A survey of quantum algorithms for PDEs

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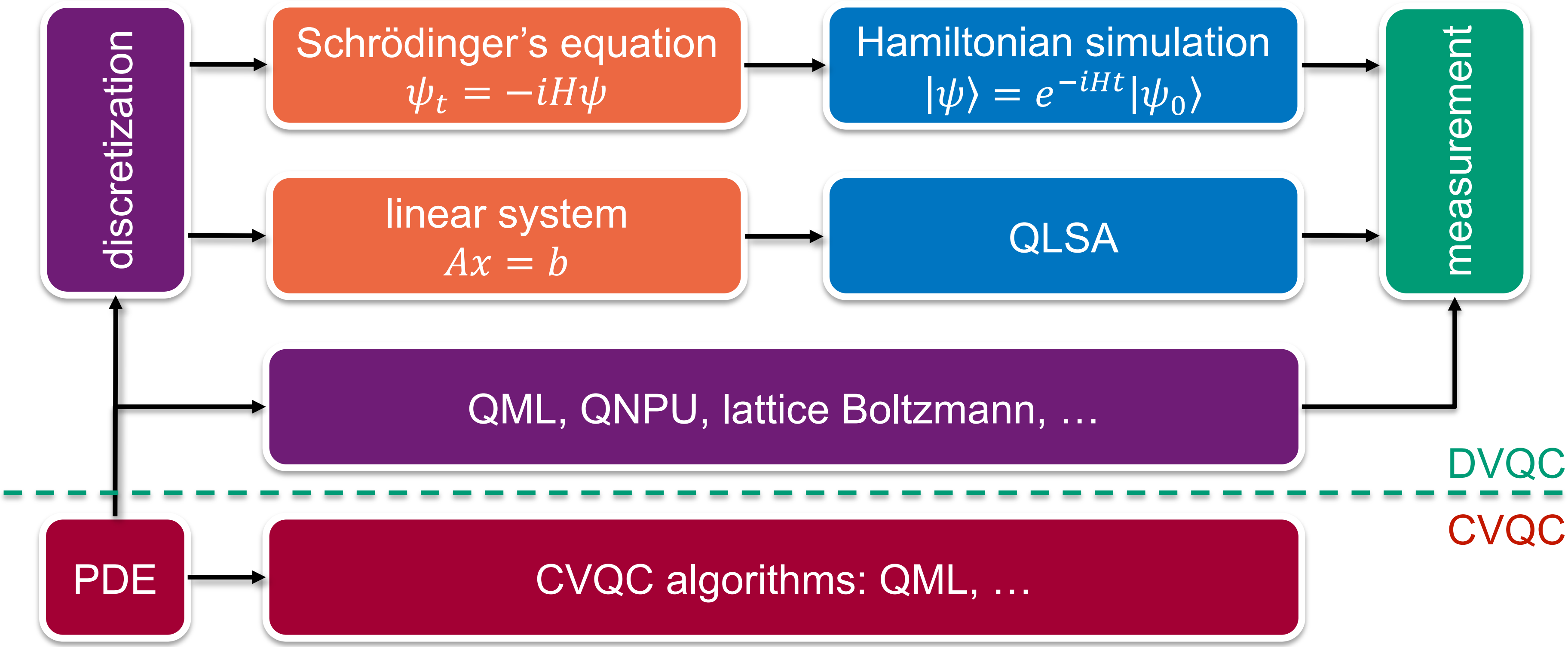
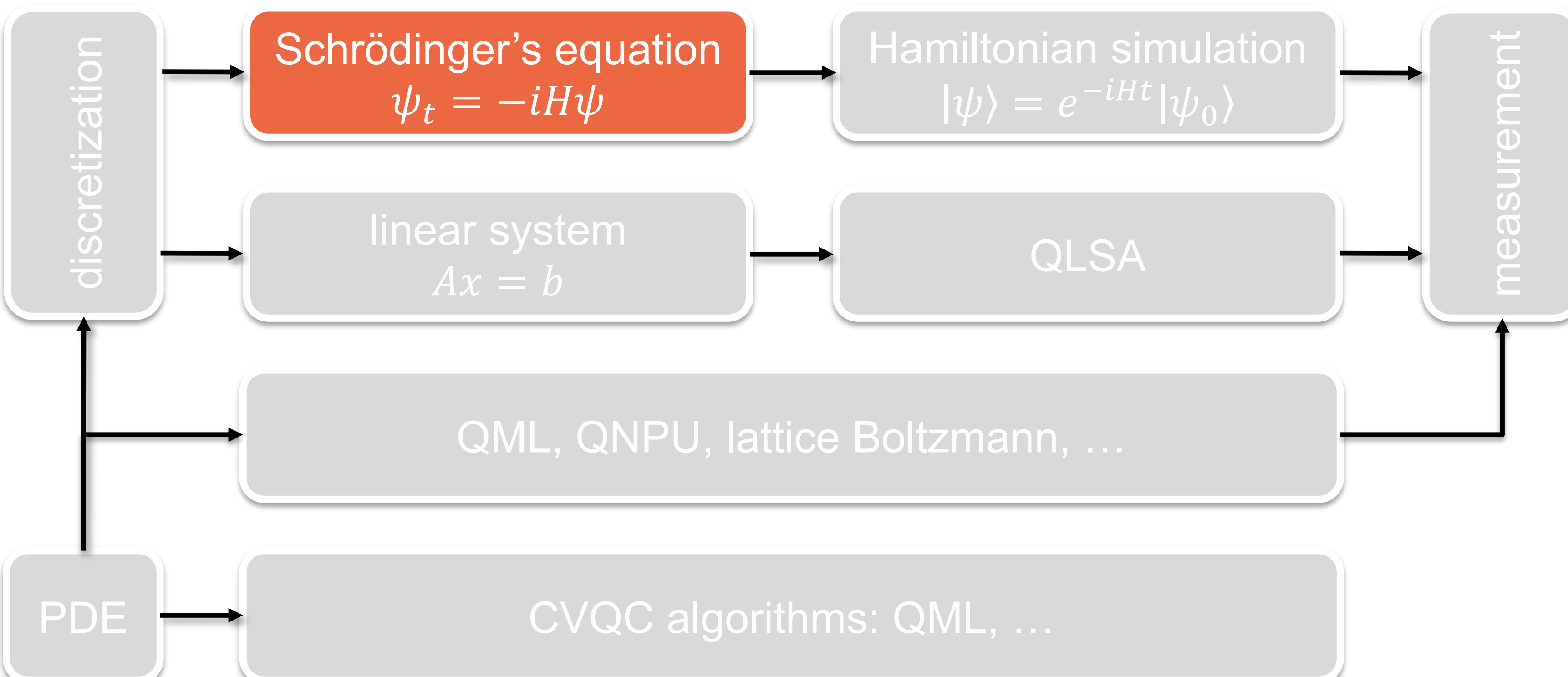
Quantum algorithms for solving PDEs



