## A survey of quantum computing for PDEs

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### Research interests and collaborations

Quantum computing in aerospace engineering applications



### Research interests and collaborations

Quantum algorithms and benchmarks for NISQ devices



### This survey is based on ...

 A review of quantum algorithms for partial differential equations in fluid and structural mechanics
 G. Balducci, B. Chen, MM, and R. de Breuker

in preparation for the special issue: Quantum Computing Applications in Computational Engineering in Frontiers in Mechanical Engineering, 2022

- Quantum Algorithms for Solving Partial Differential Equations Report by A. Pesah, 2020
- about 50 articles and reports cited in the works above



**Guest Editors** 

Prof. Dr. Matthias Möller Dr. Carmen G. Almudever Prof. Dr. Sabre Kais

> **Deadline** 31 May 2022





Different quantum computing principles

 Discrete-variable quantum computing (DVQC): eigenstates of a discrete variable form the computational basis of a finite-dimensional Hilbert space

$$|\psi\rangle = \sum_{i=0}^{2^{n-1}} c_i |b_i\rangle, \qquad \sum_{i=0}^{2^{n-1}} |c_i|^2 = 1, \qquad \langle b_i |b_j\rangle = \delta_{ij}$$

 Continuous-variable quantum computing (CVQC): eigenstates of a continuous variable form the basis of an infinite-dimensional Hilbert space

$$|\psi\rangle = \int_{-\infty}^{\infty} c(x) |x\rangle dx$$
,  $\langle x'|x\rangle = \delta(x'-x)$ 

### DVQC: Gate-based universal quantum computers

Mathematical model

 $|\psi_{out}\rangle = U_m \cdot \dots \cdot U_1 |\psi_0\rangle$ 

 Hardware realizations with ~100 superconducting qubits, e.g., by IBM, Google, Rigetti, Intel, …



### DVQC: Gate-based universal quantum computers

Mathematical model

 $|\psi_{out}\rangle = U_m \cdot \ldots \cdot U_1 |\psi_0\rangle$ 

- Hardware realizations with ~100 superconducting qubits, e.g., by IBM, Google, Rigetti, Intel, …
- QTRL 4-5 / 9 (expected in 2035)



<u>https://www.fz-juelich.de/ias/jsc/EN/Research/ModellingSimulation/QIP/QTRL/\_node.html</u> Copyright: Kristel Michielsen, Thomas Lippert – Forschungszentum Jülich

## **DVQC: Quantum annealing**

Mathematical model

 $|\psi_0\rangle = \underset{|\psi\rangle}{\arg\min} \langle \psi | H | \psi \rangle$ 

• Path of Hamiltonians for  $t \in [0, T]$  $H(t) = (1 - f(t))H_I + f(t)H_P$ 

with easy-to-compute ground state  $|\psi_0\rangle$  for the initial Hamiltonian  $H_I$ 

• Ground-state evolution  

$$H(t)|\psi(t)\rangle = -i\frac{d}{dt}|\psi(t)\rangle$$

$$E_{I}$$

$$E_{0}$$

$$E_{0}$$

# **DVQC: Quantum annealing**

Mathematical model

 $|\psi_0\rangle = \underset{|\psi\rangle}{\arg\min} \langle \psi | H | \psi \rangle$ 

- Hardware realizations by D-Wave with up to 5000 qubits
- **OTRL** QCs (QAs) exceed power of QTRL9 classical computers Quantum Technology **Readiness Levels** Scalable version of QC (QA) QTRL8 completed and qualified in test describing the maturity of Quantum Computing Prototype QC (QA) built solving Technology QTRL7 small but user-relevant problems Components integrated in small QTRL6 quantum processor w/ error correction Components integrated in small QTRL5 quantum processor w/o error correction Multi-qubit system fabricated; classical devices QTRL4 for qubit manipulation developed QTRL3 Imperfect physical qubits fabricated Applications / technologically relevant QTRL2 algorithms formulated Theoretical framework for quantum computation QTRL1 (annealing) formulated

• QTRL 8-9

<u>https://www.fz-juelich.de/ias/jsc/EN/Research/ModellingSimulation/QIP/QTRL/\_node.html</u> Copyright: Kristel Michielsen, Thomas Lippert – Forschungszentum Jülich

