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14. ABSTRACT

This three-year project consisted on the development and application of quantum computer algorithms for chemical applications. In particular, we developed algorithms for chemical reaction dynamics, electronic structure and protein folding. The first quantum computing for chemistry experiment was also realized. With the goal of simulating energy transfer in photosynthetic complexes, we developed the theory of quantum stochastic walks, and collaborated with experimentalists in its implementation. The project provided a suite of quantum algorithms and

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Report Title

Quantum Computing for Quantum Chemistry

ABSTRACT

This three-year project consisted on the development and application of quantum computer algorithms for chemical applications. In particular, we developed algorithms for chemical reaction dynamics, electronic structure and protein folding. The first quantum computing for chemistry experiment was also realized. With the goal of simulating energy transfer in photosynthetic complexes, we developed the theory of quantum stochastic walks, and collaborated with experimentalists in its implementation. The project provided a suite of quantum algorithms and early demonstrations that show clearly that quantum computing would have a considerable impact in the area of theoretical chemistry.

List of papers submitted or published that acknowledge ARO support during this reporting period. List the papers, including journal references, in the following categories:

(a) Papers published in peer-reviewed journals (N/A for none)

I. Kassal and A. Aspuru-Guzik, "Quantum algorithm for molecular properties and geometry optimization," J. Chem. Phys. 131, 224102 (2009).

B.P. Lanyon, J.D. Whitfield, G.G. Gillett, M.E. Goggin, M.P. Almeida, I. Kassal, J.D. Biamonte, M. Mohseni, B.J. Powell, M. Barbieri, A. Aspuru-Guzik and A.G. White, "Towards quantum chemistry on a quantum computer," Nature Chem. 2, 106-111 (2010).

J.D. Whitfield, C.A. Rodriguez-Rosario and A. Aspuru-Guzik, "Quantum stochastic walks: A generalization of classical random walks and quantum walks," Phys. Rev. A 81, 022323 (2010).

M. Mohseni, A.T. Rezakhani, J.T. Barreiro, P.G. Kwiat and A. Aspuru-Guzik, "Quantum process estimation via generic two-body correlations," Phys. Rev. A 81, 032102 (2010).

M.A. Broome, A. Fedrizzi, B.P. Lanyon, I. Kassal, A. Aspuru-Guzik and A.G. White, "Discrete Single-Photon Quantum Walks with Tunable Decoherence," Phys. Rev. Lett. 104, 153602 (2010).

A. Perdomo-Ortiz, S.E. Venegas-Andraca and A. Aspuru-Guzik, "A study of heuristic guesses for adiabatic quantum computation," Quantum Inf. Process. In press. Preprint: arXiv:0807.0354 (2008).

Number of Papers published in peer-reviewed journals: 6.00

(b) Papers published in non-peer-reviewed journals or in conference proceedings (N/A for none)

A. Aspuru-Guzik, "Quantum information for chemistry and biology," The Quantum Times 4, 1-3 (2009).

Number of Papers published in non peer-reviewed journals: 1.00

(c) Presentations

"The Role of Quantum Coherence in Photosynthetic Energy Transfer," Canadian Society for Chemistry Conference, Toronto, Canada, 31 May 2010.

"Quantum computation for quantum chemistry," American Physical Society Division of Atomic, Molecular and Optical Physics Annual Meeting, Houston TX, 29 May 2010.

"The Role of Quantum Coherence in Photosynthetic Complexes," Department of Chemistry, University of Southern California, Los Angeles CA, 19 April 2010.

"Quantum Computing for Chemistry," Norman Hascoe Distinguished Lecture, Department of Chemistry, University of Connecticut, Storrs CT, 12 April 2010.

"Progress towards the efficient preparation of thermal states on quantum and classical computers," CECAM Workshop: Tensor network methods for quantum chemistry, Zurich Switzerland, 31 March 2010.

"Quantum computing for quantum chemistry and molecular dynamics, a new approach for obtaining exponential speedups in exact molecular simulation: Experiment and theory," Thomas Kuhn Paradigm Shift Award Symposium, American Chemical Society National Meeting, San Francisco CA, 21 March 2010.

"Quantum Information and Quantum Computation for Chemistry," Chemical Sciences and Engineering Division, Argonne National Laboratory, Argonne IL, 26 January 2010.

Plenary: "Quantum computer algorithms for statistical mechanics research," Winter Meeting on Statistical Physics, Taxco Guerrero Mexico, 6 January 2010.

"Quantum computation for chemistry," Physics Department, National Autonomous University of Mexico, 21 August 2009.