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

Quantum algorithms for solving PDEs



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

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

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

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

- 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)

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

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

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

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

- 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]

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

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

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

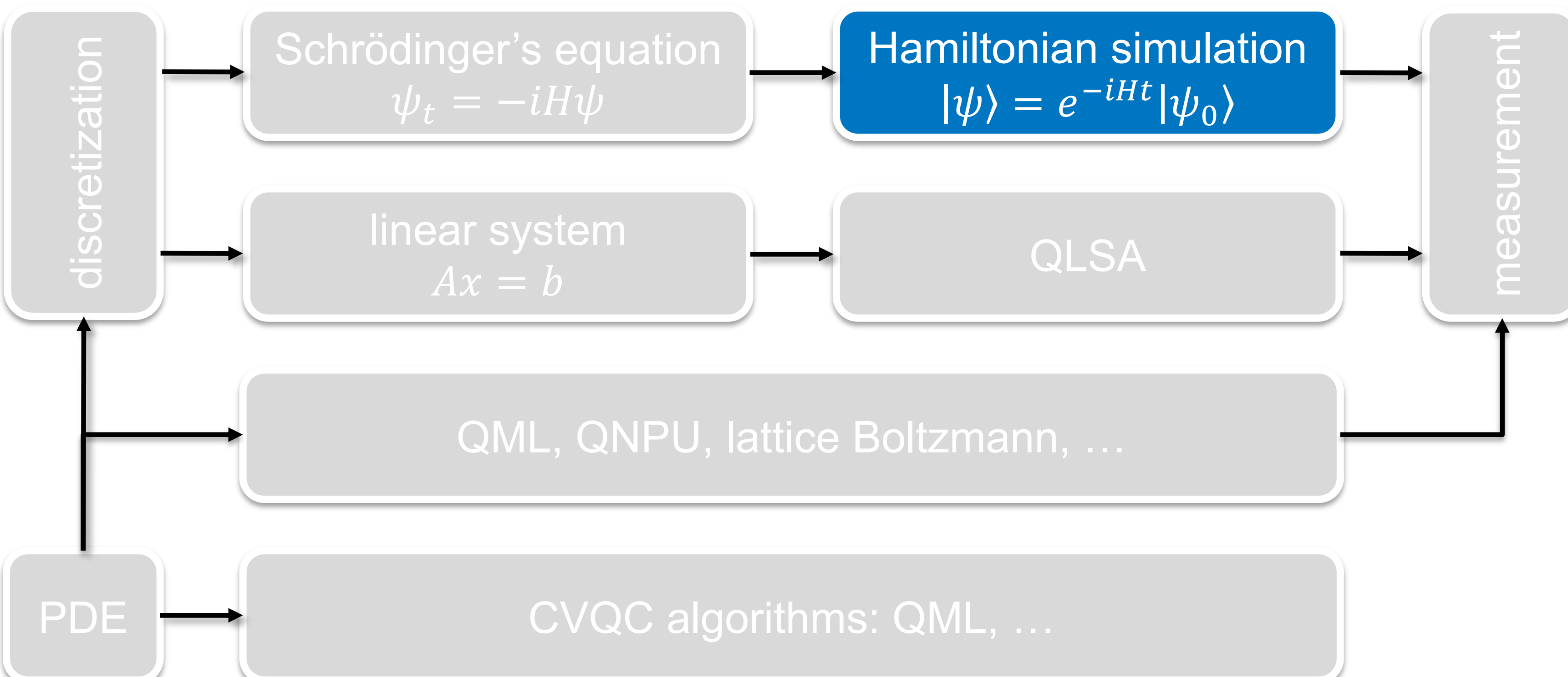
- Wave equation

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

- **Example**: graph Laplacian

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

Quantum algorithms for solving PDEs



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

Hamiltonian simulation (approach #1)

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

- Decomposition into k-local Hamiltonians [Lloyd 1996]

$$H = \sum_{\ell=1}^{L} H_\ell \, ,$$

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

- 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)

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

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

- Truncated Taylor expansion

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

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

$$H = \sum\nolimits_{\ell} \alpha_\ell H_\ell \quad \Rightarrow \quad H^n = \sum\nolimits_{\ell_1,\ldots,\ell_n} \alpha_{\ell_1} \ldots \alpha_{\ell_k} H_{\ell_1} \ldots H_{\ell_n}$$

Hamiltonian simulation (complexity)

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

	Gate complexity [1]	Query complexity [2]-[5]
1st-order Trotter	$\mathcal{O}(t^2/\epsilon)$	$\mathcal{O}\left(s^3 t (st/\epsilon)^{\frac{k}{2}}\right)$
Taylor expansion	$\mathcal{O}\left(\frac{t\log^2(t/\epsilon)}{\log\log t/\epsilon}\right)$	$\mathcal{O}\left(\frac{s^2\Vert H\Vert_{\max}\log s^2\Vert H\Vert_{\max}/\epsilon}{\log\log s^2\Vert H\Vert_{\max}/\epsilon}\right)$
Quantum walk	$\mathcal{O}(t/\sqrt{\epsilon})$	$\mathcal{O}(s\Vert H\Vert_{\max}\, t/\sqrt{\epsilon})$
Quantum signal processing	$\mathcal{O}(t + \log 1/\epsilon)$	$\mathcal{O}\left(st\Vert H\Vert_{\max} + \frac{\log 1/\epsilon}{\log\log 1/\epsilon}\right)$

[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

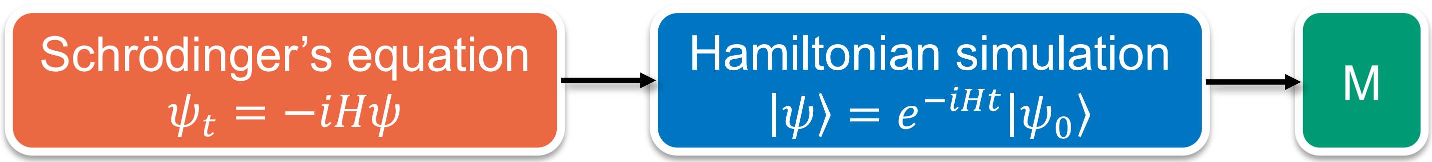
$$\dot{\boldsymbol{x}}(t) = \begin{pmatrix} f_1(\boldsymbol{x}) \\ \vdots \\ f_N(\boldsymbol{x}) \end{pmatrix}, \qquad f_j(\boldsymbol{x}) = \sum_{k,l=1}^{N} a_{kl}^{(j)} x_k x_l\,, \qquad \sum_{j=1}^{N} |x_j|^2 = 1$$