# CVQC

- Hardware realizations by Xanadu (photonic), concepts for trapped ions [Maslennikov et al. 2019]
- Comprehensive introduction by <u>S.Buck et al.</u> (2021)
- Quantum search by <u>A.K. Pati et al.</u>
   (2020) and <u>D. Su et al.</u> (2018)



## Different interpretations of the word "quantum algorithm"

- Theoretical analysis of an algorithm <u>HHL paper</u> (2008) claims exponential speedup for "solving" Ax=b under conditions on the matrix A
- Application-specific theoretical analysis <u>Montanaro et al.</u> (2016) shows that no exponential speedup for P<sub>k</sub>-FEM can be achieved for fixed dimension
- Application-specific circuit + cost estimation <u>Cao et al.</u> (2013) present textbook quantum circuits for solving Poisson's equation with FDM
- Execution of application-specific circuit on QVM <u>Wang et al.</u> (2020) demonstrate a fast Poisson solver on Sunway TaihuLight (yes, it works <sup>(2)</sup>)
- Execution of application-specific circuit on QPU <u>Morrell et al.</u> (2021) show that solving a 2x2 system on IBM-Q fails due to noise (doesn't work Section 2)

### What should we aim for?



NISQ future QCs

## Quantum algorithms for solving PDEs



Inspired by A. Pesah's report "Quantum Algorithms for Solving Partial Differential Equations" 2020.

## Quantum algorithms for solving PDEs



Inspired by A. Pesah's report "Quantum Algorithms for Solving Partial Differential Equations" 2020.

**Given**: 
$$\dot{x} = Ax$$
,  $x(t_0) = x_0$ 

Von Neumann measurement [von Neumann 1932, Childs et al. 2002]

$$\begin{pmatrix} 0 & iA^{\dagger} \\ -iA & 0 \end{pmatrix} \Rightarrow H = iA^{\dagger} \otimes |0\rangle_{P} \langle 1| - iA \otimes |1\rangle_{P} \langle 0|$$

Schrödinger's equation

 $|\psi_t| = -iH\psi$ 

State after Hamiltonian simulation [Leyton, Osborne 2008]

$$|\Psi\rangle = e^{iHt}|\psi\rangle|0\rangle_{P} = \sum_{k=0}^{\infty} \frac{(iHt)^{k}}{k!}|\psi\rangle|0\rangle_{P} = |\psi\rangle|0\rangle_{P} + tA|\psi\rangle|1\rangle_{P} - \cdots$$

- Post-selection on "1" after measurement on the ancillary qubit
- Procedure from [HHL 2008] to correct for first-order truncation
- **Caveat**: success probability  $\frac{1}{2}t^2$  (roughly  $16/t^2$  'fresh' states  $|\psi\rangle$  needed)

**Given**: 
$$\dot{x} = Ax$$
,  $x(t_0) = x_0$ 

- Matrix decomposition  $A = A_H + A_A$
- Baker–Campbell–Hausdorff formula

$$e^{iAt} = e^{iA_H t} \cdot e^{iA_A t}, \quad \text{if} [A_H, A_A] = 0$$

• Hamiltonian simulation of  $A_H$  and  $A_A$  via unitary dilation of  $\hat{O} = e^{iA_A t}$ 

$$\begin{pmatrix} \hat{O} & \sqrt{1-\hat{O}^2} \\ \sqrt{1-\hat{O}^2} & -\hat{O} \end{pmatrix} |\psi\rangle|0\rangle = \hat{O}|\psi\rangle|0\rangle + \sqrt{1-\hat{O}^2}|\psi\rangle|1\rangle$$

Black-Scholes equation [Gonzalez-Conde et al. 2021]

$$f_t = af + bf_x - cf_{xx} = (ib(-i\partial_x) + aI + c(-i\partial_x)^2)f$$

• **Caveat**: exponential scaling in t if  $[A_H, A_A] \neq 0$  [Berry 2014]

**Given**: 
$$\dot{x} = Ax$$
,  $x(t_0) = x_0$ 



Derivative of Schrödinger's equation [Costa et al. 2019]

$$\psi_{tt} = -H^2 \psi$$

Hermitian matrix

$$H = \begin{pmatrix} 0 & B \\ B^{\dagger} & 0 \end{pmatrix} \quad \Rightarrow \quad H^2 = \begin{pmatrix} BB^{\dagger} & 0 \\ 0 & B^{\dagger}B \end{pmatrix}$$

