Atos

Quantum Learning Machine

Atos

Trusted partner for your Digital Journey

Quantum computing – a promise

Quantum computing relies on one promise:

Quantum computing is based on the promise that, when quantum computers are available, it will be possible to solve some complex problems faster than the current most powerful HPC systems.

It will massively reduce the complexity of some problems currently intractable to classical computers.



A brief story of quantum computing

 <i>1981</i>: First basic model of a quantum computer <i>R. Feynman</i> 	<i>2017:</i> Atos introduced Quantum Learning Machine	 ~ 2023: Physical qubit NISQ devices era (Noisy Quantum accelerator Atos NISQ introduction 	s <i>Intermediate-Scale Quantum)</i> rindustrialization on
Discovery phase	NISQ era		FTQC era
1994 : Quantum algorithm development to factorize large numbers. <i>P. Shor</i>	m <i>Today</i> : Sin e Learning • NISQ pr	nulation g systems rototypes	 2035+: Logical qubits FTQC (Fault Tolerant Quantum Computers)



Quantum computing – a few fundamental notions



Quantum computing acceleration

• We see quantum computing as an accelerator of classical computing



It is unlikely classical computing will be replaced any time soon by quantum computing...



Why investing in quantum computing now?

Quantum computing is an opportunity, now available for businesses...



Artificial Intelligence created an unprecedented competitive gap on the market



Quantum Computing: when QPUs are available, organizations with the greatest expertise may get an order-of-magnitude edge

Investing in Quantum Computing is urgent

- · Access existing commercial quantum simulation capabilities,
- Test newly available hardware platforms, and software applications,
- Develop new algorithms

To create competitive advantage



Quantum Computing applications Numerous cross-industry impacts



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Quantum Computing applications Numerous cross-industry impacts



Quantum Computing Applications

	Machine Learning	Combinatorial Optimization	Security	Chemistry
Public Sector & Defense	Neural networks	Process optimization	CryptanalysisQuantum key distribution	Materials scienceNanotechnologies
Manufacturing	 Traffic simulation E-charging station and parking search Autonomous driving 	 Logistics (scheduling, planning, production distribution routing) Supply chain 	Software validationVerification and fault analysis	 Batteries Polymers Catalysts, enzyme design
Resources & Services	 Smart grids Energy management Network design 	Yield managementFlight schedulingOil well optimization	Cybersecurity	Carbon dioxide captureLubricants
Healthcare & Life Sciences	Personalized medicineGenomics	Virtual screeningClinical trial database search	Post-quantum cryptography	Molecular modelingProtein foldingDrug discovery
Financial Services & Insurance	 Fraud detection Trading strategies Asset pricing Market simulation 	 Portfolio optimization Risk assessment	Cryptocurrency	
Telecom, Media & Utilities	Personalized content	 5G antenna location Chip layout optimization 	Post-quantum cryptography	And many more to come

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Chemistry One of today's most active application area!



GOAL

Compute the exact energy of large molecules

- This is intractable today
- Cost: 2 qubits per orbital even without error correction!

STAR ALGORITHMS

Variational Quantum Algorithms (VQE and derivatives)

IMPACT

New discovery and energy savings in synthesis for fertilizers, lubricants, ...





Pharmaceuticals



GOAL

Predict and simulate the exact protein folding

Proteins exist in an astronomical number of possible arrangements.

IMPACT

Enable revolutionary new applications in pharmaceuticals, genetic engineering and personalized medicine

e.g: Improve the treatment of Alzheimer's-, Parkinson's disease and Cancer



TODAY/PAST (pre-quantum)

After RSA768 in 2010, RSA795 in 2019, RSA829 is the factorization world record (2,700 years of cores on tens of thousands powerful machines running NFS, in 2020)

2140324650240744961264423072839333563008614715144755017797754920 8814180234471401366433455190958046796109928518724709145876873962 6192155736304745477052080511905649310668769159001975940569345745 2230589325976697471681738069364894699871578494975937497937



-

Cryptography



2



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6413528947707158027879019017057738908482501474294344720811685963 2024532344630238623598752668347708737661925585694639798853367