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

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

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

Leyton and Osborne *2008*



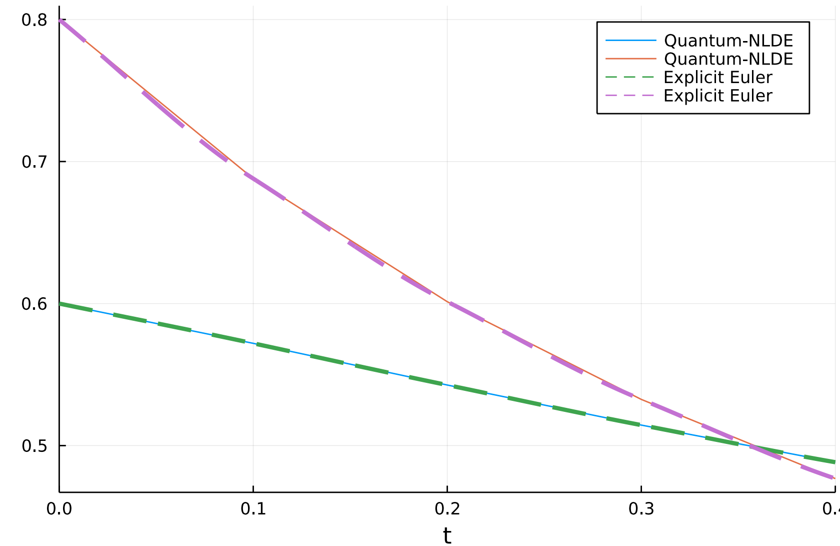
- Explicit Euler method

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

- 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 $\delta < \big(3\mathcal{O}(1)\big)^{-m}$ to ensure that the m-th iterate is exponentially close to the desired state

QuDiffEq

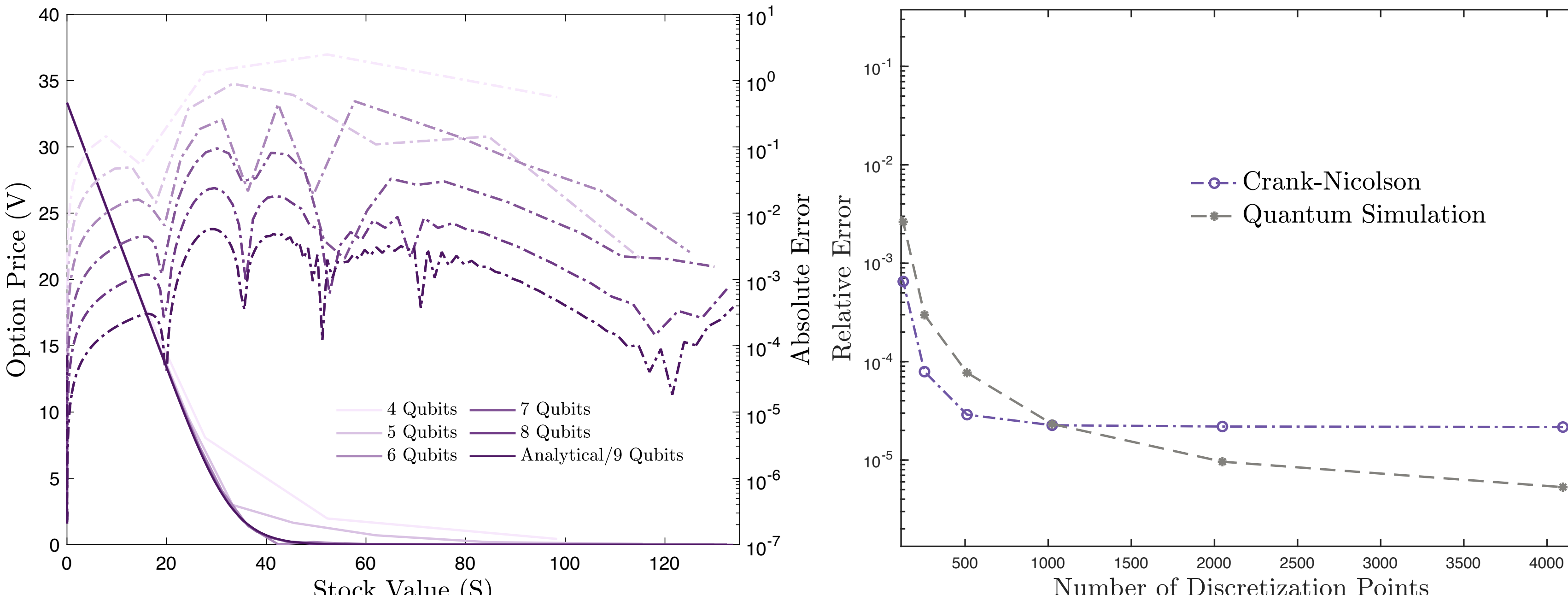
- Quantum algorithms for linear and nonlinear differential equations
- Papers with Code
  - [Leyton, Osborne 2008]
  - [Berry et al. 2010]
  - [Xin et al. 2018]



$$\dot{x}_1 = x_2 - 3x_1^2$$
$$\dot{x}_2 = -x_2^2 - x_1 x_2$$

Gonzalez-Conde et al. 2022

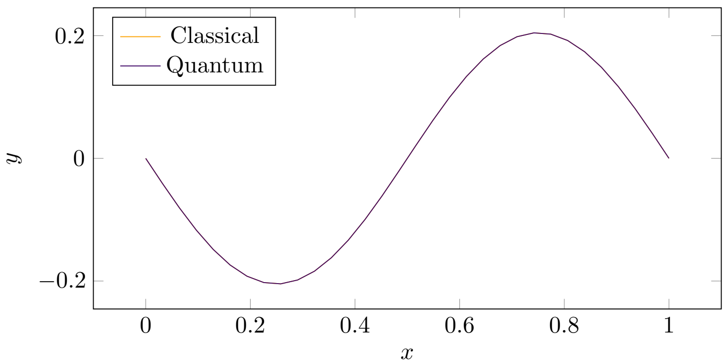
Black-Scholes equation for European put options

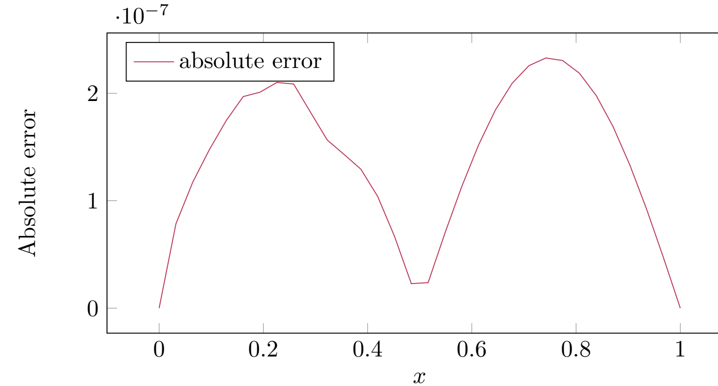


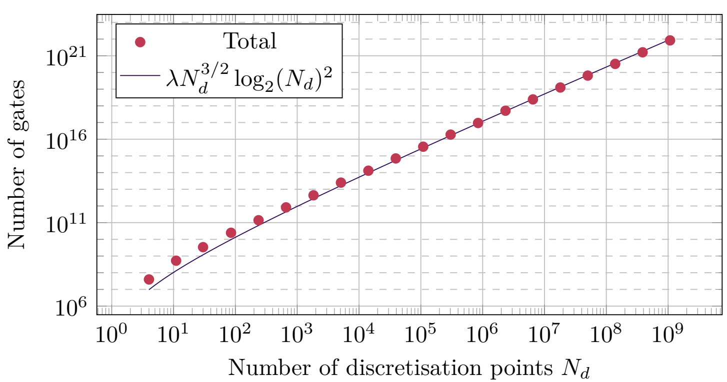
Precision comparable to classical methods with 10 qubits and 94 entangling gates on fault-tolerant QC. Complexity $\mathcal{O}(\text{poly } n)$. Success probability 0.6.