Wave equation

$$\partial_{tt} f = -\Delta f \approx A f \Rightarrow \text{ find } A = B B^{\dagger}$$

• **Example**: graph Laplacian

$$B_{ev} = \begin{cases} 1 & e = (v, w), v < w \\ -1 & e = (v, w), v > w \end{cases} \Rightarrow B_{ev} = \begin{pmatrix} 1 & -1 & 0 & 0 \\ 0 & \ddots & \ddots & 0 \\ 0 & 0 & 1 & -1 \end{pmatrix}$$

## Quantum algorithms for solving PDEs



Inspired by A. Pesah's report "Quantum Algorithms for Solving Partial Differential Equations" 2020.

## Hamiltonian simulation (approach #1)

- **Given**: Hamiltonian H ( $2^n \times 2^n$  Hermitian on n qubits), time t, and error  $\epsilon$
- **Goal**: find an algorithm to approximate U such that  $||U e^{iHt}|| \le \epsilon$
- Decomposition into local Hamiltonians [Lloved 1996]

$$H = \sum_{\ell=1}^{L} H_{\ell}, \qquad \left(e^{A\frac{t}{r}}e^{B\frac{t}{r}}\right)^{r} = e^{(A+B)t + \frac{1}{2}[A,B]\frac{t^{2}}{r} + \mathcal{O}\left(\frac{t^{3}}{r^{2}}\right)}$$

Hamiltonian simulation

 $|\psi\rangle = e^{-iHt}|\psi_0\rangle$ 

Suzuki-Trotter decomposition [Suzuki 1991]

$$e^{-iHt} \approx \left(\prod_{\ell=1}^{L} e^{-iH_{\ell}\frac{t}{r}}\right)^{r}, \qquad r \gg 1$$

## Hamiltonian simulation (approach #2)

- **Given**: Hamiltonian H ( $2^n \times 2^n$  Hermitian on n qubits), time t, and error  $\epsilon$
- **Goal**: find an algorithm to approximate U such that  $||U e^{iHt}|| \le \epsilon$
- Truncated Taylor expansion

$$e^{iHt} = I - iHt - \frac{1}{2}H^2t^2 + \frac{i}{6}H^3t^3 + \cdots$$

Linear combination of unitary operators [Berry et al. 2015]

$$H = \sum_{\ell} \alpha_{\ell} H_{\ell} \quad \Rightarrow \quad H^n = \sum_{\ell_1, \dots, \ell_n} \alpha_{\ell_1} \dots \alpha_{\ell_k} H_{\ell_1} \dots H_{\ell_n}$$

# Hamiltonian simulation (complexity)



Hamiltonian simulation

 $|\psi\rangle = e^{-iHt} |\psi_0\rangle$ 

[1] <u>Childs</u> 2017, [2] <u>Kothari</u> 2017, [3] <u>Berry</u> 2015, [4] <u>Berry</u> 2015, [5] <u>Low</u> 2017

### Leyton and Osborne 2008

First-order systems of the form

$$\dot{\boldsymbol{x}}(t) = \begin{pmatrix} f_1(\boldsymbol{x}) \\ \vdots \\ f_N(\boldsymbol{x}) \end{pmatrix}, \qquad f_j(\boldsymbol{x}) = \sum_{k,l=1}^N a_{kl}^{(j)} x_k x_l, \qquad \sum_{j=1}^N |x_j|^2 = 1$$

• **Example**: Orszag-McLaughlin dynamical system

$$\dot{x}_j = x_{j+1}x_{j+2} + x_{j-1}x_{j-2} - 2x_{j+1}x_{j-1}, \qquad j = 1, \dots N$$

- $|a_{ij}| = O(1)$  and *A* is *s*-sparse, i.e., each  $f_j$  involves at most s/2 monomials and each variable  $x_j$  appears in at most s/2 polynomials  $f_j$
- Lipschitz constant:  $||F(x y)|| \le O(1) \cdot ||x y||$  in ball  $||x|| \le 1$ ,  $||y|| \le 1$
- We assume that the initial state can be prepared efficiently

