Classical & Quantum Algorithms for Hamiltonian Simulation

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Hamiltonian simulation

Solution of the Schrödinger equation,

$$\mathrm{i}\partial_t \psi \;=\; \mathrm{H}(t)\,\psi, \qquad \mathrm{H}(t)^* = \mathrm{H}(t), \qquad \psi(t) \in \mathscr{H}.$$

Feynman, R. P. Simulating physics with computers. *Int J Theor Phys* **21**, 467-488 (1982).

> the real difficulty is this: If we had many particles, we have R particles, for example, in a system, then we would have to describe the probability of a circumstance by giving the probability to find these particles at points $x_1, x_2, \ldots, x_R$ at the time t. That would be a description of the probability of the system. And therefore, you'd need a k-digit number for every configuration of the system, for every arrangement of the R values of x. And therefore if there are N points in space, we'd need N^R configurations.

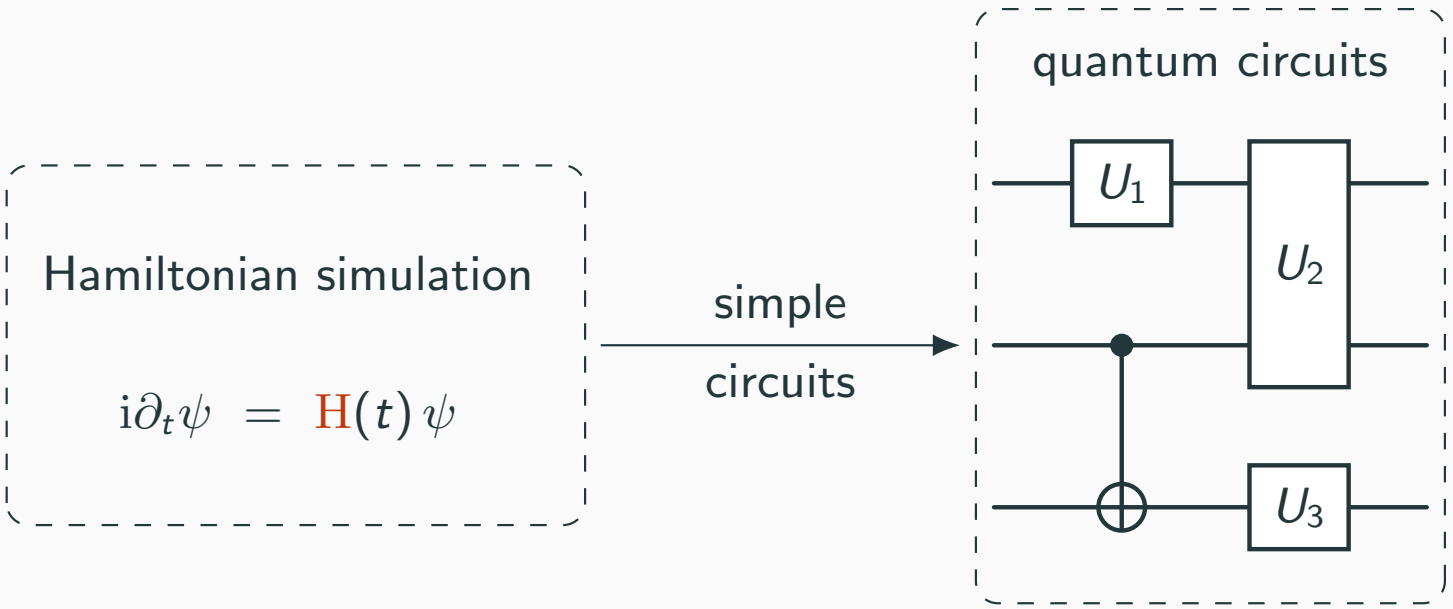
n-body problems

- PDE, $\psi \in \mathbb{C}^{N^{3n}}$ after spatial discretisation with N points in each direction,
- ODE, $\psi \in \mathbb{C}^{2^n}$ for 2-level systems (e.g. spin systems).

Why quantum algorithms for Hamiltonian simulation?

4. QUANTUM COMPUTERS—UNIVERSAL QUANTUM SIMULATORS

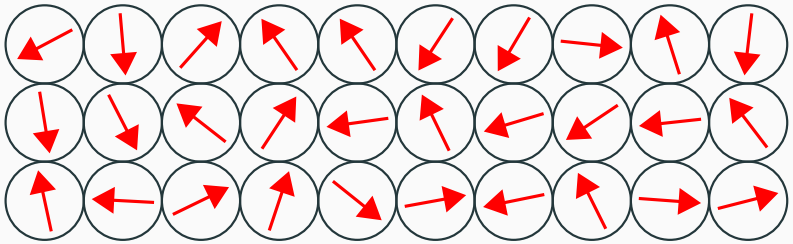
The first branch, one you might call a side-remark, is, Can you do it with a new kind of computer—a quantum computer? (I'll come back to the other branch in a moment.) Now it turns out, as far as I can tell, that you can simulate this with a quantum system, with quantum computer elements.

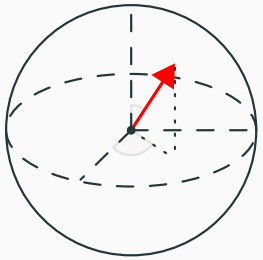


- Linear growth in number of qubits vs exponential in classical computing
- Provides a *straightforward* approach for beating the curse of dimensionality in quantum physics and chemistry simulations

Example: spin systems

- A uniquely quantum phenomenon that has no classical counterpart.





$\rho = \frac{1}{2}(I + \boldsymbol{s} \cdot \boldsymbol{\sigma}) \in \mathbb{C}^{2\times 2}$,

$\boldsymbol{s} \in \mathbb{R}^3$,

and $\boldsymbol{\sigma} = (X, Y, Z)$

are 2×2 Pauli matrices.