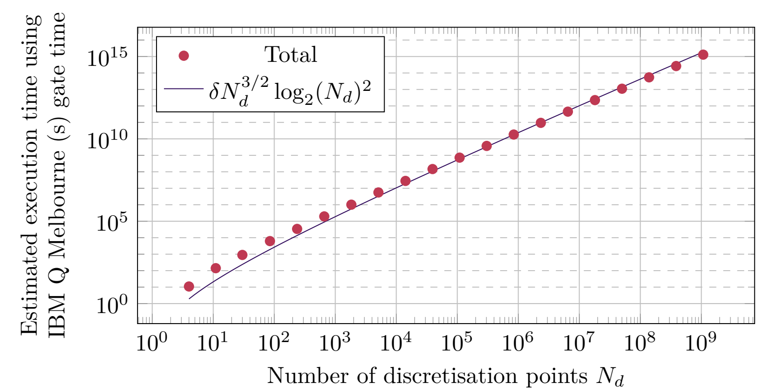
[Suau et al.](#) 2022

Wave equations

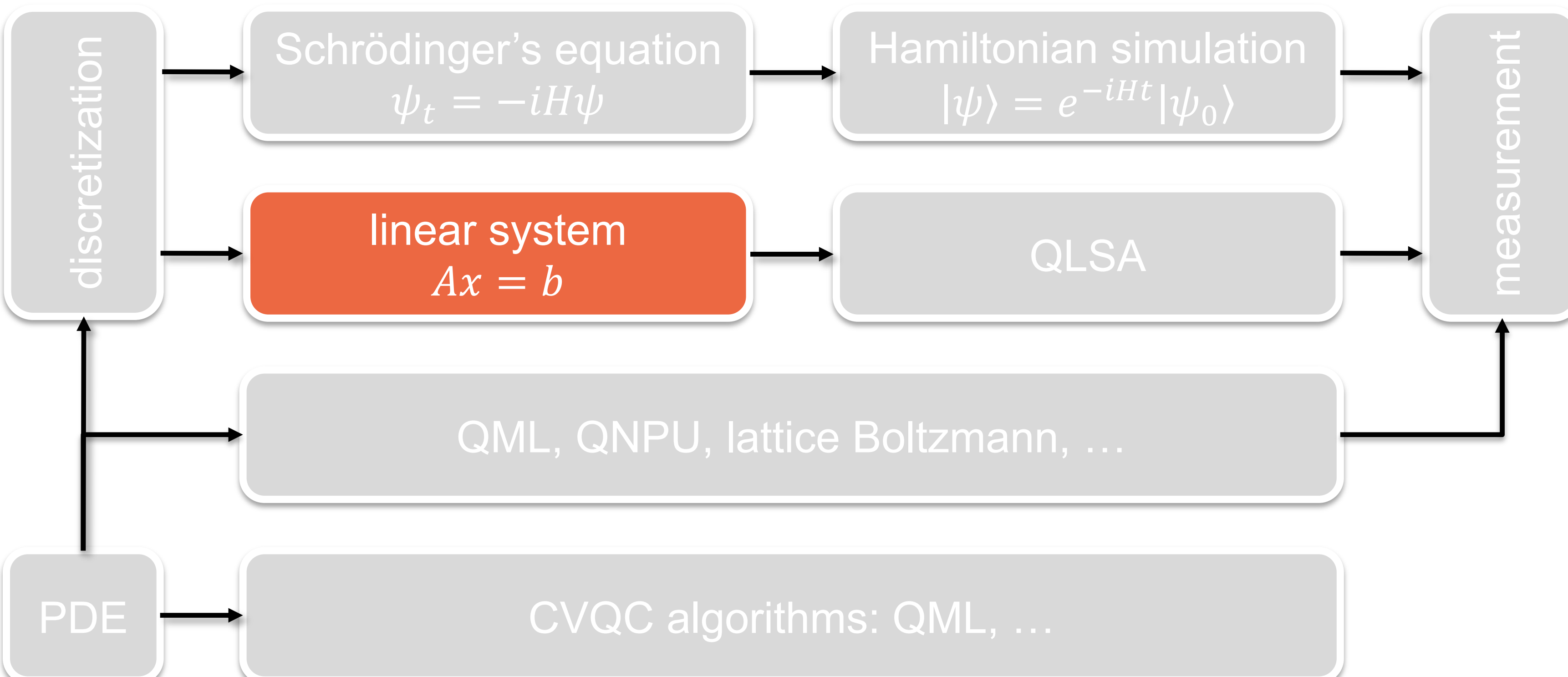








Quantum algorithms for solving PDEs



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

linear system
$Ax = b$

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

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

- Unroll Euler method in time

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

- 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]

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

linear system
$Ax = b$

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

- 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]

$$C_{m,k,p}(\Delta t A)|x\rangle = |0\rangle|x_0\rangle + \Delta t \sum_{j=0}^{m-1} |j(k+1)+1\rangle|b\rangle$$

$$\begin{pmatrix}
I &&&&&&&&&& \\
-\Delta tA & I &&&&&&&&& \\
& -\Delta tA/2 & I &&&&&&&& \\
&& -\Delta tA/3 & I &&&&&&& \\
-I & -I & -I & -I & I &&&&&& \\
&&&& -\Delta tA & I &&&&& \\
&&&&& -\Delta tA/2 & I &&&& \\
&&&&&& -\Delta tA/3 & I &&& \\
&&&& -I & -I & -I & -I & I && \\
&&&&&&&& -I & I & \\
&&&&&&&&& -I & I
\end{pmatrix}_{2,3,2}, \quad
\begin{pmatrix}
|x_0\rangle \\ \Delta t|b\rangle \\ 0 \\ 0 \\ 0 \\ \Delta t|b\rangle \\ 0 \\ 0 \\ 0 \\ 0 \\ 0
\end{pmatrix}$$