### Leyton and Osborne 2008

Schrödinger's equation  $\psi_t = -iH\psi$ 

Hamiltonian simulation  
$$|\psi\rangle = e^{-iHt} |\psi_0\rangle$$
 M

Explicit Euler method

$$|\psi'\rangle = e^{iH\Delta t}|\psi\rangle|0\rangle \Rightarrow |\psi(t+\Delta t)\rangle = |\psi(t)\rangle + \Delta tA|\psi(t)\rangle$$

• Success probability of a single step  $\frac{1}{2}\Delta t^2$ ; 16/ $\Delta t^2$  'fresh'  $|\psi\rangle$  needed

• Temporal scaling 
$$\left(\frac{16}{\Delta t^2}\right)^m$$
, spatial scaling  $\left(\frac{16}{\Delta t^2}\right)^m \log N$  for  $m$  steps

• Hamiltonian simulation must be performed with error  $\delta < (3\mathcal{O}(1))^{-m}$  to ensure that the *m*-th iterate is exponentially close to the desired state



# QuDiffEq

- Quantum algorithms for linear and nonlinear differential equations
- Papers with Code
  - [Leyton, Osborne 2008]
  - [Berry et al. 2010]
  - [Xin et al. 2018]



$$\begin{aligned} x_1 &= x_2 - 3x_1^2 \\ \dot{x}_2 &= -x_2^2 - x_1 x_2 \end{aligned}$$

# Gonzalez-Conde et al. 2022



#### Black-Scholes equation for European put options



Precision comparable to classical methods with 10 qubits and 94 entangling gates on fault-tolerant QC. Complexity O(poly n). Success probability 0.6.





#### Wave equations



## Quantum algorithms for solving PDEs



Inspired by A. Pesah's report "Quantum Algorithms for Solving Partial Differential Equations" 2020.

### **Given**: $\dot{x} = Ax + b$ , $x(t_0) = x_0$

Unroll Euler method in time

$$\begin{pmatrix} I & 0 & 0 & 0\\ -(I + \Delta tA) & I & 0 & 0\\ \vdots & \ddots & \ddots & \ddots & \ddots\\ 0 & 0 & -(I + \Delta tA) & I \end{pmatrix} \begin{pmatrix} x_0 \\ x_1 \\ \vdots \\ x_m \end{pmatrix} = \begin{pmatrix} x_{in} \\ \Delta tb \\ \vdots \\ \Delta tb \end{pmatrix}$$

• Apply HHL-type algorithm to obtain the solution at all times

$$|x\rangle = \sum_{j=0}^{m} |t_j\rangle |x_j\rangle$$

 Application and analysis for the heat equation yields poor scaling with precision [Linden et al. 2020] even with the improved variant of the QLSA 'solver' [Berry et al. 2017]

linear system  
$$Ax = b$$

 $\mathcal{O}(\text{poly}(1/\epsilon))$ 

**Solution**: 
$$x(t) = e^{At}x_0 + (e^{At} - I)A^{-1}k$$

linear system Ax = b

 $O(\operatorname{poly} \log(1/\epsilon))$ 

Truncated exponentials

$$e^{z} \approx \sum_{j=0}^{k} \frac{z^{j}}{j!}, \qquad (e^{z} - 1)z^{-1} \approx \sum_{j=1}^{k} \frac{z^{j-1}}{j!}$$

• Linear system [Berry et al. 2017]  $C_{m,k,p}(\Delta tA)|x\rangle = |0\rangle|x_0\rangle + \Delta t \sum_{j=0}^{m-1} |j(k+1)+1\rangle|b\rangle$ 



**Given**: 
$$\dot{x} = A(t)x + b(t)$$
,  $x(t_0) = x_0$ 

linear system Ax = b $\mathcal{O}(\text{poly } \log(1/\epsilon))$ 

Chebyshev pseudo-spectral approximation

$$x(t) = \sum_{k=0}^{n} c_k T_k(t) \quad \Rightarrow \quad \dot{x}(t_l) = A(t_l) x(t_l) + b(t_l), \qquad t_l = \cos\frac{l\pi}{n}$$