- The phenomenon that powers
  - magnetic resonance imaging (MRI)
  - spintronics
  - quantum computing
- Responsible for ferromagnetism.
- Suspected to be involved in detection of Earth's magnetic field by birds (quantum biology).
- Fay, Lindoy, Manolopolous, Hore 2020: '*the accurate simulation of anisotropic magnetic field effects relevant to magnetoreception seems to require full quantum mechanical calculations*'

Quantum computing comes home

For n interacting spins, state space is exponentially large, $\rho \in \mathbb{C}^{2^n \times 2^n}$.

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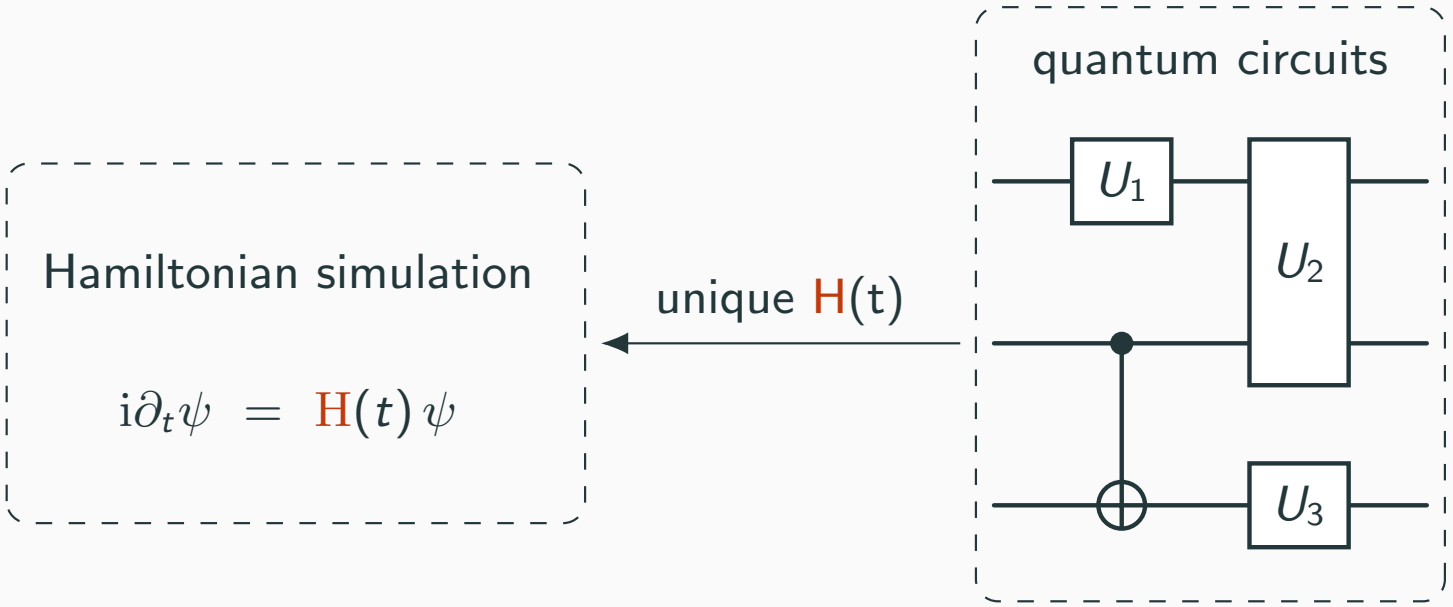
Resurgence of interest in quantum algorithms for Hamiltonian simulation.

Berry et al. 15, Low & Chuang 17, 19, Low & Wiebe 18, Smith et al. 19, Kieferova et al. 19, Berry et al. 20, Chen et al. 21, Haah et al. 21, Jin & Li 21, Jin et al. 21, Dong et al. 21,22, An et al. 22, Watkins et al. 22, Mizuta et al. 23,...

Hamiltonian simulation of two-level systems is among early candidates for demonstrating quantum advantage. (Childs et al. 18, Seetharam et al. 21).

- Claim by IBM (14 June 2023): Kim, Eddins, Anand, Wei, van den Berg, Rosenblatt, Nayfeh, Wu, Zaletel, Temme & Kandala (2023), 'Evidence for the utility of quantum computing before fault tolerance', Nature 618, 500–505.
- Claim by DWave (1 March 2024): King et al, 'Computational supremacy in quantum simulation', arXiv:2403.00910

Why is Hamiltonian simulation central to quantum computing?



- Every gate has an underlying Hamiltonian
- Every quantum circuit is a Hamiltonian Simulation (except measurement)
- Due to the unitary nature of quantum computing, Hamiltonian simulation is a natural building block for quantum algorithms
- Important subroutine in quantum algorithms – QPE (Kitaev 95), HHL (Harrow, Hassidim, Lloyd 09)

Outline

Hamiltonian Simulation

$$\mathrm{i}\partial_t \psi \;=\; \mathrm{H}(\psi, t)\,\psi, \qquad \psi(t) \in \mathscr{H}.$$

1. **Linear**
$$\partial_t u = A u$$
2. Driven
$$\partial_t u = A(t) u$$
3. Non-linear
$$\partial_t u = A u + N(u)$$

The Schrödinger equation

$$\partial_t u = -\mathrm{i}\mathrm{H}u, \qquad u(0) = u_0, \qquad \mathrm{H}^* = \mathrm{H},$$

can be thought of as an ODE

$$\partial_t u = \mathcal{A}u, \qquad u(0) = u_0, \qquad \mathcal{A} = -\mathrm{i}\mathrm{H}$$

The exact solution of this ODE is given by the matrix exponential

$$u(t) = \mathrm{e}^{t\mathcal{A}} u_0 = \sum_{k=0}^{\infty} \frac{(t\mathcal{A})^k}{k!}.$$

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exp maps Lie algebra $\mathrm{i}\mathrm{H} \in \mathfrak{su}(n)$ to Lie group $\mathrm{e}^{-\mathrm{i}t\mathrm{H}} \in \mathrm{U}(n)$, leading to:

- Unitary evolution
$$\langle u(t), v(t) \rangle = \langle u(0), v(0) \rangle$$
- Conservation of norm
$$\|u(t)\|_2 = \|u(0)\|_2 = 1$$
- Conservation of energy
$$\langle u(t), \mathrm{H}u(t) \rangle = \langle u(0), \mathrm{H}u(0) \rangle$$

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$\mathrm{e}^z \approx 1 + z$ $\qquad$ $u_1 = (I - \mathrm{i}h\mathrm{H})u_0$ $\qquad$ F.E. $\|u_n\|_2 \to \infty$

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Geometric Numerical Integration:

The design of numerical methods that conserve certain properties exactly, even if numerical error in solution is finite

Computing e^A or $\mathrm{e}^A u_0$

C. Moler & C. V. Loan, *Nineteen Dubious Ways to Compute the Exponential of a Matrix, Twenty-Five Years Later*, SIAM Review (2003).