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

linear system
$Ax = b$

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

- Chebyshev pseudo-spectral approximation

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

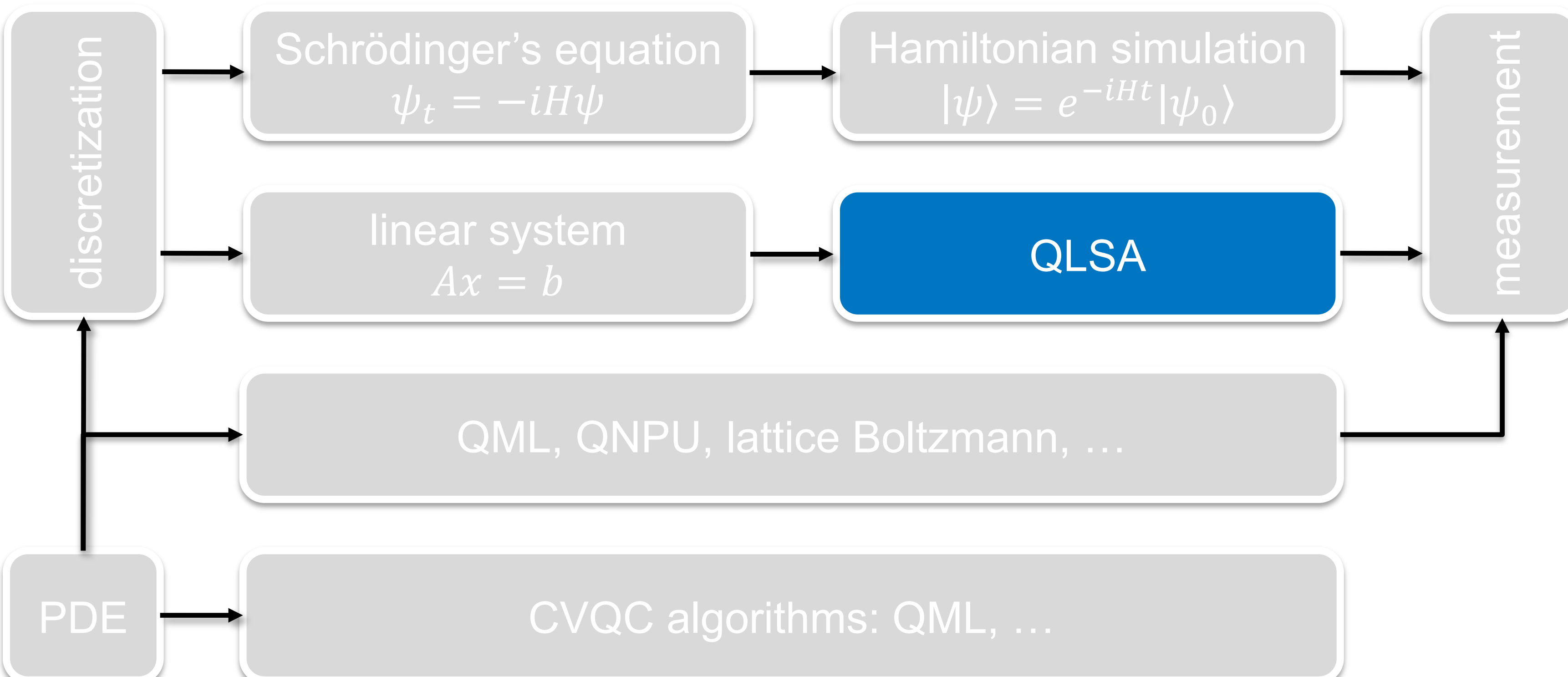
- Rescaled differential equation (Childs and Liu 2020)

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

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



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Quantum linear 'solver' algorithm

- **Problem**: $a = \langle x^{\dagger} | M | x \rangle \quad s.t. \quad A|x\rangle = |b\rangle$
- Original HHL algorithm [Harrow et al. 2008]
- Improved versions of HHL
  - VTAA [Ambainis 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

- $\mathcal{O}(s\sqrt{\kappa}N \log 1/\epsilon)$
- $\mathcal{O}(s^2\kappa^2 \log(N)/\epsilon)$
- $\mathcal{O}(s^2\kappa \log^3 \kappa \log(N)/\epsilon^3)$
- $\mathcal{O}(\kappa^2 \log(\kappa)/\epsilon)$
- $\mathcal{O}(\kappa \,\mathrm{poly}\log(\kappa/\epsilon))$
- $\mathcal{O}(\mathrm{poly}\log(1/\epsilon))$
- $\mathcal{O}\left(\kappa^2\sqrt{N}\mathrm{poly}\log(N)/\epsilon\right)$

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

- General states cannot be prepared efficiently, not even approximated

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

  uniformly controlled rotations [Mottonen et al. 2004] using $\mathcal{O}(2^n)$ 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 $\mathcal{O}(\text{poly } n)$ gates

- Reducing time complexity by adding ancillary qubits
  - Low-depth approach: $\mathcal{O}(n^2)$ using $\mathcal{O}\left(2^{n^2}\right)$ ancillae [Zhang et al. 2021]
  - s-sparse states: $\Theta(\log ns)$ using $\mathcal{O}(ns \log s)$ 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?

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

versus

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

- 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 ⇒ 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 $\kappa = \mathcal{O}(\log N)$
- $s = ?$
- $1/\epsilon = \mathcal{O}(N)$ in most discretization schemes ⇒ no exponential speedup

No exponential speedup for elliptic problems for fixed d

algorithm	w/o preconditioner	optimal preconditioner
Conjugate Gradients	$\tilde{\mathcal{O}}\left(\left(\frac{\lvert x\rvert_2}{\epsilon}\right)^{\frac{d+1}{2}}\right)$	$\tilde{\mathcal{O}}\left(\left(\frac{\lvert x\rvert_2}{\epsilon}\right)^{\frac{d}{2}}\right)$
Childs et al. 2017	$\tilde{\mathcal{O}}\left(\left(\frac{\lVert x\rVert_1 \lvert x\rvert_2^2}{\epsilon^3}\right)\right)$	$\tilde{\mathcal{O}}\left(\frac{\lVert x\rVert_1}{\epsilon}\right)$

[Montanaro, Pallister 2016]:

