## A survey of quantum computing for PDEs

Matthias Möller

Delft University of Technology
Delft Institute of Applied Mathematics

## 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

## Different quantum computing principles

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

$$
|\psi\rangle=\sum_{i=0}^{2^{n}-1} c_{i}\left|b_{i}\right\rangle, \quad \sum_{i=0}^{2^{n}-1}\left|c_{i}\right|^{2}=1, \quad\left\langle b_{i} \mid b_{j}\right\rangle=\delta_{i j}
$$

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

$$
|\psi\rangle=\int_{-\infty}^{\infty} c(x)|x\rangle d x, \quad\left\langle x^{\prime} \mid x\right\rangle=\delta\left(x^{\prime}-x\right)
$$

## DVQC: Gate-based universal quantum computers

- Mathematical model

$$
\left|\psi_{\text {out }}\right\rangle=U_{m} \cdot \ldots \cdot U_{1}\left|\psi_{0}\right\rangle
$$

- Hardware realizations with $\sim 100$ superconducting qubits, e.g., by IBM, Google, Rigetti, Intel, ...



## DVQC: Gate-based universal quantum computers

- Mathematical model

$$
\left|\psi_{\text {out }}\right\rangle=U_{m} \cdot \ldots \cdot U_{1}\left|\psi_{0}\right\rangle
$$

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

https://www.fz-juelich.de/ias/jsc/EN/Research/ModellingSimulation/QIP/QTRL/ node.html Copyright: Kristel Michielsen, Thomas Lippert - Forschungszentum Jülich


## DVQC: Quantum annealing

- Mathematical model

$$
\left|\psi_{0}\right\rangle=\underset{|\psi\rangle}{\arg \min }\langle\psi| H|\psi\rangle
$$

- 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 $\left|\psi_{0}\right\rangle$ for the initial Hamiltonian $H_{I}$
- Ground-state evolution



## DVQC: Quantum annealing

- Mathematical model

$$
\left|\psi_{0}\right\rangle=\underset{\mid 1, \omega)}{\arg \min }\langle\psi| H|\psi\rangle
$$

- Hardware realizations by D-Wave with up to 5000 qubits
- QTRL 8-9

https://www.fz-juelich.de/ias/jsc/EN/Research/ModellingSimulation/QIP/QTRL/ node.html Copyright: Kristel Michielsen, Thomas Lippert - Forschungszentum Jülich


## CVQC

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



## Different interpretations of the word "quantum algorithm"

- Theoretical analysis of an algorithm - HHL paper (2008) claims exponential speedup for "solving" $A x=b$ under conditions on the matrix $A$
- Application-specific theoretical analysis - Montanaro et al. (2016) shows that no exponential speedup for $P_{k}$-FEM can be achieved for fixed dimension
- Application-specific circuit + cost estimation - Cao et al. (2013) present textbook quantum circuits for solving Poisson's equation with FDM
- Execution of application-specific circuit on QVM - Wang et al. (2020) demonstrate a fast Poisson solver on Sunway TaihuLight (yes, it works :)
- Execution of application-specific circuit on QPU - Morrell et al. (2021) show that solving a $2 \times 2$ system on IBM-Q fails due to noise (doesn't work (-3)


## What should we aim for?


M. Troyer: super-quadratic speedup is a must because

- operations will be 10-12 orders of magnitude slower
- I/O will be 10.000x slower

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.

## Schrödinger's equation

Given: $\dot{x}=A x, x\left(t_{0}\right)=x_{0}$

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

$$
\left(\begin{array}{cc}
0 & i A^{\dagger} \\
-i A & 0
\end{array}\right) \Rightarrow H=i A^{\dagger} \otimes|0\rangle_{P}\langle 1|-i A \otimes|1\rangle_{P}\langle 0|
$$

- State after Hamiltonian simulation [Leyton, Osborne 2008]

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

- 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)


## Schrödinger's equation

Given: $\dot{x}=A x, x\left(t_{0}\right)=x_{0}$

- Matrix decomposition $A=A_{H}+A_{A}$
- Baker-Campbell-Hausdorff formula

$$
e^{i A t}=e^{i A_{H} t} \cdot e^{i A_{A} t}, \quad \text { if }\left[A_{H}, A_{A}\right]=0
$$

