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Perspectives on Full Stack Quantum Software Development

Teratec Quantum Computing Initative, Paris

31 March 2022

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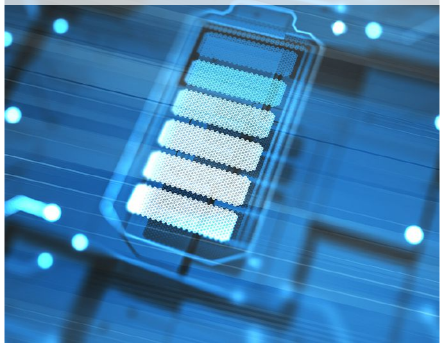
Quantum computing will impact a broad set of industries; the earliest applications are expected within R&D departments enabling the development of next gen products/services

Some examples of products and services which will be impacted by quantum computing

Battery Development



CO2 Storage Engineering

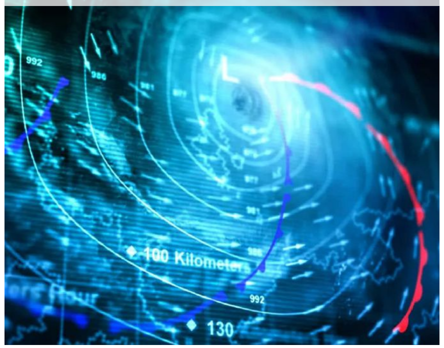
Smart Infra Management

Financial Trading

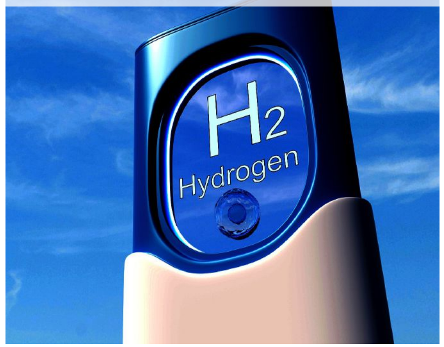
Anomaly Detection

Aerodynamics Optimization

Weather Forecasting



Fuel Cell Development



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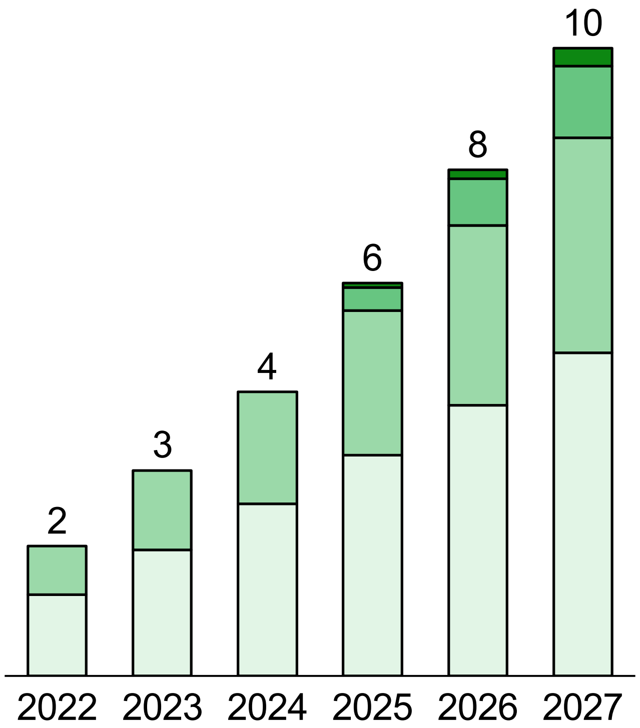
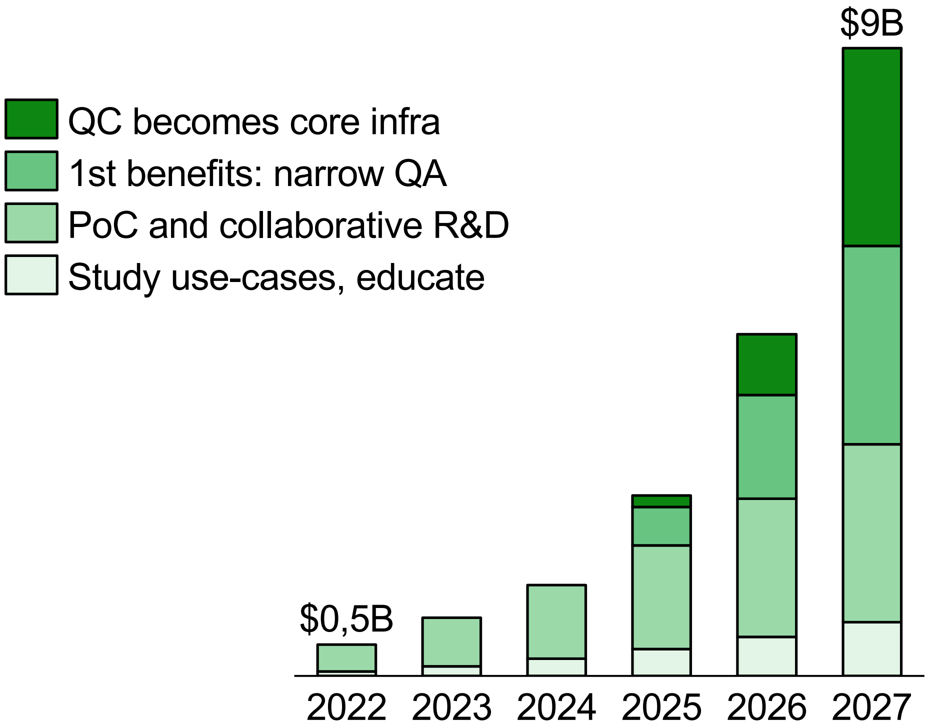
By 2027 ~10,000 companies are expected to engage with quantum and the adressable market will be in the order of $9B