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

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

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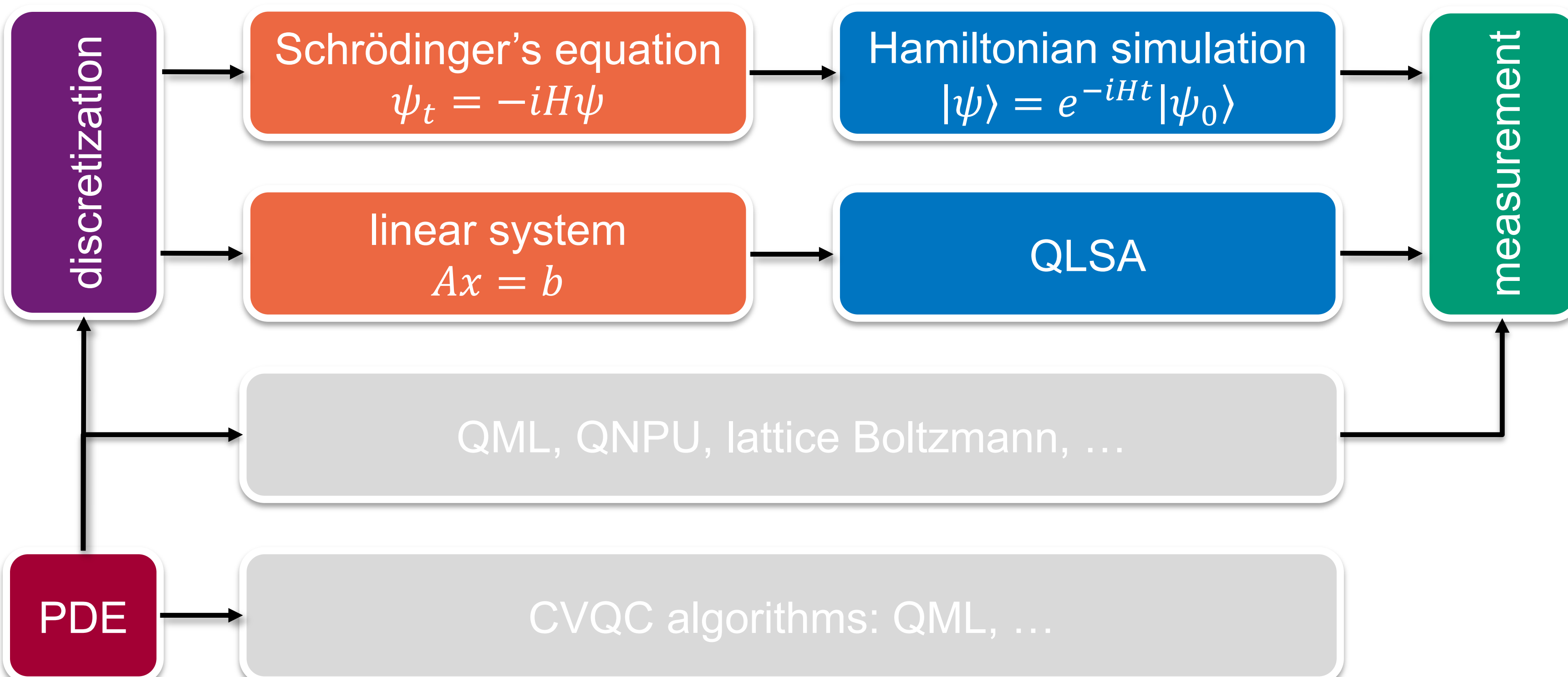

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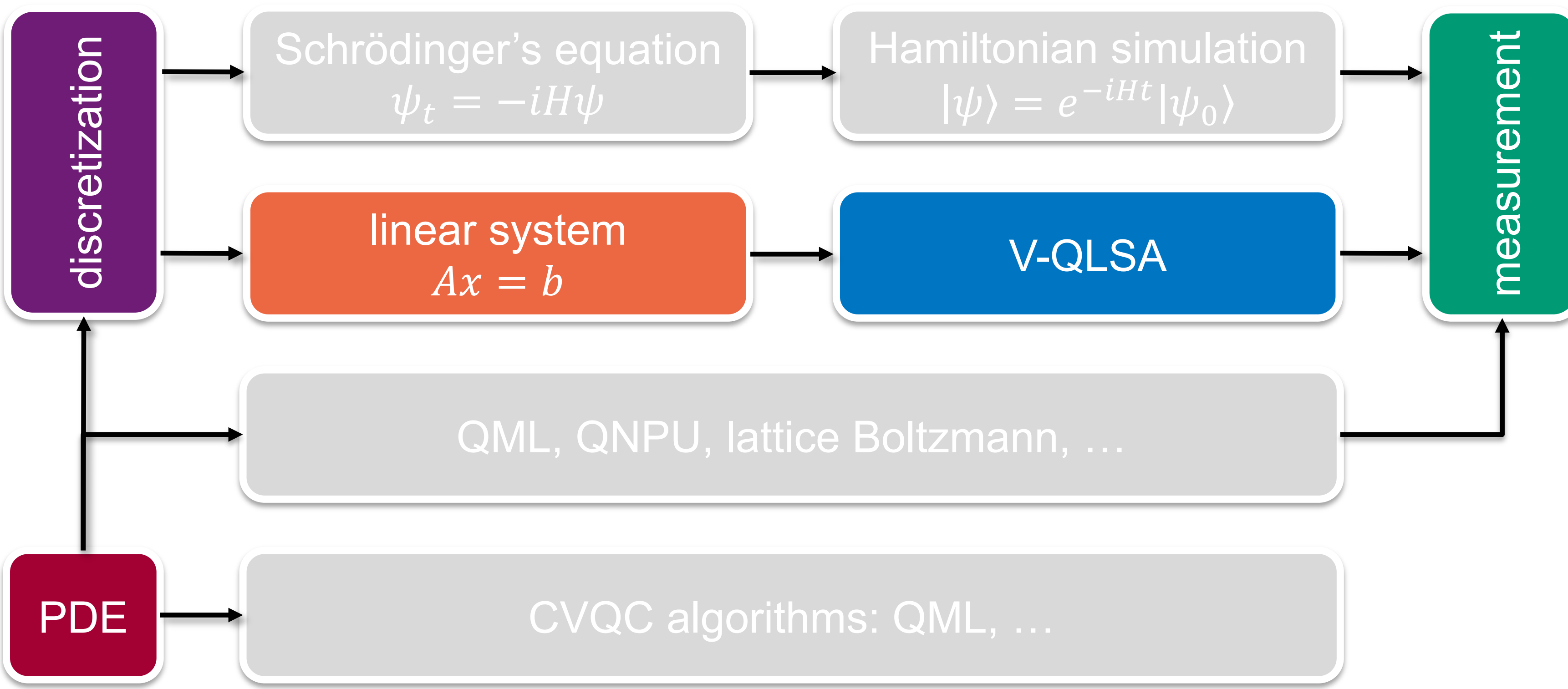