- Hamiltonian simulation of $A_{H}$ and $A_{A}$ via unitary dilation of $\hat{O}=e^{i A_{A} t}$

$$
\left(\begin{array}{cc}
\hat{O} & \sqrt{1-\hat{o}^{2}} \\
\sqrt{1-\hat{o}^{2}} & -\hat{O}
\end{array}\right)|\psi\rangle|0\rangle=\hat{O}|\psi\rangle|0\rangle+\sqrt{1-\hat{o}^{2}}|\psi\rangle|1\rangle
$$

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

$$
f_{t}=a f+b f_{x}-c f_{x x}=\left(i b\left(-i \partial_{x}\right)+a I+c\left(-i \partial_{x}\right)^{2}\right) f
$$

- Caveat: exponential scaling in $t$ if $\left[A_{H}, A_{A}\right] \neq 0$ [Berry 2014]

Given: $\dot{x}=A x, x\left(t_{0}\right)=x_{0}$

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

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

- Hermitian matrix

$$
H=\left(\begin{array}{cc}
0 & B \\
B^{\dagger} & 0
\end{array}\right) \Rightarrow H^{2}=\left(\begin{array}{cc}
B B^{\dagger} & 0 \\
0 & B^{\dagger} B
\end{array}\right)
$$

- Wave equation

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

- Example: graph Laplacian

$$
B_{e v}=\left\{\begin{array}{cc}
1 & e=(v, w), v<w \\
-1 & e=(v, w), v>w \\
0 & \text { otherwise }
\end{array} \Rightarrow B_{e v}=\left(\begin{array}{cccc}
1 & -1 & 0 & 0 \\
0 & \ddots & \ddots & 0 \\
0 & 0 & 1 & -1
\end{array}\right)\right.
$$

## Quantum algorithms for solving PDEs



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

## Hamiltonian simulation

## Hamiltonian simulation (approach \#1)

- Given: Hamiltonian $H\left(2^{n} \times 2^{n}\right.$ Hermitian on $n$ qubits), time $t$, and error $\epsilon$
- Goal: find an algorithm to approximate $U$ such that $\left\|U-e^{i H t}\right\| \leq \epsilon$
- Decomposition into local Hamiltonianc II Invd 19061

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

- Suzuki-Trotter decomposition [Suzuki 1991]

$$
e^{-i H t} \approx\left(\prod_{\ell=1}^{L} e^{-i H_{\ell} \frac{t}{r}}\right)^{r}, \quad r \gg 1
$$

## Hamiltonian simulation (approach \#2)

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

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

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

$$
H=\sum_{\ell} \alpha_{\ell} H_{\ell} \Rightarrow H^{n}=\sum_{\ell_{1}, \ldots, \ell_{n}} \alpha_{\ell_{1}} \ldots \alpha_{\ell_{k}} H_{\ell_{1}} \ldots H_{\ell_{n}}
$$

## Hamiltonian simulation (complexity)

$$
|\psi\rangle=e^{-i H t}\left|\psi_{0}\right\rangle
$$

Gate complexity [1]

## Query complexity [2]-[5]

| 1st_order Trotter | $\mathcal{O}\left(t^{2} / \epsilon\right)$ | $\mathcal{O}\left(s^{3} t(s t / \epsilon)^{\frac{k}{2}}\right)$ |
| ---: | :---: | :---: |
| Taylor expansion | $\mathcal{O}\left(\frac{t \log ^{2}(t / \epsilon)}{\log \log t / \epsilon}\right)$ | $\mathcal{O}\left(\frac{s^{2}\\|H\\|_{\max } \log s^{2}\\|H\\|_{\max } / \epsilon}{\log \log s^{2}\\|H\\|_{\max } / \epsilon}\right)$ |
| Quantum walk | $\mathcal{O}(t / \sqrt{\epsilon}$ | $\mathcal{O}\left(s\\|H\\|_{\max } t / \sqrt{\epsilon}\right)$ |
| Quantum signal <br> processing | $\mathcal{O}(t+\log 1 / \epsilon)$ | $\mathcal{O}\left(s t\\|H\\|_{\max }+\frac{\log 1 / \epsilon}{\log \log 1 / \epsilon}\right)$ |

[1] Childs 2017, [2] Kothari 2017, [3] Berry 2015, [4] Berry 2015, [5] Low 2017

## Leyton and Osborne 2008

- First-order systems of the form

$$
\dot{\boldsymbol{x}}(t)=\left(\begin{array}{c}
f_{1}(\boldsymbol{x}) \\
\vdots \\
f_{N}(\boldsymbol{x})
\end{array}\right), \quad f_{j}(\boldsymbol{x})=\sum_{k, l=1}^{N} a_{k l}^{(j)} x_{k} x_{l}, \quad \sum_{j=1}^{N}\left|x_{j}\right|^{2}=1
$$