	Diagonalisation	Scaling and Squaring	**Splitting**
If	$A = UDU^*$	$\|A\| > 1$	$A = B + C$
	$\mathrm{e}^A = U\mathrm{e}^D U^*$	$\mathrm{e}^A = \left(\mathrm{e}^{A/n}\right)^n$	$\mathrm{e}^A = \lim_{n\to\infty}\left(\mathrm{e}^{B/n}\mathrm{e}^{C/n}\right)^n$
Fast when	Uu_0 and U^*u_0 cheap	$\|A\| < 1$ needed	$\mathrm{e}^B, \mathrm{e}^C$ cheap

	Asymptotic $z \to 0$	Approximate e^z on spectrum $z \in [a,b] \subseteq \sigma(A)$	Iterative Use A and u_0
Polynomial	Taylor $\sum_{k=0}^n \frac{z^k}{k!}$	Chebyshev $J_0(\mathrm{i}) + 2\sum_{k=1}^n \mathrm{i}^k J_k(-\mathrm{i})T_k(z)$	Polynomial Krylov
Rational	Padé $\frac{1+\frac{1}{2}z+\frac{1}{12}z^2}{1-\frac{1}{2}z+\frac{1}{12}z^2}$	?	Rational Krylov

Trotterisation $\leftrightarrow$ Splitting methods for matrix exponential

If e^{hA} and e^{hB} are easier to compute, approximate $\mathrm{e}^{h(A+B)}$ by

splitting	error	name	stages
$\mathrm{e}^{hA}\mathrm{e}^{hB}$	$\mathcal{O}(h^2)$	Trotter	2

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$\mathrm{e}^{a_1 hB}\mathrm{e}^{b_1 hA}\mathrm{e}^{a_2 hB}\ldots\mathrm{e}^{b_n hA}\ldots\mathrm{e}^{a_2 hB}\mathrm{e}^{b_1 hA}\mathrm{e}^{a_1 hB}$	$\mathcal{O}(h^{2p+1})$	Classical	$\mathcal{O}(2^p)$

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$\mathrm{e}^{\frac{h}{6}A}\mathrm{e}^{\frac{h}{2}B}\mathrm{e}^{\frac{2}{3}(hA+\frac{h^3}{48}[[A,B],B])}\mathrm{e}^{\frac{h}{2}B}\mathrm{e}^{\frac{h}{6}A}$	$\mathcal{O}(h^{2p+1})$	Compact	$\mathcal{O}(2^p)$
$\mathrm{e}^{\frac{h}{2}B}\mathrm{e}^{\frac{h}{2}A}\mathrm{e}^{h^3 R}\mathrm{e}^{h^5 S}\mathrm{e}^{h^3 R}\mathrm{e}^{\frac{h}{2}A}\mathrm{e}^{\frac{h}{2}B}$	$\mathcal{O}(h^{2p+1})$	Asymptotic	$\mathcal{O}(p)$

Yoshida 1990, Murua & Sanz-Serna 1999, Chin & Chen 2002, McLachlan & Quispel 2002, Omelyan, Mrygold & Folk 2003, Blanes, Casas & Murua 2008, Chartier & Murua 2009, ... Asymptotic (Zassenhaus) Bader, Iserles, Kropielnicka, & S. 2014, Found. Comp. Math.

If e^{hA} and e^{hB} conserve unitarity, then splitting conserves unitarity, norm, modified energy.

Example: Spin Hamiltonians

$$\mathcal{H} = \underbrace{\mathbf{e}^\top \mathbb{S}}_{\mathcal{H}_{\mathsf{ss}}(t)} + \underbrace{\frac{1}{2}\mathbb{S}^\top C\, \mathbb{S}}_{\mathcal{H}_{\mathsf{in}}}$$

$$= \sum_{k=1}^{n} \sum_{\alpha \in \{X,Y,Z\}} \mathrm{e}_k^\alpha\, \alpha_k + \frac{1}{2} \sum_{j,k=1}^{n} \sum_{\alpha,\beta \in \{X,Y,Z\}} C_{j,k}^{\alpha,\beta}\, \alpha_j\, \beta_k$$

where α_k acts on kth spin only,

$$\alpha_k = \underbrace{I \otimes \cdots \otimes I}_{n-k \text{ times}} \otimes \underbrace{\alpha}_{k\text{th}} \otimes \underbrace{I \otimes \cdots \otimes I}_{k-1 \text{ times}} \quad \in \mathbb{C}^{2^n \times 2^n},$$

and $\alpha = X, Y, Z$ are Pauli matrices,

$$X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad Y = \begin{pmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{pmatrix}, \quad Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

Two-level systems: Ising chains, Kitaev models, NMR/ESR, qubits (spin, superconducting, ...)

$$\partial_t u = \mathcal{A}\, u, \quad u(0) = u_0,$$

exact solution given by matrix exponential

$$u(t) = \exp(t\mathcal{A})u_0 = \sum_{k=0}^{\infty} \frac{(t\mathcal{A})^k}{k!} u_0.$$

Hamiltonian simulation:

$$\mathcal{A} \quad = \quad -\mathrm{i}\,(\ \mathbf{e}^\top \mathbb{S} \quad + \quad \frac{1}{2}\mathbb{S}^\top C\ \mathbb{S}\ ) \tag{1}$$