Addressable[1] market (# end-users[2])



Addressable[1] market (revenues)



Source: OECD datasets, quantum market studies (Hyperion, BCG, McKinsey), Pasqal team analysis
1: excluding 'restricted' countries like China, Russia, Iran, ...
2: number of active quantum end-users (companies)

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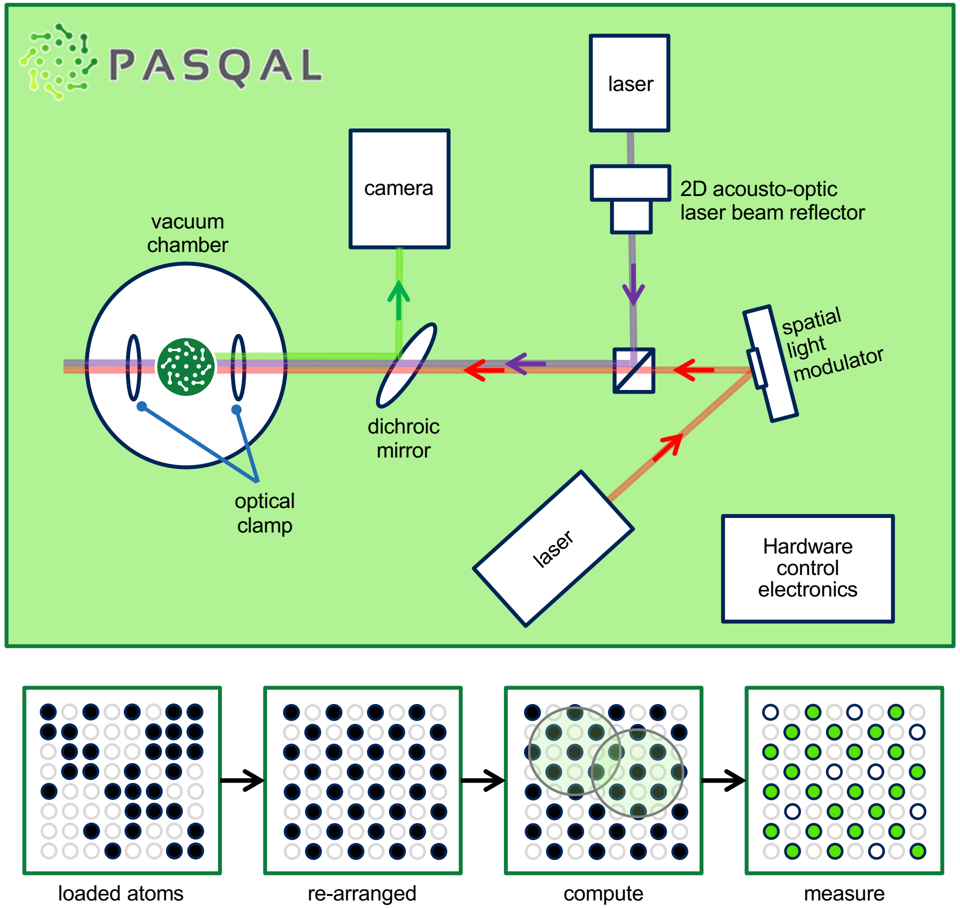
PASQAL delivers unique quantum processors based on neutral-atoms type qubits, with superior scaling, state-of-the-art performance and a high level of industrialization