333720275949781565562260106053551142279407603447675546667845209 87023841729210037080257448673296881877565718986258036932062711

▶ comp[RSA1024] \cong comp[RSA829] * 10⁵⁷

This exponential complexity is the keystone of RSA crypto algorithm (and almost all asymmetric algos)





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6413528947707158027879019017057738908482501474294344720811685963 2024532344630238623598752668347708737661925585694639798853367

333720275949781565562260106053551142279407603447675546667845209 87023841729210037080257448673296881877565718986258036932062711

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TOMORROW (post-quantum)

Shor Algorithm: polynomial time RSA-768 : almost instantaneous by using a quantum computer with several thousands logical Qubits comp[RSA1024] < comp[RSA829] * 2





TODAY/PAST (pre-quantum)

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6413528947707158027879019017057738908482501474294344720811685963 2024532344630238623598752668347708737661925585694639798853367

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Critical risk (very high impact, low prob.) for IT security everywhere



[▶] comp[RSA1024] \cong comp[RSA829] * 10^{57}

Finance



GOAL

Help investment professionals and financial institutions optimize returns while minimizing risk by analyzing an unimaginable range of scenarios

STAR ALGORITHMS

- Black-Scholes differential equation is a derivative from Schrödinger's equation
- Quantum Random Walker

IMPACT

- Optimization of trading strategies
- Portfolio optimization (optimization under constraints)
- Improved fraud detection



Oil Prospection



GOAL

Solve Partial Differential Equations with an exponential speed-up

STAR ALGORITHMS

HHL, the matrix inversion algorithm

IMPACT

Unprecedented performance and accuracy for

- Oil well optimization
- Seismic simulation





Combinatorial Optimization Example of the Travelling Salesman problem

What is the shortest path to travel to x cities?

- 14 cities = 10^11 possible routes → 100s (1GHz computer)
- 22 cities = 10^19 possible routes → 1,600 years (1GHz computer)
- 28 cities ... → Longer than the lifetime of the universe



Atos

Combinatorial

Optimization

Combinatorial Optimization

Combinatorial Optimization

GOAL

Solve NP-hard problems with an exponential speedup

STAR ALGORITHMS

QAOA, the Quantum Approximate Optimization Algorithm

IMPACT

Direct applications to:

- power management
- supply chain optimization
- optimization of industrial processes
- flight scheduling



Machine Learning

- Quantum Machine Learning (QML) is among the most active research areas
- Theoretical works have proven exponential speedup in several key applications:
 - Train neural networks of a complexity intractable to current supercomputers
 - Most statistical learning techniques have a quantum counterpart with an exponential speedup



Machine Learning

Expected timing of Quantum Advantage



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Providing end-to-end solutions for the quantum era



Atos

Atos

Atos Quantum Program



Help people **learn**, **experiment** with quantum computers, **develop** applications and algorithms,

without the need to wait for quantum machines to be physically available...



Atos Quantum program

Monitored by a top-class scientific advisory board

Atos has its quantum activities watched by the most renowned scientists in this field.

- Artur Ekert (Hughes Medal)
- Alain Aspect (World Prize)
- Serge Haroche (Nobel Prize)
- Daniel Esteve
- David Di Vincenzo





Atos Quantum program

► A global strategy

1	Quantum Programming Platform	Complete programming and simulation environment for quantum software/hardware developers and for education/training	
2	Quantum Expert Consulting Services	Assisting our customers in discovering Quantum Computing, detecting relevant use cases, assessing quantum implementation benefits on the QLM simulator	
3	New Generation Architectures	Designing the new quantum-powered accelerators for supercomputers or hybrid systems	
4	Quantum Algorithms	Atos' own research, focused on Quantum Machine Learning one of the most promising application areas of QC	
5	Quantum Safe Cryptography	Preparing the cryptographies and hardware security modules, resistant to quantum computer attacks	







Quantum Computing Programming environment

Quantum computing hardware manufacturers have created their **own proprietary programming** software and standards, based on their qubits technology

Atos offers a **universal programming environment** to avoid the vendor lock-in



Atos Quantum Program added value



What are the possible ways to use the Atos QLM?