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For non-interacting spins, since $\mathfrak{su}(2)$ is spanned by $\mathrm{i}X, \mathrm{i}Y, \mathrm{i}Z$ and

$$[X, Y] = \mathrm{i}Z, \quad [Y, Z] = \mathrm{i}X, \quad [Z, X] = \mathrm{i}Y,$$

can compute exponential analytically

$$\mathrm{e}^{t\mathcal{A}} = \bigotimes_{k=1}^{n} \mathrm{e}^{-\mathrm{i}t\mathbf{e}_k\cdot\boldsymbol{\sigma}} = \bigotimes_{k=1}^{n} \begin{pmatrix} \cos\left(\frac{t\|\boldsymbol{e}_k\|}{2}\right) - \mathrm{i}e_k^z \frac{\sin\left(\frac{\|\boldsymbol{e}_k\|}{2}\right)}{\|t\boldsymbol{e}_k\|} & (-\mathrm{i}e_k^x - e_k^y)\frac{\sin\left(\frac{t\|\boldsymbol{e}_k\|}{2}\right)}{\|\boldsymbol{e}_k\|} \\ (-\mathrm{i}e_k^x + e_k^y)\frac{\sin\left(\frac{t\|\boldsymbol{e}_k\|}{2}\right)}{\|\boldsymbol{e}_k\|} & \cos\left(\frac{t\|\boldsymbol{e}_k\|}{2}\right) + \mathrm{i}e_k^z \frac{\sin\left(\frac{t\|\boldsymbol{e}_k\|}{2}\right)}{\|\boldsymbol{e}_k\|} \end{pmatrix},$$

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Trotterisation: For $-\mathrm{i}\mathrm{H} = A + B$ we need to split

$$\exp(h(A+B)) = \mathrm{e}^{hA}\mathrm{e}^{hB} + \mathcal{O}\left(h^2\right)$$

Trotterisation:

$$\mathrm{e}^{-\mathrm{i}h(\mathcal{H}^X+\mathcal{H}^Y+\mathcal{H}^Z)} = \mathrm{e}^{-\mathrm{i}h\mathcal{H}^X}\,\mathrm{e}^{-\mathrm{i}h\mathcal{H}^Y}\,\mathrm{e}^{-\mathrm{i}h\mathcal{H}^Z} + \mathcal{O}\left(h^2\right),$$

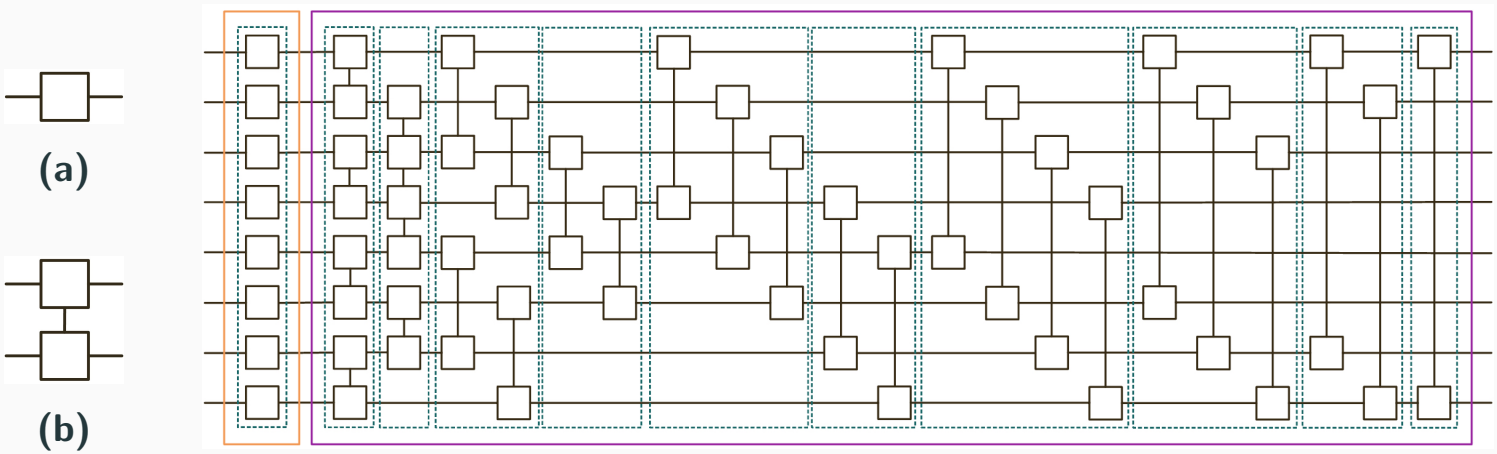
where

$$\mathcal{H}^\alpha = \mathbf{e}^\top \mathbb{S}^\alpha + \frac{1}{2}\mathbb{S}^{\alpha\top} C^{\alpha,\alpha}\, \mathbb{S}^\alpha, \qquad \alpha \in \{X, Y, Z\},$$

and

$$\mathrm{e}^{-\mathrm{i}h\mathcal{H}^\alpha} = \prod_{\ell=1}^{n} \mathrm{e}^{-\mathrm{i}h\mathbf{e}^\alpha_\ell \alpha_\ell} \prod_{j=1}^{n} \prod_{k=j+1}^{n} \mathrm{e}^{-\mathrm{i}hC^{\alpha,\alpha}_{j,k}\alpha_j\alpha_k},$$

computed exactly using n single-qubit gates and $\mathcal{O}\left(n^2\right)$ coupling gates.



(a)

(b)

(c)

High order Trotterisations

Trotterisation is one of the earliest candidates for Hamiltonian simulation.

IBM (14 June 2023) used Trotter splitting for an Ising chain: Kim, Eddins, Anand, Wei, van den Berg, Rosenblatt, Nayfeh, Wu, Zaletel, Temme & Kandala (2023), 'Evidence for the utility of quantum computing before fault tolerance', Nature 618, 500–505.

