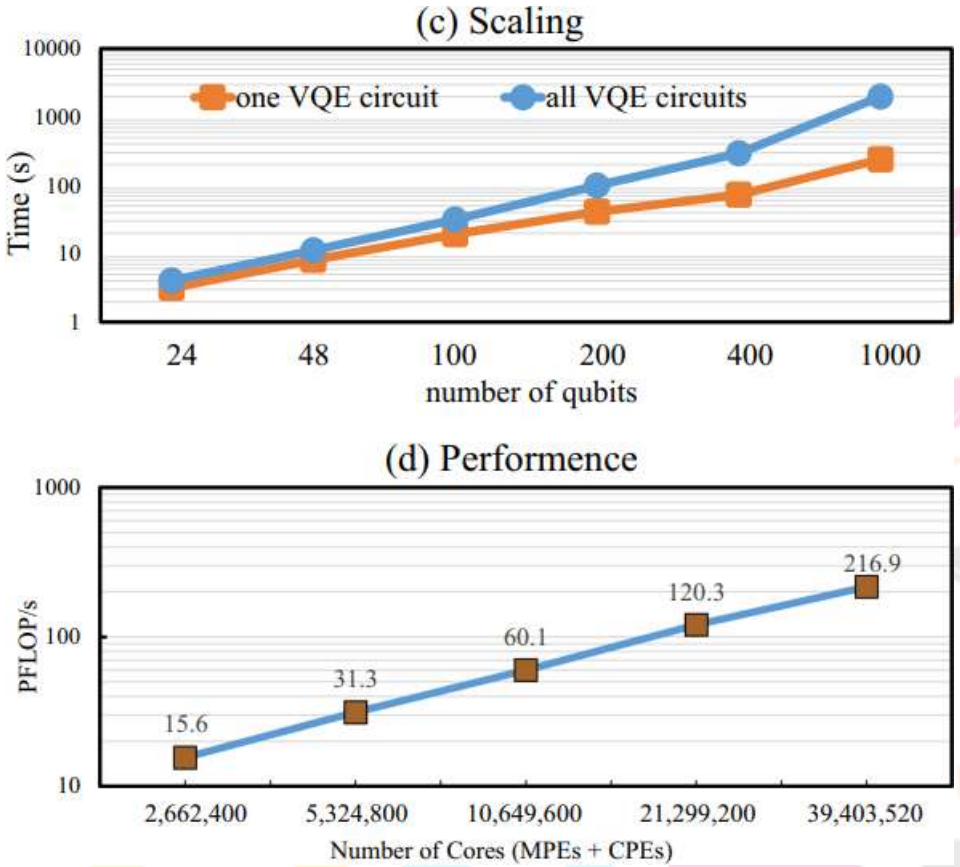


Fig.4 Performance Insights into Linear Algebra Routines.

Scientific Interpretation and Implications

The empirical findings and subsequent analysis usher in a new era in quantum computing and quantum chemistry. The unprecedented scalability achieved in quantum circuit simulations paves the way for tackling intricate quantum systems, unraveling the mysteries inherent in molecular interactions, material properties, and fundamental quantum phenomena.

The attainment of chemical accuracy across diverse basis sets underscores the transformative

potential of quantum computing in quantum chemistry simulations. The fidelity, precision, and computational efficiency showcased in our research set a new benchmark in the realm of quantum chemistry, offering a robust platform for scientific exploration, molecular design, and technological innovation.

Moreover, the approximation to the exact potential energy curve of the hydrogen molecule through FCI results in the CBS limit elucidates the intricate interplay between electronic configurations, molecular geometry, and potential energy landscapes. This approximation serves as a foundational pillar in quantum chemistry, facilitating advancements in molecular research, chemical synthesis, and materials design.

Conclusion

The culmination of our research endeavors at the confluence of quantum computing and quantum chemistry heralds a new era in scientific exploration and technological innovation. Through meticulous simulations, groundbreaking algorithms, and transformative insights, our study has illuminated the transformative potential of quantum computing in unraveling the mysteries of molecular interactions, electronic configurations, and fundamental quantum phenomena. The attainment of unprecedented scalability, computational efficiency, and chemical accuracy underscores the efficacy, precision, and promise of quantum computing in revolutionizing quantum chemistry research. As we stand on the precipice of unparalleled advancements, our research serves as a beacon of innovation, paving the way for a future where quantum computing transcends boundaries, reshaping our understanding of the quantum realm and catalyzing advancements across diverse scientific domains.

Limitation of the Study

While our research endeavors have achieved remarkable milestones, it is imperative to acknowledge the inherent limitations and challenges that encompass our study. The quantum circuit simulations, albeit groundbreaking, represent a subset of the vast quantum systems and

phenomena inherent in quantum chemistry. The computational frameworks, algorithms, and methodologies employed, while robust, necessitate further refinement and optimization to address the evolving complexities and intricacies of quantum systems. Additionally, the attainment of chemical accuracy, while exemplary, necessitates continued validation, verification, and enhancement to ensure consistency, reliability, and reproducibility across diverse molecular systems, basis sets, and computational scenarios. Recognizing these limitations provides a foundation for future research endeavors, fostering a collaborative, iterative, and forward-thinking approach to advancing quantum computing and quantum chemistry research.

Implication of the Study

The implications of our study resonate across diverse scientific, technological, and industrial sectors, heralding a paradigm shift in quantum computing and quantum chemistry research. The transformative insights, methodologies, and benchmarks established serve as foundational pillars for advancing molecular research, chemical synthesis, material design, and computational modeling. The attainment of unprecedented scalability and computational efficiency unlocks new avenues for tackling intricate quantum systems, elucidating molecular interactions, and pioneering innovations at the forefront of science and technology. Moreover, the synthesis of quantum computing and quantum chemistry catalyzes interdisciplinary collaborations, fostering synergies between theoretical insights, computational frameworks, and experimental validations. As we navigate the implications of our study, we envision a future where quantum computing augments scientific exploration, propels technological innovation, and catalyzes advancements across diverse scientific domains.

Future Recommendations

Building upon the foundational insights and milestones achieved in our study, future research endeavors could explore several avenues to further enhance, expand, and evolve the nexus of quantum computing and quantum chemistry. Emphasizing the refinement and optimization of computational frameworks, algorithms, and methodologies would bolster the scalability, efficiency, and applicability of quantum computing simulations across diverse quantum systems and phenomena. Collaborative initiatives fostering interdisciplinary collaborations between quantum physicists, computational chemists, material scientists, and industry stakeholders could catalyze innovations, drive technological advancements, and accelerate the translation of quantum computing research into real-world applications. Furthermore, investment in infrastructure, resources, and training initiatives would cultivate a vibrant ecosystem, nurturing talent, fostering innovation, and propelling the quantum computing and quantum chemistry research landscape into new frontiers of discovery, exploration, and impact. As we chart the course for future research endeavors, embracing a collaborative, iterative, and visionary approach would catalyze advancements, unlock potentials, and shape the future trajectory of quantum computing and quantum chemistry research.

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