Source: arXiv:2006.12326

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PASQAL is a full-stack quantum hardware company: our proposition comprises of hardware access, coding platforms, (turnkey) solutions, libraries and support

Pasqal product and service portfolio

Hardware

Generation 1	100/200-Q
Generation 2	512/1024-Q
Generation 3	2k/5k/10k-Q
...	
Emulators (NVIDIA)	20/50/200-Q

Services

Access	• Cloud access • On-premise install • Manage ecosystem
Platform	• Coding platform • Graphical User Interface • Software integrations[1]
Solutions	• Turnkey solutions per problem and sector • Chemistry, CFD, Finance
Libraries	• Quantum (ready) algorithms per mathematical problem • PDE, optimization, ML, ...
Support	• R&D support • Tech support • Maintenance

1: integrations with leading classical software packages (for instance the integration of our chemistry simulation platform with the software of schrodinger.com)

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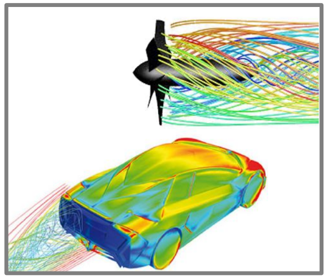
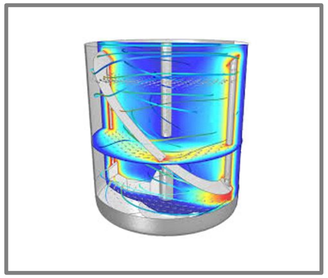
To explain the challenges of developing Q-solutions and the value of full-stack, I will use the story of how we became the world leader in quantum solvers for differential equations

Examples of industry relevant problems governed by differential equations

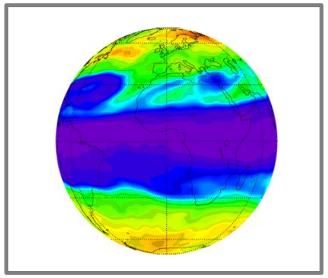
Mechanical Engineering



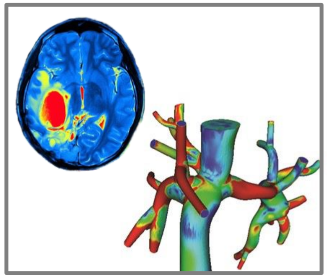
Chemical engineering



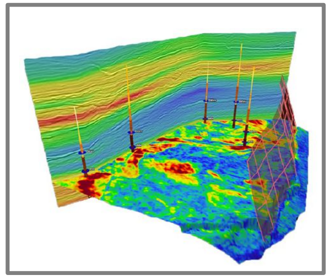
Metrology & Climate



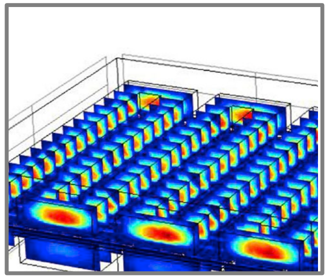
Biomedical



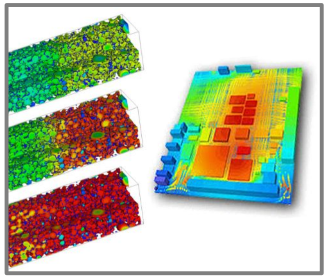
CO_2 storage & Seismic



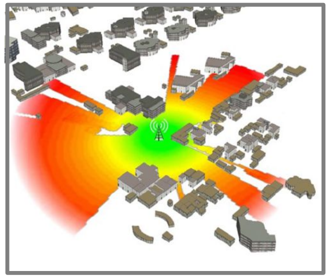
Fuel cell design



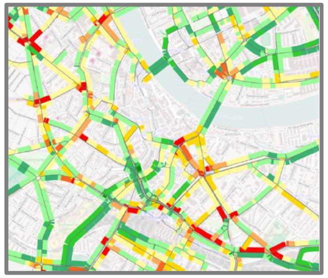
Batteries & Electronics



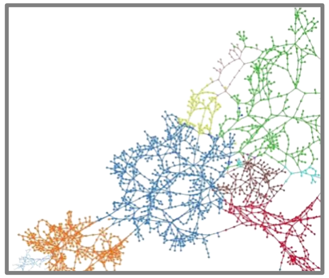
Wireless networks



Traffic flows



Power grid management



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1: DQC = differentiable quantum circuit (https://arxiv.org/abs/2011.10395)

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In 2019 different academic proposals had been made to solve PDE with quantum, however none of these proposals showed any promise for near-/mid-term quantum advantage