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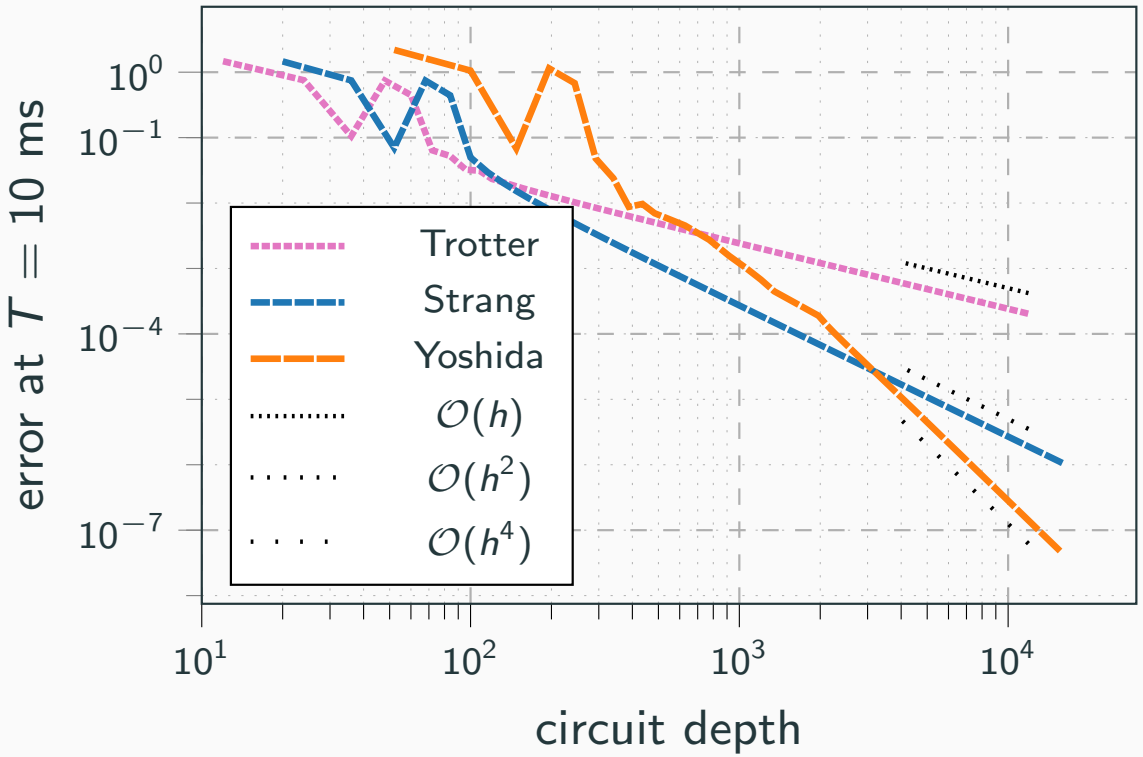

No good reason to use Trotter instead of Strang, even for NISQ

Chen, Foroozandeh, Budd & S. 2023. *Quantum simulation of highly-oscillatory many-body Hamiltonians for near-term devices*, submitted

Machine learned Trotterisations

$$\mathrm{e}^{h(A+B)} \approx \mathrm{e}^{a_1 hB}\mathrm{e}^{b_1 hA}\mathrm{e}^{a_2 hB}\ldots\mathrm{e}^{b_n hA}\ldots\mathrm{e}^{a_2 hB}\mathrm{e}^{b_1 hA}\mathrm{e}^{a_1 hB}$$

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For moderate accuracies (10^{-1}–10^{-4}), often what matters is the error constant, not the order of convergence.

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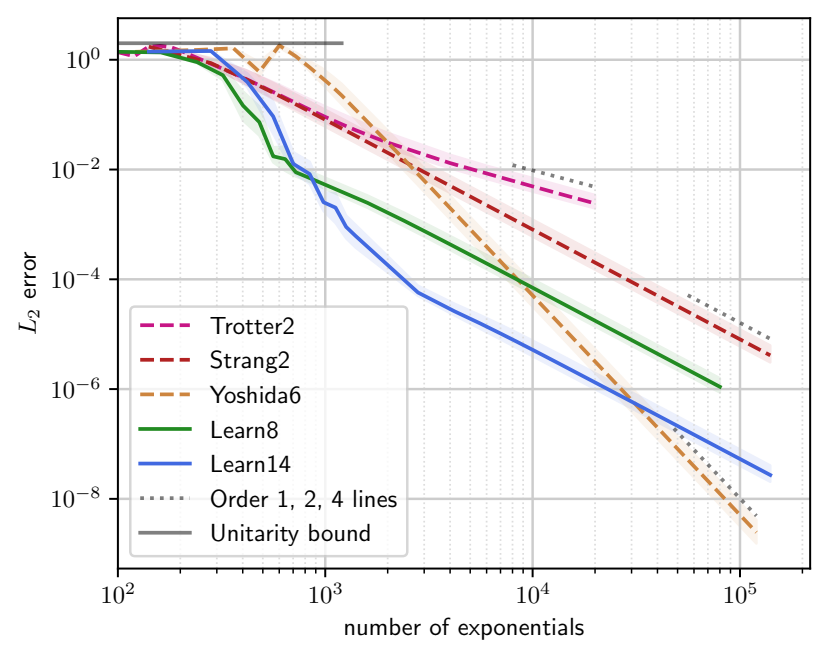
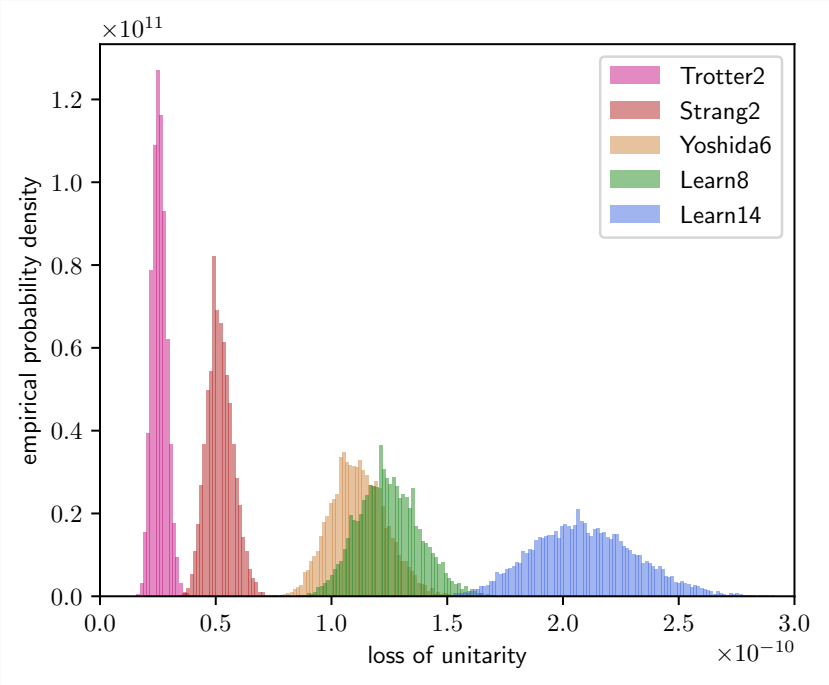
Traditionally: solve algebraic order conditions that result from Taylor expansion