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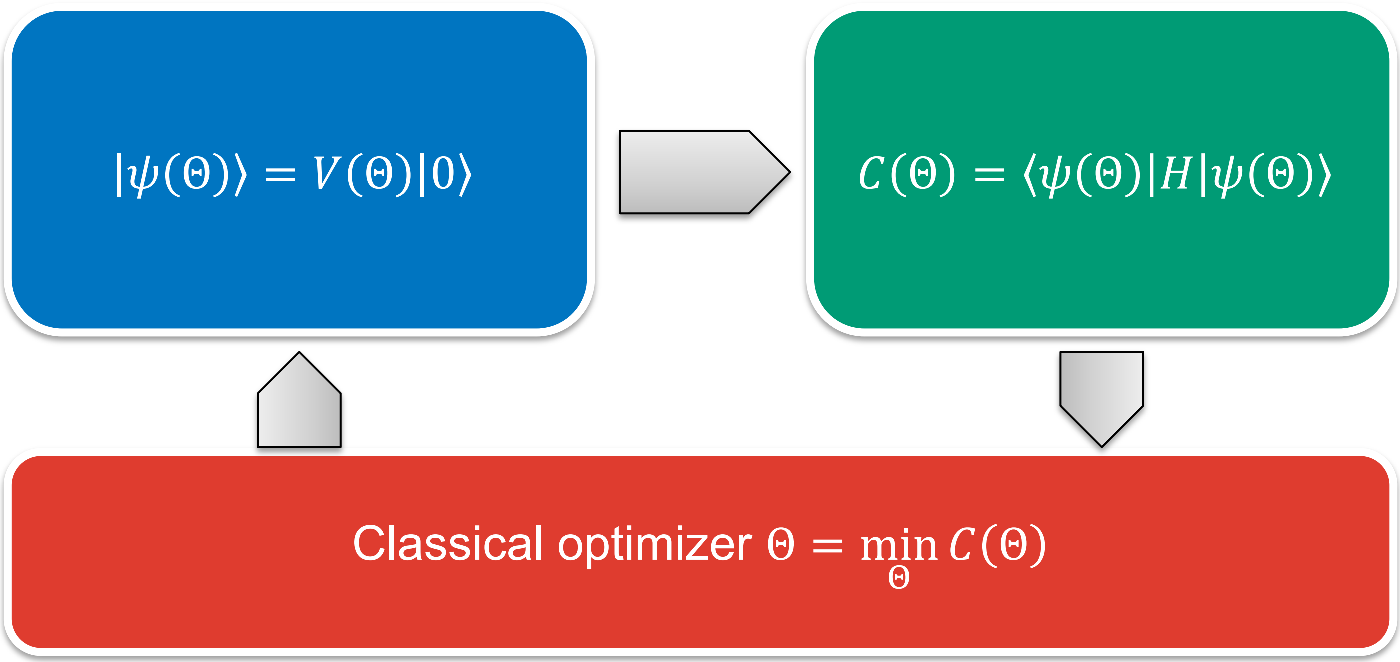
Variational quantum algorithms [Cerezo et al. 2020]



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

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

- Ground-state Hamiltonian

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

- Cost function

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

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

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- Ground-state Hamiltonian

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

- Normalized cost function

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

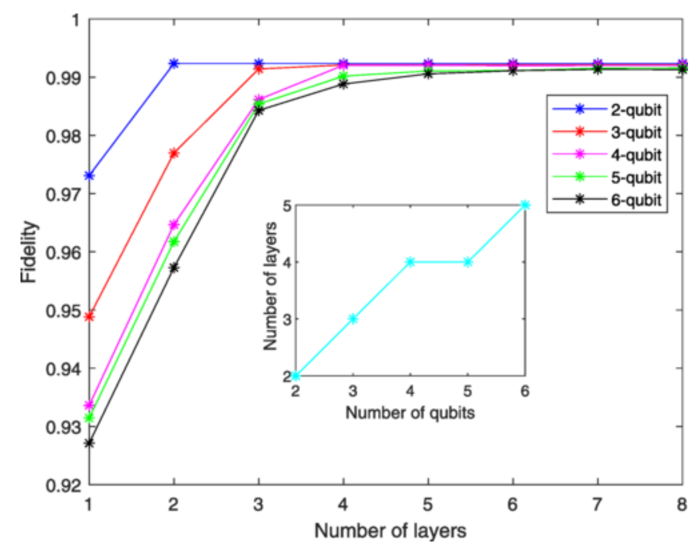
Variational quantum linear solver [Bravo-Prieto et al. 2020]

- 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 $\mathcal{O}(\log N)$ terms consisting of identities and ½ 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



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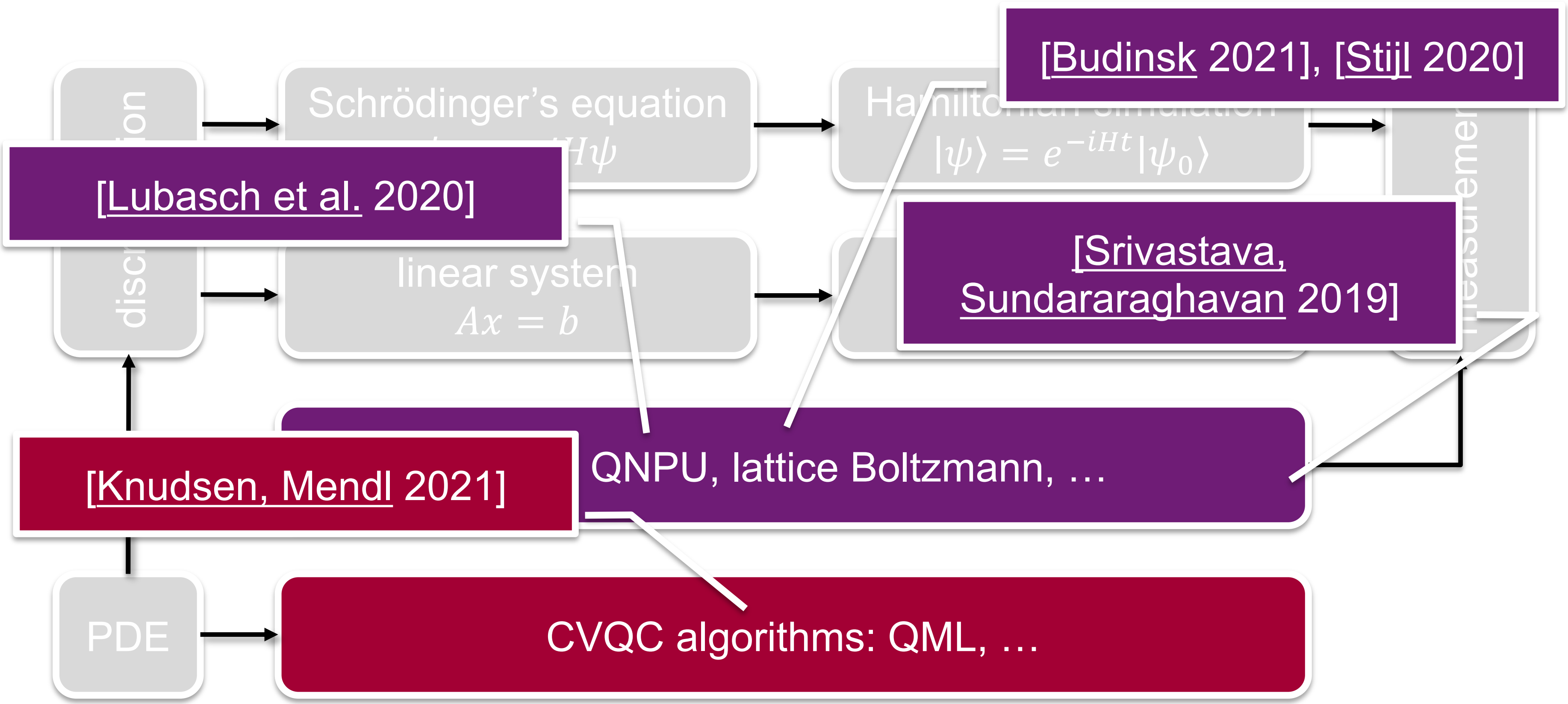