Deterministic classical solvers

- Examples include grid-based methods (finite elements) or discrete spectral methods
- Grid-based methods typically require a very large number of grid-points, while discrete spectral methods are more efficient, but struggle dealing with complex boundary conditions
- One downside of all deterministic methods is that they are not variational in nature, which means one may only hope to improve the result by increasing discretization resolution further

Variational classical solvers

- Neural network (NN) solvers are variational in nature: NN nodes are used to represent basis functions and are trained to represent a function that approximately satisfies a set of differential equations and boundaries
- These methods are slowly coming out of academia to industry, because they show good convergence for smooth functions, can deal with high degree of non-linearity[1] and can handle sharp gradients
- However, they typically require a large number of basis functions which increases computational complexity and their training time

Deterministic quantum solvers

- Many proposed quantum solvers typically employ some version the so-called HHL quantum subroutine, which can be used to solve linear systems efficiently
- However, HHL type algorithms are often only suitable for long-term fault-tolerant quantum processors
- Data is assumed to be encoded in ampltidues, posing a data input- and data output-problem
- HHL-type algorithms typically need to linearize any nonlinearity in the problem before solving it. Some recent exceptions exist [1][3]
- Derivatives are *estimated* using finite difference

Variational quantum solvers (before DQC[4])

- In 2019 a first proposal was made[2] for a variational quantum algorithm for solving nonlinear DEs
- However, similar to the deterministic quantum solvers, this proposal requires the efficient conversion of a large classical dataset into the amplitudes of a quantum wave function, which is not (yet) possible
- Additional downsides of this algorithm include inaccuracies due to numerical differentiation, and while in-principle it is NISQ-compatible, the circuit coherence requirements are unfeasible for near-term hardware

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1: e.g. arXiv:2011.06571; 2: e.g. arXiv:1907.09032; 3: e.g. arXiv:2011.03185; 4: DOI:10.1103/PhysRevA.103.052416

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We did not see that as an issue, but rather as a challenge and an opportunity; and to capture that opportunity we partnered with a brilliant academic from Exeter University

Oleksander Kyriienko

UNIVERSITY OF EXETER

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Solving nonlinear differential equations with differentiable quantum circuits

Oleksandr Kyriienko,[1,2] Annie E. Paine,[1,2] and Vincent E. Elfving[2]

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[2]*Qu & Co B.V., PO Box 75872, 1070 AW, Amsterdam, The Netherlands*

(Dated: May 20, 2021)

We propose a quantum algorithm to solve systems of nonlinear differential equations. Using a quantum feature map encoding, we define functions as expectation values of parametrized quantum circuits. We use automatic differentiation to represent function derivatives in an analytical form as differentiable quantum circuits (DQCs), thus avoiding inaccurate finite difference procedures for calculating gradients. We describe a hybrid quantum-classical workflow where DQCs are trained to satisfy differential equations and specified boundary conditions. As a particular example setting, we show how this approach can implement a spectral method for solving differential equations in a high-dimensional feature space. From a technical perspective, we design a Chebyshev quantum feature map that offers a powerful basis set of fitting polynomials and possesses rich expressivity. We simulate the algorithm to solve an instance of Navier-Stokes equations, and compute density, temperature and velocity profiles for the fluid flow in a convergent-divergent nozzle.