- Example: Orszag-McLaughlin dynamical system

$$
\dot{x}_{j}=x_{j+1} x_{j+2}+x_{j-1} x_{j-2}-2 x_{j+1} x_{j-1}, \quad j=1, \ldots N
$$

- $\left|a_{i j}\right|=\mathcal{O}(1)$ 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: $\|F(\boldsymbol{x}-\boldsymbol{y})\| \leq \mathcal{O}(1) \cdot\|x-y\|$ in ball $\|x\| \leq 1,\|y\| \leq 1$
- We assume that the initial state can be prepared efficiently


## Leyton and Osborne 2008

Schrödinger's equation
Hamiltonian simulation Hamiltonian simulation
$|\psi\rangle=e^{-i H t}\left|\psi_{0}\right\rangle$ $\psi_{t}=-i H \psi$ M

- Explicit Euler method

$$
\left|\psi^{\prime}\right\rangle=e^{i H \Delta t}|\psi\rangle|0\rangle \quad \Rightarrow \quad|\psi(t+\Delta t)\rangle=|\psi(t)\rangle+\Delta t A|\psi(t)\rangle
$$

- 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]



## 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 $\mathcal{O}($ poly $n)$. Success probability 0.6 .

## Suau et al. 2022

## Wave equations






## Quantum algorithms for solving PDEs



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

## linear system

Given: $\dot{x}=A x+b, x\left(t_{0}\right)=x_{0}$

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

- Unroll Euler method in time

$$
\left(\begin{array}{cccc}
I & 0 & 0 & 0 \\
-(I+\Delta t A) & I & 0 & 0 \\
\ddots & \ddots & \ddots & \ddots \\
0 & 0 & -(I+\Delta t A) & I
\end{array}\right)\left(\begin{array}{c}
x_{0} \\
x_{1} \\
\vdots \\
x_{m}
\end{array}\right)=\left(\begin{array}{c}
x_{i n} \\
\Delta t b \\
\vdots \\
\Delta t b
\end{array}\right)
$$

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

$$
|x\rangle=\sum_{j=0}^{m}\left|t_{j}\right\rangle\left|x_{j}\right\rangle
$$

- 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

Solution: $x(t)=e^{A t} x_{0}+\left(e^{A t}-I\right) A^{-1} b$

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

- Truncated exponentials

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

- Linear system [Berry et al. 2017]

$$
C_{m, k, p}(\Delta t A)|x\rangle=|0\rangle\left|x_{0}\right\rangle+\Delta t \sum_{j=0}^{m-1}|j(k+1)+1\rangle|b\rangle
$$

$$
\left(\begin{array}{ccccccccccc}
I & & & & & & & & & & \\
-\Delta t A & I & & & & & & & & & \\
& -\Delta t A / 2 & I & & & & & & & & \\
& & -\Delta t A / 3 & I & & & & & & & \\
-I & -I & -I & -I & I & & & & & & \\
& & & & -\Delta t A & I & & & \\
& & & & & -\Delta t A / 2 & I & & & & \\
& & & & & & -\Delta t A / 3 & I & & & \\
& & & & -I & -I & -I & -I & I & & \\
& & & & & & & & -I & I & \\
& & & & & & & & & -I & I
\end{array}\right)_{2,3,2} \quad\left(\begin{array}{c}
\left|x_{0}\right\rangle \\
\Delta 0|b\rangle \\
0 \\
0 \\
0 \\
\Delta t|b\rangle \\
0 \\
0 \\
0 \\
0 \\
0
\end{array}\right)
$$

Given: $\dot{x}=A(t) x+b(t), x\left(t_{0}\right)=x_{0}$

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

- Chebyshev pseudo-spectral approximation

$$
x(t)=\sum_{k=0}^{n} c_{k} T_{k}(t) \Rightarrow \dot{x}\left(t_{l}\right)=A\left(t_{l}\right) x\left(t_{l}\right)+b\left(t_{l}\right), \quad t_{l}=\cos \frac{l \pi}{n}
$$

- Rescaled differential equation (Childs and Liu 2020)