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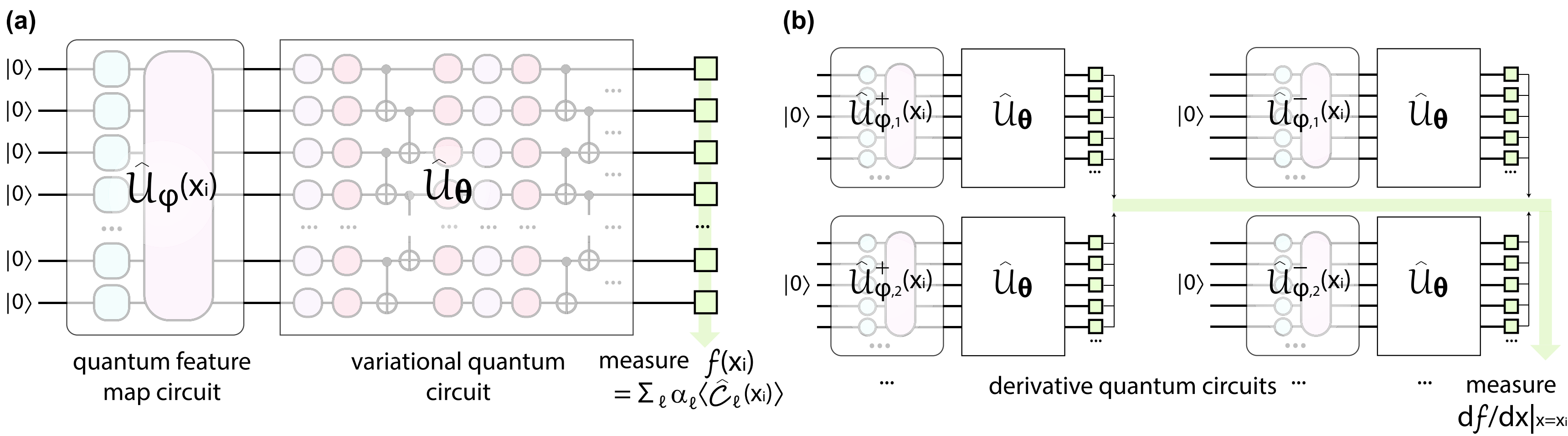
Physics-informed QNN [Kyriienko et al. 2021]



BACKUP

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

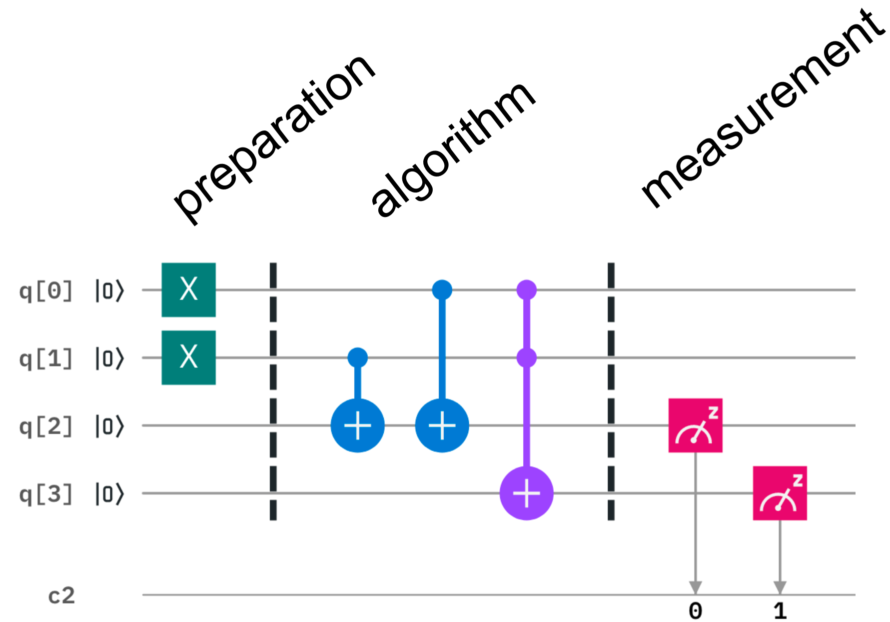
$$|\psi\rangle = \int_{-\infty}^{\infty} c(x) |x\rangle dx , \qquad \langle x' | x \rangle = \delta(x' - x)$$

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, …



DVQC: Quantum annealing

- Mathematical model

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

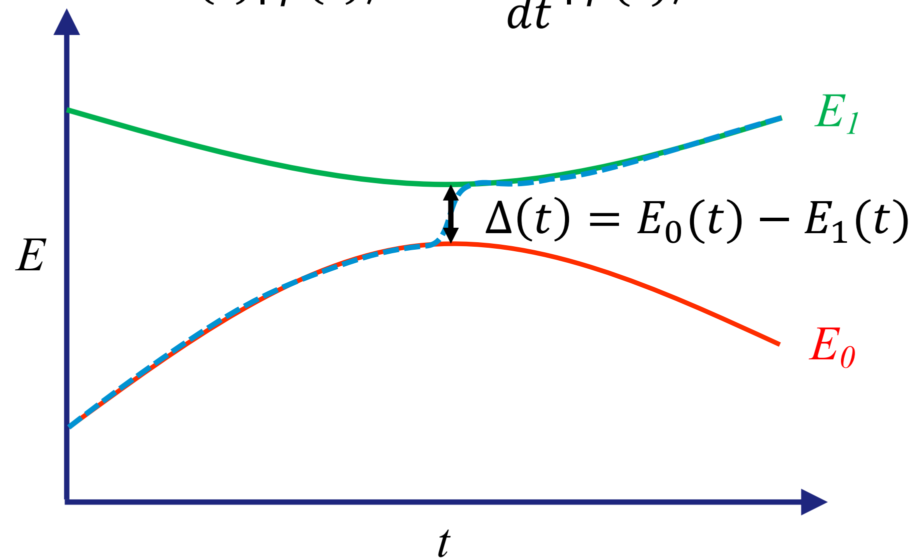
- Path of Hamiltonians for $t \in [0, T]$

$$H(t) = \big(1 - f(t)\big)H_I + f(t)H_P$$

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

- Ground-state evolution

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



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