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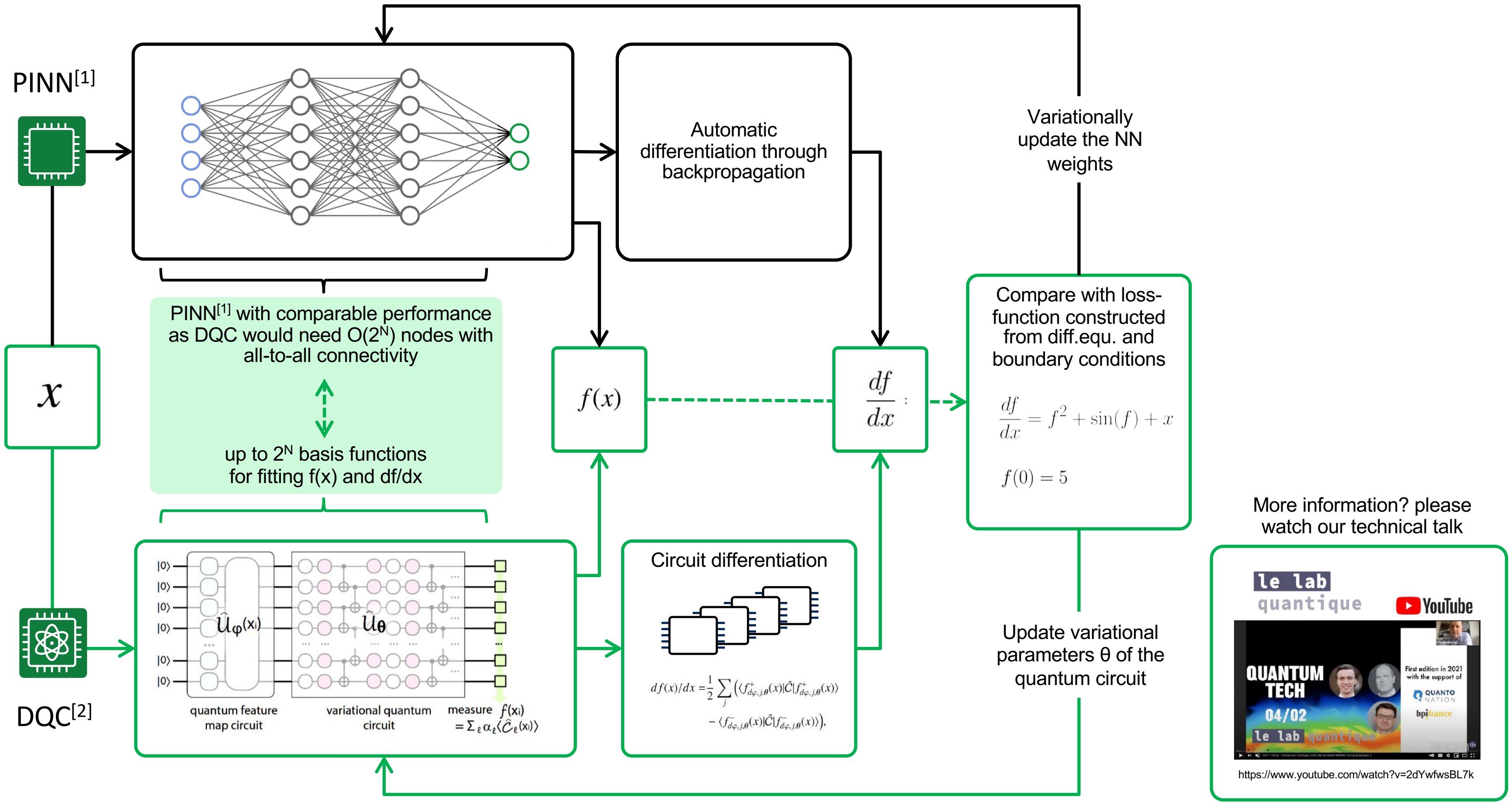
Inspired by classical neural network solvers[1] for differential equations (DE) we proposed the DQC[2] quantum method to solve DE on near-term quantum-processors



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1: PINN = Physics Informed Neural Network
2: DOI:10.1103/PhysRevA.103.052416 (note: patent filed by Qu&Co)
Note: Qu&Co has filed a patent on the DQC and QQM algorithms, please contact us if you are interested in obtaining a research license on one of these approaches

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Our (patented) DQC method[5] became the first (and so-far only) realistic option to solve complex differential equations with near-term quantum processors

Qu&Co's DQC[5] algorithm vs. its competitors	PASQAL	Lloyd et al.[1]	Jaksch et al.[2]	Childs et al.[3]	Gaitan et al.[4]
Advantage: promises superpolynomial quantum-advantage	✓	✓	✓	✓	✘
Input: deals efficiently with input data-sets and does not require QRAM	✓	✘	✘	✘	✘
Noise: suitable for current-day noisy intermediate scale quantum-processors	✓	✘	✓	✘	✘
Scaling: runtime expected feasible for industry relevant problem sizes	✓	✓	✘	✓	✓
Accuracy: uses direct differentiation rather than numerical differentation	✓	✘	✘	✘	✘
Non-linear: does not linearize the problem, but solves non-linearity directly	✓	✘	✓	✘	✓
Output: solution does not require exponential sampling from quantum-state	✓	✘	✘	✘	✘
Flexibility: compatible with wide variety of differential equation types	✓	✘	✘	✘	✘

1: e.g. arXiv:2011.06571; 2: e.g. arXiv:1907.09032; 3: e.g. arXiv:2011.03185; 4: e.g. doi:/10.1038/s41534-020-00291-0
5: DOI:10.1103/PhysRevA.103.052416