► A multi-purpose system





What is the Atos Quantum Learning Machine?

► A complete programming environment and a quantum processor emulator





A highly scalable and modular simulator

Upgrade your Atos QLM to suit your simulation needs



Atos QLM E[nhanced]

Accelerating research in the NISQ era

Discover the new GPU-optimized appliance Atos QLM E

- Accelerate your quantum simulations up to 12x
- Optimized for variational algorithms best suited for the NISQ* era (up to 30 qubits)
- Upgrade your QLM to a QLM E very easily to benefit from these enhanced features





*NISQ = Noisy

Quantum

Intermediate-Scale

Atos QLM E[nhanced]

Accelerating research in the NISQ era

Quantum Approximate
 Optimization Algorithm



- Variational Quantum
 Eigensolver / Variational
 Imaginary Time Evolution
- Variational Quantum Factoring
- Variational Quantum Classifier



Variational algorithms will be the first to be implemented on NISQ* devices



ATOS

COMING SOON: Simulated Quantum Annealing

Atos' **Quantum Annealing Simulator** Available to solve real-world production problems



Highest efficiency unrivaled precision and speed

Greatest scalability emulate more than 40,000 perfect spins in a few seconds



Portfolio optimization



Automotive/ aeronautic design



Traffic optimization Navigation Airline scheduling Yield management





Grid management



Supply chain optimization



Why the Atos QLM?

► Key benefits

			1	Hardware Agnostic	 Avoid the lock-in Evaluate your code vs several HW
 Up to 41 qubits (worst case simulation) Hybrid quantum-classical simulations 	Scalable & Futureproof	2			
$\begin{array}{c} \operatorname{Out}\left[1\right]: & \phi_{0} & -\underline{H} - \underline{PH}[\underline{\tilde{s}}] - \underline{PH}[\underline{\tilde{s}}] - \underline{PH}[\underline{\tilde{s}}] - \underline{PH}[\underline{\tilde{s}}] \\ & q_{1} & -\underline{H} - \underline{PH} \\ & q_{2} & -\underline{H} - \underline{PH} \\ & q_{3} & -\underline{H} - \underline{PH} \\ & q_{4} & -\underline{H} - \underline{PH} \\ & -\underline{H} \\ & -\underline{H} - \underline{PH} \\ & -\underline{H} $	$H[\frac{\pi}{2}] - PH[\frac{\pi}{4}] - P$		3	A user-friendly framework	 Jupyter Notebooks library Integrated Quantum Algorithms & QLIB
 Use interoperability with Qiskit or ProjectQ Develop your own connectors 	Interoperability kit	4	A C C C C		Cirq rigetti
			5	Noisy Simulation	Evaluate the impact of quantum noise on your simulation's results



Expand your Quantum Programmer Community with OmyQLM

Available for FREE to ALL Atos QLM customers



Scientists: You are currently using the Atos QLM and you want to prepare your code and run them on your laptop?



Students: You want to start programming Quantum algorithms using the same framework as your professors?



Tech enthusiasts: You want to discover Quantum programming using an accessible and user-friendly environment?



SmyQLM

An accessible approach to quantum simulation



Atos

What functionalities are included in myQLM?

► The programming environment of the Atos QLM with open source simulators



Upgrade from myQLM to advanced simulators

► Features comparison

Featu	res	myQLM freeware	Atos QLM appliance	Atos QLM E[nhanced] appliance
SN IMM	pyAQASM/AQASM/CIRC formats	\checkmark	\checkmark	✓
	Custom gates	\checkmark	\checkmark	\checkmark
JGR⊅	QLIB libraries	\checkmark	\checkmark	✓
PRO	Interoperability kit – open source	\checkmark	\checkmark	\checkmark
ц р	Custom plugins	\checkmark	\checkmark	✓
SOc ⁻	Gate set rewriter	Х	\checkmark	\checkmark
ke-/F oce	Topology constraints solver	Х	\checkmark	\checkmark
PR	Circuit Optimizer	Х	\checkmark	✓
	Simulation capabilities	Up to 20 qubits	Up to 41 qubits	Up to 41 qubits
N	Simulation performances	*	***	****
ATIC	PyLinalg – open source	\checkmark	\checkmark	✓
MUL	Advanced noiseless simulators	Х	\checkmark	× 54
SI	Noisy simulators	X	\checkmark	
ES	Acceleration up to 12x	Х	X	
	Training	Self-training	Instructor-led	Instructor-led
ZVIC	Support	Community	Subscription	Subscription
SEF	Consulting	On demand	On demand	On demand