For moderate accuracies (10^{-1}–10^{-4}), often what matters is the error constant, not the order of convergence.





Kreusser, Lockyer, Müller, & S 2024. *Learning efficient and provably convergent splitting methods*

Computing e^A or $\mathrm{e}^A u_0$

C. Moler & C. V. Loan, *Nineteen Dubious Ways to Compute the Exponential of a Matrix, Twenty-Five Years Later*, SIAM Review (2003).

	Diagonalisation	Scaling and Squaring	Splitting
If	$A = UDU^*$	$\|A\| > 1$	$A = B + C$
	$\mathrm{e}^A = U\mathrm{e}^D U^*$	$\mathrm{e}^A = \left(\mathrm{e}^{A/n}\right)^n$	$\mathrm{e}^A = \lim_{n\to\infty}\left(\mathrm{e}^{B/n}\mathrm{e}^{C/n}\right)^n$
Fast when	Uu_0 and $U^* u_0$ cheap	$\|A\| < 1$ needed	$\mathrm{e}^B, \mathrm{e}^C$ cheap

	Asymptotic $z \to 0$	Approximate e^z on spectrum $z \in [a, b] \subseteq \sigma(A)$	**Iterative** Use A and u_0
Polynomial	Taylor $\sum_{k=0}^{n} \frac{z^k}{k!}$	Chebyshev $J_0(\mathrm{i}) + 2\sum_{k=1}^{n} \mathrm{i}^k J_k(-\mathrm{i}) T_k(z)$	Polynomial Krylov
Rational	Padé $\frac{1+\frac{1}{2}z+\frac{1}{12}z^2}{1-\frac{1}{2}z+\frac{1}{12}z^2}$	?	Rational Krylov

(Polynomial) Krylov methods

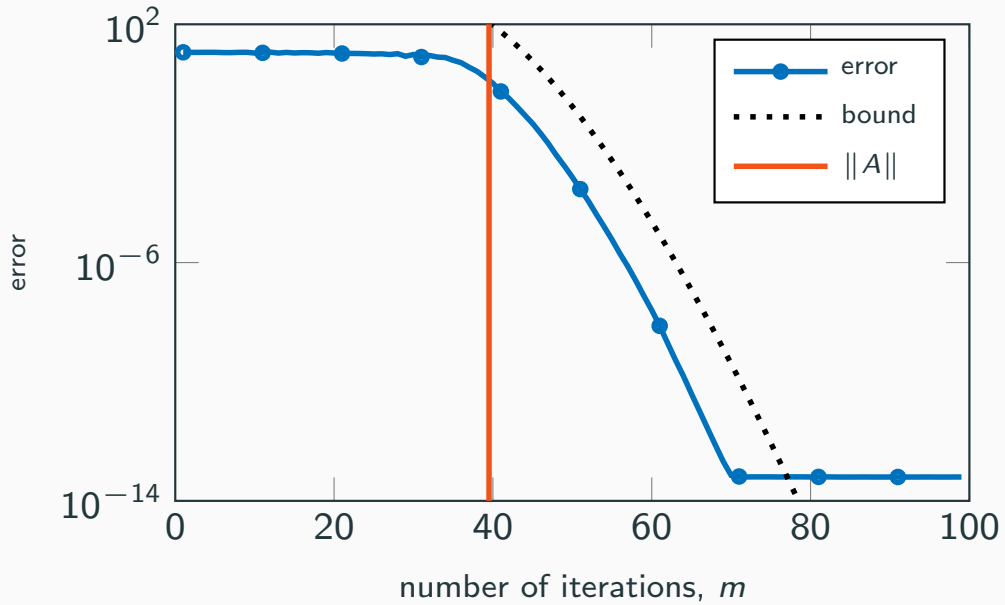
Krylov subspace

$$\mathcal{K}_m(A, u_0) = \operatorname{span}\{u_0, Au_0, \ldots, A^{m-1}u_0\}$$

with basis $\mathcal{V}_m$ and tridiagonal $\mathcal{H}_m$ has super-linear accuracy,

$$\left\| \mathrm{e}^{A}u_0 - \mathcal{V}_m \mathrm{e}^{\mathcal{H}_m}\mathcal{V}_m^* u_0 \right\| \leq C \left(\frac{\mathrm{e}\rho}{2m}\right)^m$$

conserves norm and energy but not unitarity.



accurate once $m \geq \rho = \|A\|$, is surpassed (Hochbruck & Lubich 1997).