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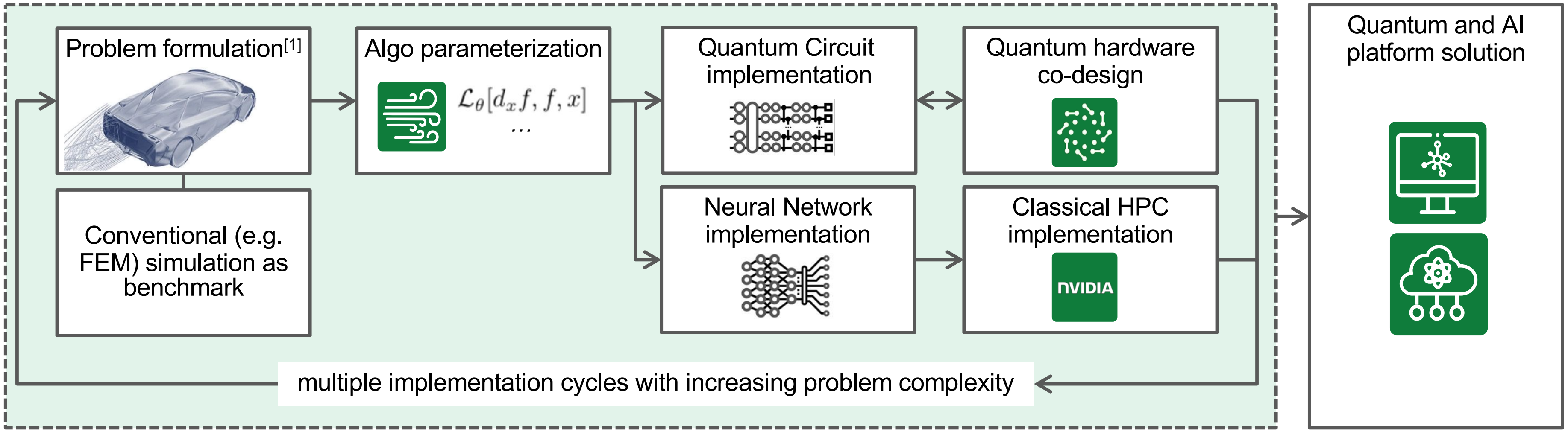
To optimally allign our quantum solutions with the needs of our clients, we typically co-develop our solutions through collaborative R&D with domain experts from our clients

Typical phasing of a Collaborative R&D (example fluid dynamics[2])



Domain expert (client) provides formulation of the governing equations plus initial/boundary conditions; alternatively it is sufficient to provide the structure of the differential equations and some experimental data

for one implementation cycle (one level of complexity), parameterization of the DQ and implementation and testing on NN and QC takes 6-12 person-months (depending on the complexity level of the problem)

co-design aimed at improved performance of the algorithm on a specific hardware set-up takes ~6 months for design and emulation and ~6 months for QPU implementation (incl. several iterations)

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1: formulation of the (structure of the) governing equations plus initial/boundary conditions (and some experimental data)
2: a similar iterative develop/test/benchmark approach would be applicable in case of other algorithms/use-cases

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So this is why, starting a couple of months after presenting the DQC method we started working with several clients on follow-on research related to multiphysics simulations

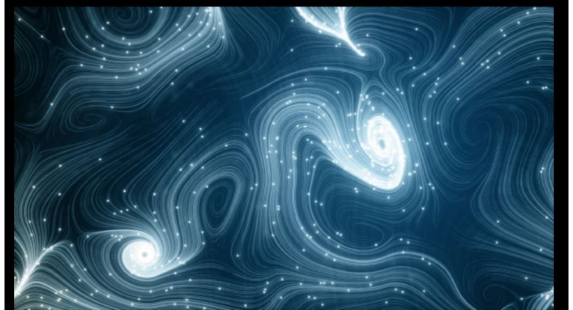
AIRBUS

Qu&Co to collaborate with Airbus on research, development and testing of quantum computational methods for flight physics simulations
08 June 2021

Amsterdam, 8 June 2021 - ***Qu&Co to collaborate with Airbus on research, development and testing of quantum computational methods for flight physics simulations***

LG

Qu&Co and LG Electronics announce multi-year research collaboration to develop and test quantum algorithms for multiphysics simulations.
15 April 2021



Amsterdam and Seoul, 15 April 2021 - *Qu&Co and LG Electronics announce multi-year research collaboration to develop and test quantum algorithms for multiphysics simulations.*