1	Quantum Computing Basis	BEGINNER ½ day	A comprehensive approach to quantum computing
2	Atos QLM Fast Start	INTERMEDIATE 2 days	Quick knowledge ramp-up on the Atos QLM appliance
3	Decoding of quantum algorithm	ADVANCED 2 days	Principles and building steps of a specific quantum algorithm
4	Proof of Concept	BUSINESS + EXPERTS 5 days → 8 months	Study the feasibility of quantum implementation relative to the customer's use cases



Center for Excellence in

Performance Programming



Center for

ATOS

The Atos QLM User Club

Building on existing synergies around the Atos QLM







started **Collaborating** early on Quantum Computing-related research topics

&

They co-signed a QLM-based research article:

Function Maximization with Dynamic Quantum Search

Charles Moussa^{1,2[0000-0002-5387-564X]} and Henri Calandra³,

and Travis S. Humble *2[0000-0002-9449-0498]

¹ TOTAL American Services Inc., Houston, Texas USA
 ² Oak Ridge National Laboratory, Oak Ridge, Tennessee USA
 ³ TOTAL SA, Courbevoie, France





The Atos QLM User Club

Launched in December 2019



Join the Atos QLM user community

- Get the latest updates on the Atos Quantum program
- Meet other Atos QLM users and share tips
- Provide Atos feedback on the features and build the future of the Atos QLM
- Explore contributions to the myQLM open source project

Henri CALANDRA & Travis HUMBLE TOTAL CALANDRA & Travis HUMBLE Presidents of the Atos QLM User Club

Will send the invitations for user group meetings Will be the voice of users

> Andy GRANT **AtoS**

Leader of the Atos QLM User Club Will organize user group meetings Will be the link between users and the Atos organization







Atos QLM: enabling research since 2017





Reuse method for quantum circuit synthesis – AMMCS 2017 Allouche C, Baboulin M, Goubault de Brugière T, Valiron B



Quantum classification of the MNIST dataset via Slow Feature Analysis – Phys Rev A 2020 Kerenidis I, Luongo A



Electron-Phonon Systems on a Universal Quantum Computer – Phys Rev Lett 2018 A. Macridin, P. Spentzouris, J. Amundson, and R. Harnik



Digital quantum computation of fermion-boson interacting systems – Phys Rev A 2018 A. Macridin, P. Spentzouris, J. Amundson, and R. Harnik



q-means: A quantum algorithm for unsupervised machine learning – *NIPS* 2019

Kerenidis I, Landman J, Luongo A, Prakash A



Synthesizing Quantum Circuits via Numerical Optimization – ICCS 2019 Goubault de Brugière T, Baboulin M, Valiron B, Allouche C



Atos QLM: enabling research since 2017





Function Maximization with Dynamic Quantum Search – QTOP 2019 C. Moussa, H. Calandra, and T. S. Humble



Practical implementation of a quantum backtracking algorithm – Sofsem 2020 S. Martiel, M. Remaud



Methods for Classically Simulating Noisy Networked Quantum Architectures – QST 2019 I. Vankov, D. Mills, P. Wallden, and E. Kashefi



To quantum or not to quantum: towards algorithm selection in near-term quantum optimization – arXiv 2001.08271 C. Moussa, H. Calandra, and V. Dunjko



Quantum circuits synthesis using Householder transformations – CPC 2020 T. Goubault de Brugière, M. Baboulin, B. Valiron, and C. Allouche



Running large quantum circuits on small quantum computers – *ISVLSI* 2020

F.-M. Le Régent, T. Ayral, Z. H. Saleem, Y. Alexeev, and M. Suchara



Assessing the potential of Rydberg atoms for adiabatic quantum computing of an NP-hard problem— arXiv 2006.11190 B. Marchand, F. Serret, and T. Ayral