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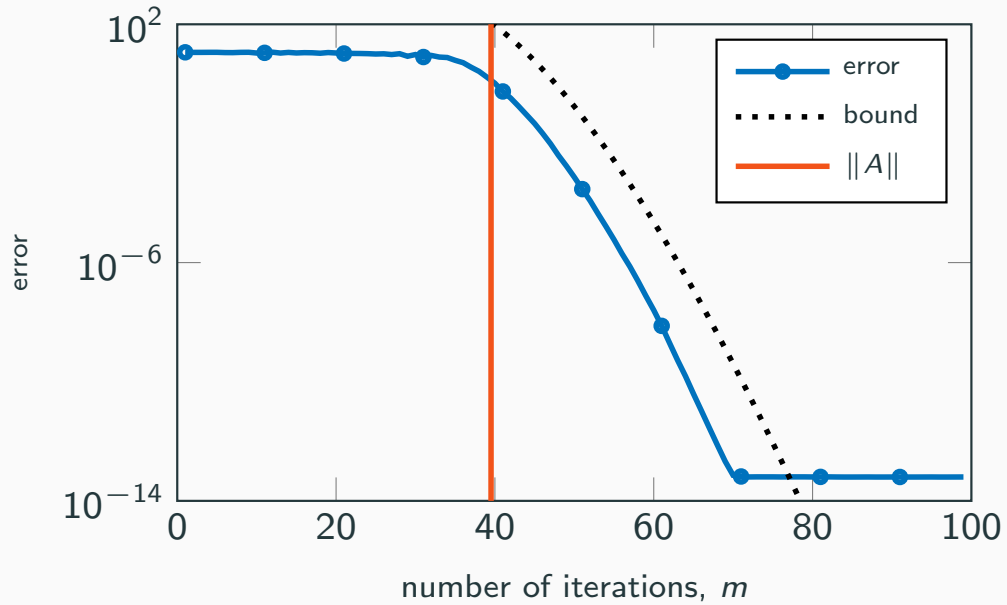

accurate once $m \geq \rho = \|A\|$, is surpassed (Hochbruck & Lubich 1997). High accuracy for small steps, but ineffective for large steps.

Shift-and-Invert (Sal) method

$$\mathcal{Q}_m(A, u_0) = \mathcal{K}_m((A - \alpha I)^{-1}, u_0),$$

is equivalent to Polynomial Krylov with shift-inverted matrix $(A - \alpha I)^{-1}$ and

$$\underbrace{\mathrm{e}^{hA} u_0}_{\varphi_h^A(u_0)} \quad \approx \quad \underbrace{\mathcal{V}_m \mathrm{e}^{h(\alpha I - H_m^{-1})} \mathcal{V}_m^* u_0}_{\Phi_h^A(u_0, \alpha)}$$

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How should we choose the shift α? Learning (Botchev, Grimm & M. Hochbruck 2013, Katrutsa, Botchev, & Oseledets 2019), Rational Krylov fitting (Berljafa & Güttel 2017)

Optimise an approximation of the local error:

$$\underbrace{\left\| \varphi_h^A(u_n) - \Phi_h^A(u_n, \alpha_n) \right\|}_{\text{true local error } \mathcal{L}(h, u_n, \alpha)} \quad \propto \quad \underbrace{\left\| \partial_t \Phi_h^A(u_n, \alpha_n) - A \Phi_h^A(u_n, \alpha_n) \right\|}_{\text{defect based estimate of local error } L(h, u_n, \alpha)}$$

$$\alpha_n^* = \operatorname{argmin}_{\alpha \in \Omega} \, L(h, u_n, \alpha)$$

adaptive (i.e., on-the-fly), unsupervised approach.

energy not conserved, error estimate asymptotic and expensive.

Rational Krylov methods: Rayleigh quotient

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Rayleigh quotient:

$$A_m = \mathcal{V}_m^* A \mathcal{V}_m.$$

The Rayleigh approximation:

$$\mathrm{e}^{hA} v \approx \beta \mathcal{V}_m \mathrm{e}^{hA_m} \mathcal{V}_m^* u_0.$$

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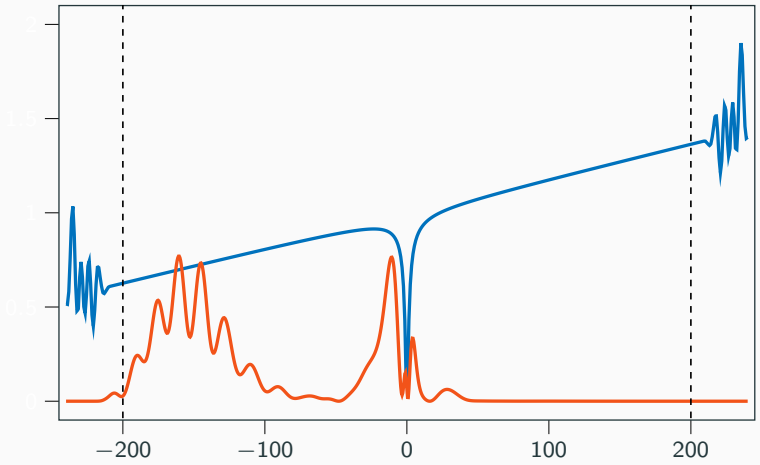
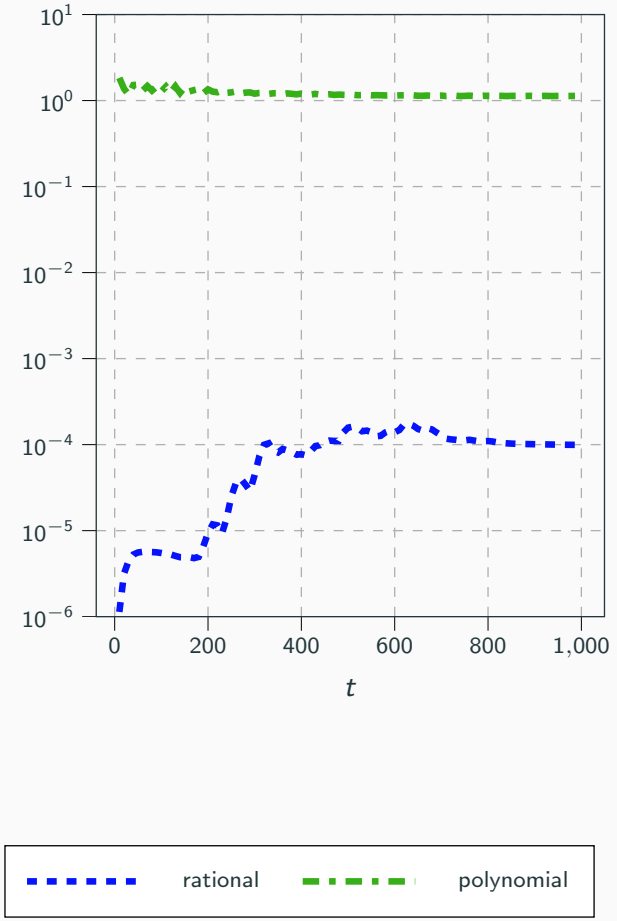
In practice, both Shift-and-Invert and Rayleigh quotion approaches work well with cheaper surrogates