Rescaled differential equation (<u>Childs and Liu</u> 2020)

$$\dot{x}(\gamma(t)) = -\frac{t^{n+1}-t^n}{2} [A(\gamma(t))x(\gamma(t)) + b(\gamma(t))],$$

where  $\gamma: [t^n, t^{n+1}] \mapsto [-1, 1]$  is defined as  $\gamma: t \mapsto 1 - \frac{2(t-t^n)}{t^{n+1}-t^n}$ 

• Combined with the  $C_{m,k,p}$ -approach from [Berry et al. 2017] this extends their work to ODEs with time-dependent coefficient matrices and vectors

## Quantum algorithms for solving PDEs



Inspired by A. Pesah's report "Quantum Algorithms for Solving Partial Differential Equations" 2020.

# **Quantum linear 'solver' algorithm**

- **Problem**:  $a = \langle x^{\dagger} | M | x \rangle$  s.t.  $A | x \rangle = | b \rangle$
- Original HHL algorithm [Harrow et al. 2008]
- Improved versions of HHL
  - VTAA [<u>Ambainis</u> 2010]
  - AQC [Subasi et al. 2019]
  - AQC [An and Lin 2019]
- QLSA w/o phase estimation [Childs et al. 2017]
- Dense matrices [Wossnig et al. 2018]

QLSA

 $\mathcal{O}(s\sqrt{\kappa}N\log 1/\epsilon)$ 

 $\mathcal{O}(s^2\kappa^2\log(N)/\epsilon)$ 



### **Original HHL algorithm**



Figure 1 from [Morrell and Wong 2021]

#### QLSA

# State preparation: $|\psi_{init}\rangle = U_{prep}|0\rangle$

General states cannot be prepared efficiently, not even approximated

 $N \text{ grid points} \Rightarrow n = \log N \text{ qubits} \Rightarrow |U_{prep}| = \mathcal{O}(N)$ 

uniformly controlled rotations [Mottonen et al. 2004] using  $O(2^n)$  gates

- Certain states of the form  $|\psi\rangle = \sum_i \sqrt{p_i} |i\rangle$  can be prepared efficiently, e.g., using quantum GANs [Zoufal et al. 2019] using O(poly n) gates
- Reducing time complexity by adding ancillary qubits
  - Low-depth approach:  $O(n^2)$  using  $O(2^{n^2})$  ancillae [Zhang et al. 2021]
  - s-sparse states:  $\Theta(\log ns)$  using  $O(ns \log s)$  ancillae [Zhang et al. 2022]

### Does any of this work in practice?

- QLSA for Ax = b
  - HW-realization for 2×2 matrix [Cai et al. 2013], [Barz et al. 2013], [Pan et al. 2013], and 8×8 matrix [Wen et al. 2018]
  - 2×2, 4×4, and 8×8 on IBM, Rigetti, IonQ [Cornelissen et al. 2021]
  - Other authors report that "due to imperfection and noise in a real quantum computer [ibmq\_santiago], the hardware execution of the same circuit does not give satisfactory results" [Morrell and Wong 2021]
- Okay, so no chance for solving ODEs / transient PDEs with QC in near term
- How about solving Poisson's equation discretized by FDM / FEM?



### versus

 $\mathcal{O}(\operatorname{poly}\log(1/\epsilon))$ 

- General state preparation is exponentially expensive, i.e., O(N)
  - Polynomials/functions with local support can be prepared efficiently
- $\kappa = O(N^{d/2})$  in standard FEM  $\Rightarrow$  no exponential speedup
  - Quantum-SPAI precondioner, i.e. PAx = Pb [Clader et al. 2013]
    - $\mathcal{O}(s^2)$  queries to *PA*-oracle;  $\mathcal{O}(s^3)$  runtime

• 
$$\kappa = \mathcal{O}(1)$$
 or  $\kappa = \mathcal{O}(\log N)$ 

- *s* = ?
- $1/\epsilon = O(N)$  in most discretization schemes  $\Rightarrow$  no exponential speedup