"The role of quantum coherence in photosynthetic energy transfer," Chemistry Department, National Autonomous University of Mexico, 20 August 2009.

Number of Presentations: 10.00

Non Peer-Reviewed Conference Proceeding publications (other than abstracts):

Number of Non Peer-Reviewed Conference Proceeding publications (other than abstracts): 0

Peer-Reviewed Conference Proceeding publications (other than abstracts):

Number of Peer-Reviewed Conference Proceeding publications (other than abstracts): 0

(d) Manuscripts

J.D. Whitfield, J. Biamonte and A. Aspuru-Guzik, "Quantum Computing Resource Estimate of Molecular Energy Simulation," Submitted to J. Chem. Phys. Preprint: arXiv:1001.3855 (2010).

J.D. Biamonte, V. Bergholm, J.D. Whitfield, J. Fitzsimons and A. Aspuru-Guzik, "Adiabatic Quantum Simulators," Submitted to Phys. Rev. Lett. Preprint: arXiv:1002.0368 (2010).

M.H. Yung, D. Nagaj, J.D. Whitfield and A. Aspuru-Guzik, "Simulation of Classical Thermal States on a Quantum Computer: A Renormalization Group Approach," Submitted to Phys. Rev. Lett. Preprint: arXiv:1005.0020 (2010).

I. Kassal, J.D. Whitfield, A. Perdomo-Ortiz, M.-H. Yung and A. Aspuru-Guzik, "Simulating Chemistry Using Quantum Computers," Submitted to Annu. Rev. Phys. Chem. Preprint: arXiv:1007.2648 (2010).

Number of Manuscripts: 4.00

Patents Submitted

Patents Awarded

Graduate Students

NAME	PERCENT_SUPPORTED
Ivan Kassal	1.00
FTE Equivalent:	**1.00**
Total Number:	**1**

Names of Post Doctorates

NAME	PERCENT_SUPPORTED
FTE Equivalent:	
Total Number:	

Names of Faculty Supported

NAME	PERCENT_SUPPORTED	National Academy Member
Alan Aspuru-Guzik	0.08	No
FTE Equivalent:	**0.08**	
Total Number:	**1**	

Names of Under Graduate students supported

NAME	PERCENT_SUPPORTED
FTE Equivalent:	
Total Number:	

Student Metrics

This section only applies to graduating undergraduates supported by this agreement in this reporting period

The number of undergraduates funded by this agreement who graduated during this period: 0.00

The number of undergraduates funded by this agreement who graduated during this period with a degree in science, mathematics, engineering, or technology fields:..... 0.00

The number of undergraduates funded by your agreement who graduated during this period and will continue to pursue a graduate or Ph.D. degree in science, mathematics, engineering, or technology fields:..... 0.00

Number of graduating undergraduates who achieved a 3.5 GPA to 4.0 (4.0 max scale):..... 0.00

Number of graduating undergraduates funded by a DoD funded Center of Excellence grant for Education, Research and Engineering:..... 0.00

The number of undergraduates funded by your agreement who graduated during this period and intend to work for the Department of Defense 0.00

The number of undergraduates funded by your agreement who graduated during this period and will receive scholarships or fellowships for further studies in science, mathematics, engineering or technology fields:..... 0.00

Names of Personnel receiving masters degrees

NAME

Total Number:

Names of personnel receiving PHDs

NAME

Total Number:

Names of other research staff

NAME	PERCENT_SUPPORTED

FTE Equivalent:

Total Number:

Sub Contractors (DD882)

Inventions (DD882)

ARO Grant No. W911NF-07-1-0304
Quantum Computing for Quantum Chemistry
Alán Aspuru-Guzik

FINAL TECHNICAL REPORT

Our first publication was *Polynomial-time quantum algorithm for the simulation of chemical dynamics* Proc. Natl. Acad. Sci. 105 (2008) 18681, in which we showed that quantum computers could offer an exponential speed-up for the simulation of chemical dynamics. While the Born-Oppenheimer approximation can be used, it surprisingly makes the computation more difficult for reactions with more than a few atoms. A detailed resource estimate showed that about 100 qubits would be needed to solve problems inaccessible to classical computers.

Real-space quantum simulation techniques require a grid-based preparation of initial states. The PNAS paper proposed a method for preparing chemically relevant states on a quantum computer, and this direction was fleshed out in *Preparation of many-body states for quantum simulation* J. Chem. Phys. 130 (2009) 194105. We provided a technique for translating a concise description of a quantum state---for example, a few quantum numbers---into the grid-based quantum state. Provided a few broadly applicable conditions are met, the procedure works for eigenstates, superpositions, and mixed states.