Proof of Concept in the pharmaceutical industry

Demonstrate that Quantum can either tackle problems that traditional computing cannot solve or prove that it is exponentially faster

Goal: evaluate the use of Quantum Computing in research and analysis of human disease patterns



DIGITAL LEADER AWARD 2019 GEWINNER KATEGORIE I SOCIETY BAYER & RWTH AACHEN MIT ATOS FÜR GEMEINSAME KOOPERATION ZUR BESCHLEUNIGUNG DER MEDIZINISCHEN FORSCHUNG MIT QUANTUM COMPUTING

BAYER & RWTH WITH ATOS FOR JOINT COOPERATION TO ACCELERATE MEDICAL RESEARCH USING QUANTUM COMPUTING





Proof of Concept in the pharmaceutical industry



Project driver and evaluation

Propose and implement **quantum algorithm** corresponding to proposed problem

Atos

• Evaluate QC approach

RWITHAACHEN UNIVERSITY

- Agree on **problem translation** suited for quantum algorithm
- Compare classical machine learning algorithm with Atos quantum implementation

Atos



Study of disease propagation mechanisms

Observed morbidities Patient clustering depending on observed morbidities

Quantumaccelerated clustering Underlying relationship between morbidities

••••

 Development of new diagnostic methods
 Improved therapy of complex multifactorial diseases





Study of disease propagation mechanisms

- Targeting an algorithm suited for Noisy Intermediate-Scale Quantum (NISQ) devices
 - to be less sensitive to noise/quantum errors
 - to exploit near term quantum devices
- Since quantum speed-up is only expected for larger problems than current use cases, focus on the qualitative benefit of quantum algorithm approach
- Combinatorial optimization through the Quantum Approximate Optimization Algorithm (QAOA), hybrid classical-quantum algorithm





Hierarchical clustering approach





Hybrid classical-quantum approach

- Defining pre-processing of the data with medical data analysis expert (Aachen)
- Atos Quantum Learning Machine is crucial for studying parameters effects and get improved results





Variation of the minimum state probability in function of numbers of measurements for classical evaluation



QC – based clusters exhibit significantly (p<.01) **superior performance compared to classical clustering**



Groups used to estimate the evolution



2

3

Leads to groups of diseases with minimum correlation between groups

Results



of co-morbidities









Quantum Learning-as-a-Service

- 1. Work with STFC and Industry to **develop quantum algorithms** in a technology agnostic way
- 2. Develop a library of quantum algorithms
- 3. Training and knowledge transfer **workshops** on QLM using CEPP services
- 4. Provide access to the QLM
 - PaaS model
 - Quantum consulting
 - Expertise for quantum algorithm development

Already a successful initiative: many prospects and an ongoing PoC







Quantum Learning-as-a-Service

- \checkmark Bought a QLM38 in 2019
- ✓ Established a Quantum-Learningas-a-service (QLaaS) business around the QLM
- Have gathered major British industries interests



Hartree Centre & Science & Technology Facilities Council

"Quantum Algorithms for Aerospace Applications "The **Quantum Learning Machine** will provide a platform on which we can **develop new quantum algorithms** with potential impacts across our business. We have a long track-record of successful collaborations with the Hartree Centre and with the support of Atos we look forward to research that takes us in new and exciting directions."

Leigh Lapworth, Head of Computational Sciences – Rolls-Royce









Providing external research teams access to the Atos QLM

"Argonne [...] has an onpremise Atos QLM-35 quantum simulator, a stateof-the-art environment capable of simulating quantum algorithms using up to 35 qubits"

Fermilab



Digital quantum computation of fermionboson interacting systems – 2018 Macridin A, Spentzouris P, Amundson J, Harnik R



Electron-Phonon Systems on a Universal Quantum Computer – 2018 Macridin A, Spentzouris P, Amundson J, Harnik R







Our customers are our best promoters

"The Atos Quantum Learning Machine provides a unique platform for testing new quantum programming ideas"

Travis Humble, ORNL's Quantum Computing Institute Director





Thank you

Jan Wender jan.wender@atos.net

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