# No exponential speedup for elliptic problems for fixed d

algorithm	w/o preconditioner	optimal preconditioner
Conjugate Gradients	$\tilde{\mathcal{O}}\left(\left(\frac{ x _2}{\epsilon}\right)^{\frac{d+1}{2}}\right)$	$\tilde{\mathcal{O}}\left(\left(\frac{ x _2}{\epsilon}\right)^{\frac{d}{2}}\right)$
Childs et al. 2017	$\tilde{\mathcal{O}}\left(\left(\frac{\ x\ _1 \ x\ _2^2}{\epsilon^3}\right)\right)$	$\tilde{\mathcal{O}}\left(\frac{\ x\ _1}{\epsilon}\right)$

[Montanaro, Pallister 2016]:

 $\tilde{\mathcal{O}}(h(n)) = \mathcal{O}(h(n)\log^k n)$ 

- State preparation + q-SPAI preconditioner + PA-oracle in  $O(\log(1/\epsilon))$
- To distinguish between two  $\epsilon$ -close states requires  $O(\sqrt{1/\epsilon})$  queries

## Quantum algorithms for solving PDEs



Inspired by A. Pesah's report "Quantum Algorithms for Solving Partial Differential Equations" 2020.

## Quantum algorithms for solving PDEs



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### Variational quantum algorithms

### [Cerezo et al. 2020]



## Variational quantum linear solver [Bravo-Prieto et al. 2020]

Efficient(!) decomposition into unitaries + efficient(!) state preparation

$$A = \sum_{k} \alpha_{k} A_{k} , \qquad |b\rangle = B |0\rangle$$

Cost function

$$\begin{array}{ll} |\Phi\rangle \perp |b\rangle &\Rightarrow & \mathcal{C}(\Theta) \text{ large} \\ |\Phi\rangle \parallel |b\rangle &\Rightarrow & \mathcal{C}(\Theta) \text{ small} \end{array} \right\} \quad |\Phi\rangle = A |\psi(\Theta)\rangle$$

Ground-state Hamiltonian

$$H = A^{\dagger} (\mathbb{I} - |b\rangle \langle b|) A$$

Cost function

$$\mathcal{C}(\Theta) = \langle \psi(\Theta) | H | \psi(\Theta) \rangle = \langle \Phi | \Phi \rangle - \langle \Phi | b \rangle \langle b | \Phi \rangle$$

### Variational quantum linear solver [Bravo-Prieto et al. 2020]

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Cost function

$$\begin{array}{ll} |\Phi\rangle \perp |b\rangle &\Rightarrow & \mathcal{C}(\Theta) \text{ large} \\ |\Phi\rangle \parallel |b\rangle &\Rightarrow & \mathcal{C}(\Theta) \text{ small} \end{array} \right\} \quad |\Phi\rangle = A |\psi(\Theta)\rangle$$

Ground-state Hamiltonian

$$H = A^{\dagger} (\mathbb{I} - |b\rangle \langle b|) A$$

Normalized cost function

$$\hat{C}(\Theta) = 1 - \frac{|\langle \Phi | b \rangle|^2}{\langle \Phi | \Phi \rangle}$$

Variational quantum linear solver [Bravo-Prieto et al. 2020]

Towards an implementable cost function

$$\langle \Phi | \Phi \rangle = \sum_{k,l} c_k^* c_l \langle 0 | V^{\dagger}(\Theta) A_k^{\dagger} A_l V(\Theta) | 0 \rangle$$
  
 
$$\langle \Phi | b \rangle = \sum_{k,l} c_k^* c_l \langle 0 | B^{\dagger} A_l V(\Theta) | 0 \rangle \langle 0 | B^{\dagger} A_k V(\Theta) | 0 \rangle$$

- [Liu et al. 2021]:
  - Decomposition of the *d*-dimensional Poisson matrix (FDM) into O(log N) terms consisting of identities and ½ spin operators |1>(0| and |0>(1|
  - Difficulties to convergence the classical optimizer for 50-100 qubits
  - Fully connected measurement circuits



# Quantum algorithms for solving PDEs



Inspired by A. Pesah's report "Quantum Algorithms for Solving Partial Differential Equations" 2020.

### Summary and recommendations

- ODEs / transient PDEs (long term)
  - 'smart' time integrators that reduce the condition number (QLSA)
- Steady-state PDEs (near to mid term)
  - 'smart' discretization that reduce the condition number (QLSA)
  - problems that admit efficient matrix decompositions (V-QLSA)
- Service to QC
  - improve VQAs using classical CSE techniques