In *Quantum algorithm for molecular properties and geometry optimization* J. Chem. Phys. 131 (2009) 224102, we applied the quantum gradient estimation algorithm to chemical problems to show that energy derivatives could be computed with a significant speed-up. In a d-dimensional system, the nth derivative would require only 2^{n-1} energy computations, as opposed to the classical $O\left(d^{\lfloor n/2\rfloor }\right)$ cost. In particular, calculating gradients and Hessians with respect to nuclear coordinates could be used to optimize the geometry of any molecule using a constant number of energy evaluations.

A major landmark in our research direction was the first experimental implementation of a quantum chemical calculation on a quantum computer, in *Towards quantum chemistry on a quantum computer* Nature Chem. 2 (2010) 106. Our collaborators at the University of Queensland implemented the iterative phase estimation algorithm on a two-qubit optical quantum computer in order to compute the potential energy surface of the hydrogen molecule in a minimal basis. While this implementation required a fair amount of classical pre-processing, the technique is scalable to larger systems.

Further expounding on the scalable extensions, we have submitted *Quantum Computation for Molecular Energy Simulations* (preprint at arxiv:1001.3855) to the Journal of Molecular Physics. In this article we provide a detailed explanation of the path to scalable digital quantum simulation as well as the explicit gate sequence for the hydrogen molecule using five qubits. Estimates for other chemical systems are also given.

The use of adiabatic quantum computers for quantum simulation was explored in *Adiabatic quantum simulators* (preprint at arxiv:1002.0368). We used an adiabatic process together with a method reminiscent of Ramsey spectroscopy to suitable replace the gate-model physics simulation algorithms. This provided a novel quantum algorithmic component needed to exploit several important results from the complexity of finding ground states.

Simulating Markov processes with quantum computer is another research topic that we have touch upon in *Simulation of Classical Thermal States on a Quantum Computer: A Transfer Matrix Approach* (preprint at arxiv:1005.0020). Most of the algorithms to date are based on

adaptations of the quantum search algorithm which obtain a quadratic speedup with respect to the eigenvalue gap of the Markov chain. Our contribution was to explore the Transfer Matrix approach in the quantum setting thereby obtaining an algorithm that was gap independent and quadratic faster than its classical counterpart.

We reviewed the state of the field in *Simulating chemistry using quantum computers*, which was submitted to *Ann. Rev. Phys. Chem.* (preprint at arxiv:1007.2648).

We have also focused on exploring and implementing quantum computing using quantum walks.

In *Discrete single-photon quantum walks with tunable decoherence* Phys. Rev. Lett. 104 (2010) 153602, we described, in collaboration with researchers at the University of Queensland, an experimental, quantum-optical implementation of a discrete-time quantum walk. This was the first demonstration that used a truly quantum walker, and is distinguished by the ability to add controllable amounts of decoherence at each step. This allowed us to study the transition between the quantum and classical random walks as the decoherence became strong.

Recent experiments on photosynthetic light-harvesting complexes observed long-lived excitonic coherences at room temperature. This observation has lead to speculations that a possible quantum search operation analogous to the Grover search was performed by the light-harvesting complex. In *Environment-assisted quantum walks in energy transfer of photosynthetic complexes*, J. Chem. Phys. 129 (2008) 174106, we found that the criteria for such a search are not met in a strict sense. We established however the connection of exciton transfer in multichromophoric networks to another quantum information concept, the continuous time quantum walk. To this end, we extended the unitary quantum walk to a decohered quantum walk.

Motivated by the experiments on the Fenna-Matthews-Olson (FMO) light-harvesting complex of green sulfur bacteria, we developed and discussed the fundamentals of environment-assisted quantum transport (ENAQT) in *Environment-assisted quantum transport*, New J. Phys. 11 (2009) 033003. The efficiency of quantum transport can be enhanced by the presence of a fluctuating environment. For example, in the case of transport through statically disordered structures, adding pure dephasing can enhance transport efficiency, which would otherwise be limited by quantum localization. For the FMO complex, we found that maximal transport efficiency can be obtained at dephasing rates corresponding to room temperature values.

In *Role of quantum coherence and environmental fluctuations in chromophoric energy transport*, J. Phys. Chem. B 113 (2009) 9942, we developed a method to quantify the biological importance of quantum coherence by its contribution to the efficiency of the primary photosynthetic event. We found a contribution of around 10% for a spatially uncorrelated model of the FMO complex. Furthermore, we studied the robustness of the exciton transport with respect to slow protein conformation changes, the effect of spatial correlations, and the importance of various transfer pathways.