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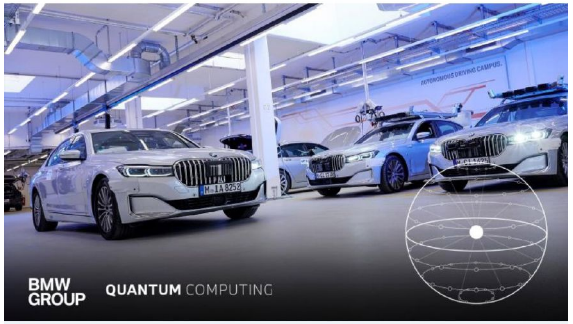
Worldwide Business Development and Go-To-Market Strategy for Quantum ...
3mo · Edited ·

Congratulations to the teams at Accenture, 1QBit-NTT Ltd.-NTT DATA, QC Ware Corp. and Qu & Co on winning the BMW Group quantum computing challenge announced today at the #q2b21 conference. ...see more



Winners announced in the BMW Group Quantum Computing Challenge | Amazon Web Services
aws.amazon.com · 4 min read

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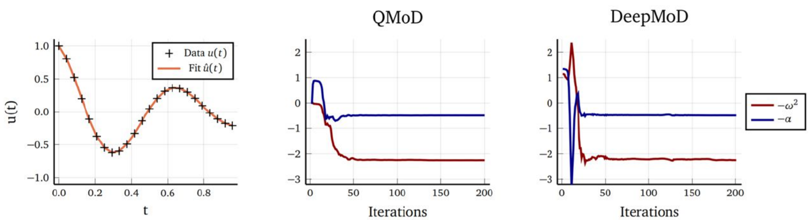
Good example of the value of co-development (client 'feedback') is the DQC extension to parameter inference and model discovery, which are much more realistic problem settings

Parameter inference

- Parameter inference aims to learn uncertain parameters of a parameterized Differential Equation (ODE/PDE/SDE) based on information gained from observations/data

$$\frac{d^2u_d}{dt_d^2} = -\omega^2 u_d - \alpha \frac{du_d}{dt_d}$$



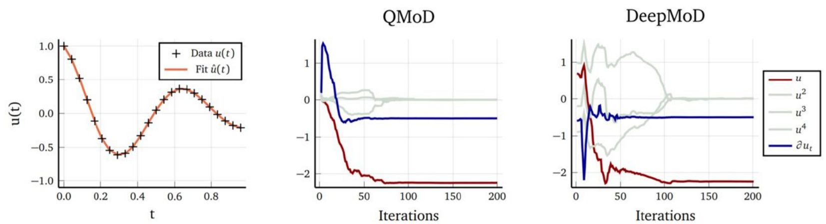
Equation	Model	Basis function: u	$\frac{du}{dt}$
$\frac{d^2u}{dt^2} = -\omega^2 t_c^2 u - \alpha t_c^2 \frac{du}{dt}$	QMoD	$\omega = \sqrt{2.249} = 1.499$	$\alpha = 0.500$
	DeepMoD	$\omega = \sqrt{2.247} = 1.498$	$\alpha = 0.500$
	Truth	$\omega = 1.5$	$\alpha = 0.5$

Model discovery

- Model Discovery aims to learn generalizations to given input datasets, using constrains based on differential equation models, including ODE/PDE/SDE

$$\frac{d^2u_d}{dt_d^2} = \boxed{?}$$

$$\varphi(u) = \left[t_c^2 u(t), \quad u_c t_c^2 u^2(t), \quad u_c^2 t_c^2 u^3(t), \quad u_c^3 t_c^2 u^4(t), \quad t_c \frac{du}{dt} \right]^T$$



Equation	Model	Basis function: u	u^2	u^3	u^4	$\frac{du}{dt}$
$\frac{d^2u}{dt^2} = -\omega^2 t_c^2 u - \alpha t_c^2 \frac{du}{dt}$	QMoD	$\omega = \sqrt{2.239} = 1.496$	$< 10^{-3}$	$< 10^{-3}$	$< 10^{-3}$	$\alpha = 0.497$
	DeepMoD	$\omega = \sqrt{2.242} = 1.498$	$< 10^{-3}$	$< 10^{-3}$	$< 10^{-3}$	$\alpha = 0.496$
	Truth	$\omega = 1.5$	0	0	0	$\alpha = 0.5$

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Source: arXiv:2111.06376; Note: PASQAL has filed a patent on the DQC and QMoD algorithms, please contact us if you are interested in obtaining a research license on one of these approaches

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After the merger between PASQAL and Qu&Co, our attention shifted to aligning software and hardware to find ways to reach the point of quantum advantage much faster