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

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

- 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

- Original HHL algorithm [Harrow et al. 2008]
- Improved versions of HHL
- VTAA [Ambainis 2010]
- AQC [Subasi et al. 2019]

$$
\mathcal{O}\left(s^{2} \kappa \log ^{3} \kappa \log (N) / \epsilon^{3}\right)
$$

$$
\mathcal{O}\left(\kappa^{2} \log (\kappa) / \epsilon\right)
$$

- AQC [An and Lin 2019]
- QLSA w/o phase estimation [Childs et al. 2017]
- Dense matrices [Wossnig et al. 2018]
$\mathcal{O}(\kappa$ poly $\log (\kappa / \epsilon))$
$\mathcal{O}($ poly $\log (1 / \epsilon))$
$\mathcal{O}\left(\kappa^{2} \sqrt{N}\right.$ poly $\left.\log (N) / \epsilon\right)$


## Original HHL algorithm

## QLSA



Figure 1 from [Morrell and Wong 2021]

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

- General states cannot be prepared efficiently, not even approximated

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

uniformly controlled rotations [Mottonen et al. 2004] using $\mathcal{O}\left(2^{n}\right)$ 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 $\mathcal{O}$ (poly $n$ ) gates
- Reducing time complexity by adding ancillary qubits
- Low-depth approach: $\mathcal{O}\left(n^{2}\right)$ using $\mathcal{O}\left(2^{n^{2}}\right)$ ancillae [Zhang et al. 2021]
- $s$-sparse states: $\Theta(\log n s)$ using $\mathcal{O}(n s \log s)$ ancillae [Zhang et al. 2022]


## Does any of this work in practice?

- QLSA for $A x=b$
- HW-realization for $2 \times 2$ matrix [Cai et al. 2013], [Barz et al. 2013], [Pan et al. 2013], and $8 \times 8$ matrix [Wen et al. 2018]
- $2 \times 2,4 \times 4$, and $8 \times 8$ 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?
- General state preparation is exponentially expensive, i.e., $\mathcal{O}(N)$
- Polynomials/functions with local support can be prepared efficiently
- $\kappa=\mathcal{O}\left(N^{d / 2}\right)$ in standard FEM $\Rightarrow$ no exponential speedup
- Quantum-SPAI precondioner, i.e. $P A x=P b$ [Clader et al. 2013]
- $\mathcal{O}\left(s^{2}\right)$ queries to $P A$-oracle; $\mathcal{O}\left(s^{3}\right)$ runtime
- $\kappa=\mathcal{O}(1)$ or $\kappa=\mathcal{O}(\log N)$
- $s=$ ?
- $1 / \epsilon=\mathcal{O}(N)$ 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 | $\tilde{\mathcal{O}}\left(\left(\frac{\\|x\\|_{1}\|x\|_{2}^{2}}{\epsilon^{3}}\right)\right)$ | $\tilde{\mathcal{O}}\left(\frac{\\|x\\|_{1}}{\epsilon}\right)$ |

\tilde{\mathcal{O}}(h(n))=\mathcal{O}\left(h(n) \log ^{k} n\right)
\]

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



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

## Variational quantum algorithms

[Cerezo et al. 2020]

$$
|\psi(\Theta)\rangle=V(\Theta)|0\rangle
$$



Classical optimizer $\Theta=\min _{\Theta} C(\Theta)$

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

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

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

- Cost function

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

- Ground-state Hamiltonian

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

- Cost function

$$
C(\Theta)=\langle\psi(\Theta)| H|\psi(\Theta)\rangle=\langle\Phi \mid \Phi\rangle-\langle\Phi \mid b\rangle\langle b \mid \Phi\rangle
$$

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

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

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

- Cost function

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

- Ground-state Hamiltonian

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

- Normalized cost function

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

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

- Towards an implementable cost function

$$
\begin{aligned}
& \langle\Phi \mid \Phi\rangle=\sum_{k, l} c_{k}^{*} c_{l}\langle 0| V^{\dagger}(\Theta) A_{k}^{\dagger} A_{l} V(\Theta)|0\rangle \\
& \langle\Phi \mid b\rangle=\sum_{k, l} c_{k}^{*} c_{l}\langle 0| B^{\dagger} A_{l} V(\Theta)|0\rangle\langle 0| B^{\dagger} A_{k} V(\Theta)|0\rangle
\end{aligned}
$$

- [Liu et al. 2021]:
- Decomposition of the $d$-dimensional Poisson matrix (FDM) into $\mathcal{O}(\log N)$ terms consisting of identities and $1 / 2$ spin operators $|1\rangle\langle 0|$ and $|0\rangle\langle 1|$
- 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