In *Quantum Stochastic Walks: A generalization of classical random walks and quantum walks*, Phys. Rev. A 81 (2010) 022323 we explored the theoretical connections between the classical and quantum walks using the appropriate framework of probabilistic quantum evolution. We used this framework to look at quantum-to-classical transition for the walk on a line and the glued tree graph of depth three. Using this model we showed that mixed quantum classical transport can retard the walk for short times on certain graphs.

ARO-Funded Publications (2007-2010)

1. H. Wang, S. Kais, A. Aspuru-Guzik and M.R. Hoffmann, "Quantum algorithm for obtaining the energy spectrum of molecular systems," *Phys. Chem. Chem. Phys.* **10**, 5388-5393 (2008).

2. M. Mohseni, P. Rebentrost, S. Lloyd and A. Aspuru-Guzik, "Environment-assisted quantum walks in photosynthetic energy transfer," *J. Chem. Phys.* **129**, 174106 (2008).

3. I. Kassal, S.P. Jordan, P.J. Love, M. Mohseni and A. Aspuru-Guzik, "Polynomial-time quantum algorithm for the simulation of chemical dynamics," *Proc. Natl. Acad. Sci. USA* **105**, 18681-18686 (2008).

4. P. Rebentrost, M. Mohseni, I. Kassal, S. Lloyd and A. Aspuru-Guzik, "Environment-assisted quantum transport," *New J. Phys.* **11**, 033003 (2009).

5. N.J. Ward, I. Kassal and A. Aspuru-Guzik, "Preparation of many-body states for quantum simulation," *J. Chem. Phys.* **130**, 194105 (2009).

6. P. Rebentrost, M. Mohseni and A. Aspuru-Guzik, "Role of Quantum Coherence and Environmental Fluctuations in Chromophoric Energy Transport," *J. Phys. Chem. B* **113**, 9942-9947 (2009).

7. I. Kassal and A. Aspuru-Guzik, "Quantum algorithm for molecular properties and geometry optimization," *J. Chem. Phys.* **131**, 224102 (2009).

8. B.P. Lanyon, J.D. Whitfield, G.G. Gillett, M.E. Goggin, M.P. Almeida, I. Kassal, J.D. Biamonte, M. Mohseni, B.J. Powell, M. Barbieri, A. Aspuru-Guzik and A.G. White, "Towards quantum chemistry on a quantum computer," *Nature Chem.* **2**, 106-111 (2010).

9. J.D. Whitfield, C.A. Rodriguez-Rosario and A. Aspuru-Guzik, "Quantum stochastic walks: A generalization of classical random walks and quantum walks," *Phys. Rev. A* **81**, 022323 (2010).

10. M. Mohseni, A.T. Rezakhani, J.T. Barreiro, P.G. Kwiat and A. Aspuru-Guzik, "Quantum process estimation via generic two-body correlations," *Phys. Rev. A* **81**, 032102 (2010).

11. M.A. Broome, A. Fedrizzi, B.P. Lanyon, I. Kassal, A. Aspuru-Guzik and A.G. White, "Discrete Single-Photon Quantum Walks with Tunable Decoherence," *Phys. Rev. Lett.* **104**, 153602 (2010).

12. A. Perdomo-Ortiz, S.E. Venegas-Andraca and A. Aspuru-Guzik, "A study of heuristic guesses for adiabatic quantum computation," *Quantum Inf. Process*. In press. Preprint: arXiv:0807.0354 (2008).

13. J.D. Whitfield, J. Biamonte and A. Aspuru-Guzik, "Quantum Computing Resource Estimate of Molecular Energy Simulation," Submitted to *J. Chem. Phys.* Preprint: arXiv:1001.3855 (2010).

14. J.D. Biamonte, V. Bergholm, J.D. Whitfield, J. Fitzsimons and A. Aspuru-Guzik, "Adiabatic Quantum Simulators," Submitted to *Phys. Rev. Lett.* Preprint: arXiv:1002.0368 (2010).

15. M.H. Yung, D. Nagaj, J.D. Whitfield and A. Aspuru-Guzik, "Simulation of Classical Thermal States on a Quantum Computer: A Renormalization Group Approach," Submitted to *Phys. Rev. Lett.* Preprint: arXiv:1005.0020 (2010).

16. I. Kassal, J.D. Whitfield, A. Perdomo-Ortiz, M.-H. Yung and A. Aspuru-Guzik, "Simulating Chemistry Using Quantum Computers," Submitted to *Annu. Rev. Phys. Chem.* Preprint: arXiv:1007.2648 (2010).