Source: press announcement of PASQAL + Qu&Co merger in January 2022

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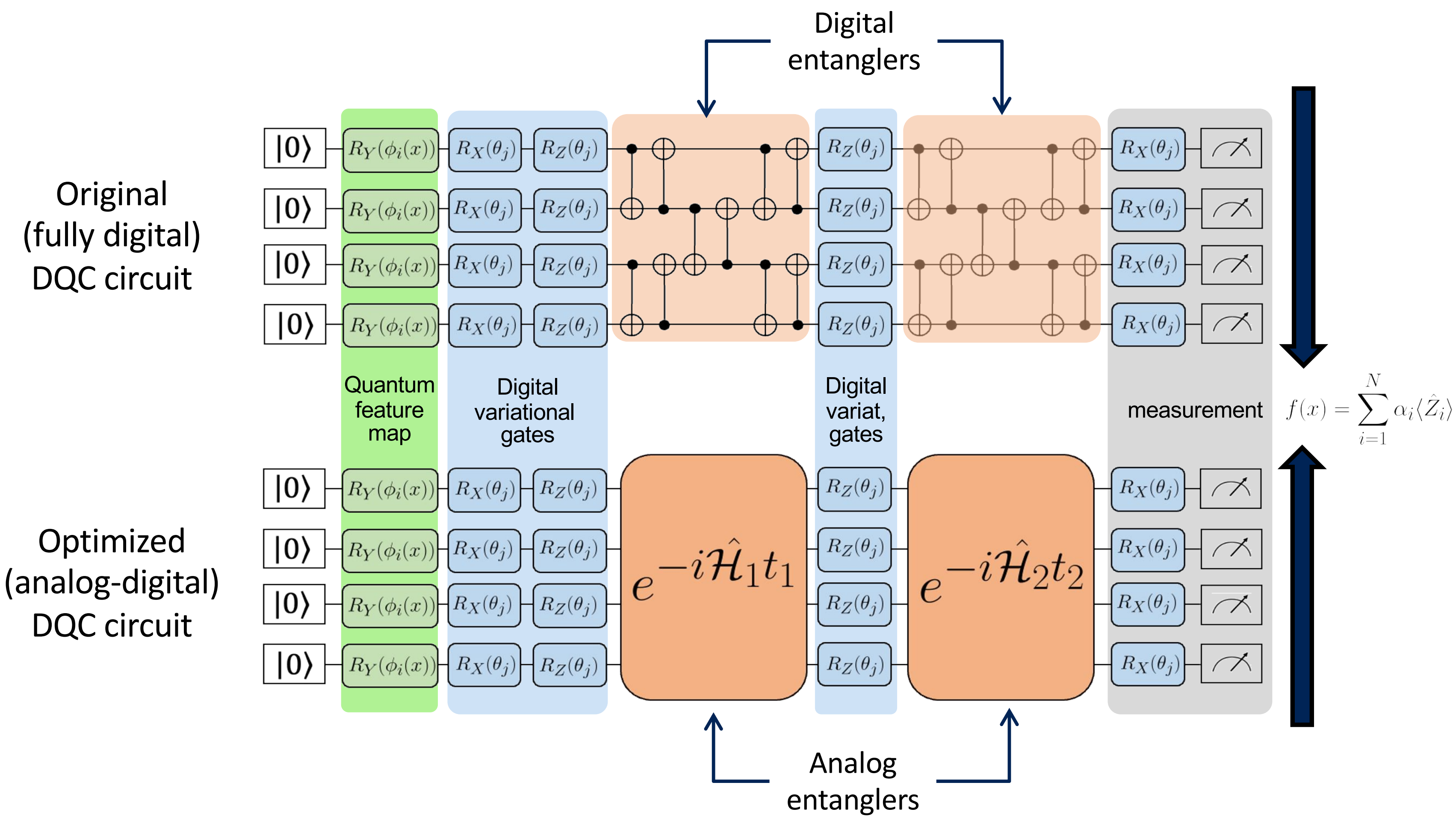
Good example of the value of combined hardware-software research is our latest patent: replacing digital by analog entanglers to make DQC much more efficient and noise-robust



Note: PASQAL has filed a patent on the DQC method and on its analog-digital equivalent, please contact us if you are interested in obtaining a research license on one of these approaches

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In conclusion: we believe that the key reason why PASQAL will succeed in realizing industry-relevant Q-advantage in the next few years is our full-stack approach

Neutral atoms **quantum processors** with unique capabilities (like analog-digital mode)

Work with leading academics to develop **unique and proprietary algos**

Applications **co-developed** with clients to ensure **industry relevance**

Core technology

Unique algorithms

Client involvement

Industrialized hardware

Hardware-software alignment

Software solutions

industrialized hardware, accesible through **cloud** or on-premise

Software-Hardware alignment to realize **quantum advantage** years sooner

Turnkey solutions and **integrations** with leading classical software to **drive adoption**

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