Tennyson, Jawecki, Dolgov, & S., '*Optimal poles for the Shift-and-Invert method*', in preparation

Computing the matrix exponential

If we have good scalar approximations on the spectrum

$$\mathrm{e}^{\mathrm{i}x} \approx f(\mathrm{i}x), \quad x \in \sigma(\mathrm{H})$$

Then we have good approximation of the matrix exponential,

$$\mathrm{e}^{-\mathrm{i}t\mathrm{H}} = U\mathrm{diag}\left(\mathrm{e}^{-\mathrm{i}tE_k}\right)U^{-1} \approx U\mathrm{diag}(f(\mathrm{i}tE_k))U^{-1} = f(\mathrm{i}t\mathrm{H})$$

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- Based on polynomial Chebyshev approximation.
- Cannot conserve unitarity, norm, energy.
- May have stability issues (due to noise outside spectrum).

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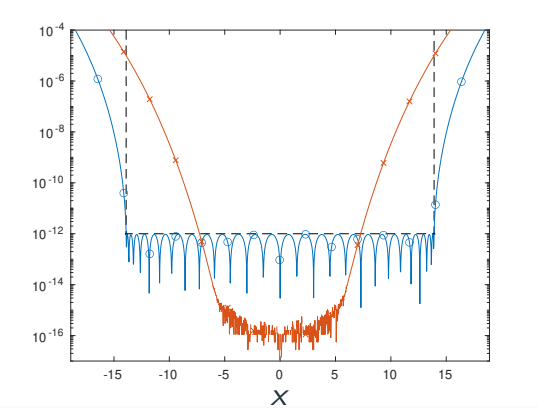
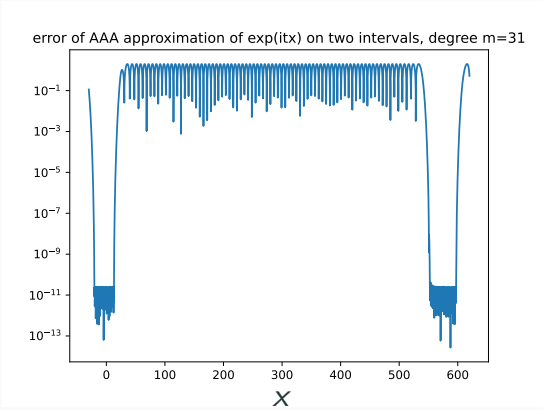
AAA & AAA–Lawson

AAA & AAA–Lawson (Nakatsukasa, Sète & Trefethen 2018, Nakatsukasa & Trefethen 2020) are *greedy* algorithms for rational approximations (i.e. fitting) based on the Loewner matrix framework.

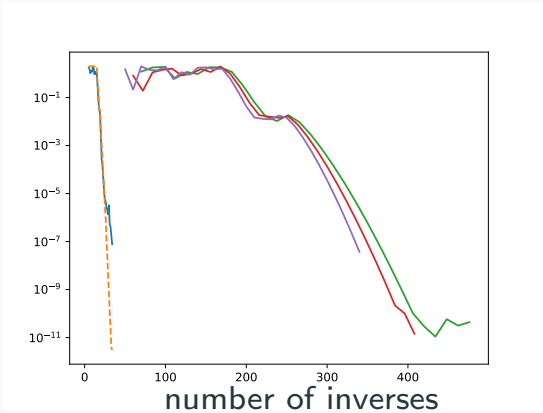
Padé vs AAA–Lawson



AAA–Lawson



(31, 31) AAA–Lawson vs Padé



Loewner matrix based rational approximations and interpolations are unitary (to machine precision when using a modified AAA/AAA–Lawson algorithm).

Jawecki & S 2023. *Unitarity of some barycentric rational approximants*, IMA J. Num. Anal.

Includes Antoulas & Anderson 1986, Mayo & Antoulas 2007, NST 2018 (AAA), NT 2020 (AAA–Lawson), JS (*submitted*) (interpolation at Chebyshev nodes, modified BRASIL algorithm, modified AAA–Lawson), ...

Best unitary rational approximation

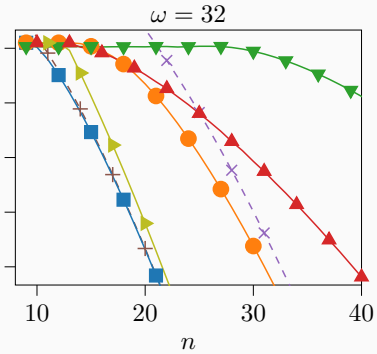
Theorem. For $\omega \in (0, (n+1)\pi)$, there exists a unique unitary best approximation $r \in \mathcal{U}_n$, i.e.,

$$\|r - \exp(\omega\cdot)\| = \inf_{u \in \mathcal{U}_n} \|u - \exp(\omega\cdot)\|, \qquad \|f\| := \sup_{x \in [-1,1]} |f(\mathrm{i}x)|,$$

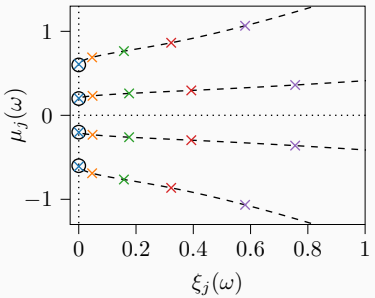
whose phase error equioscillates at $2n+2$ points, where max approx error is achieved. Moreover, r has minimal degree n, and distinct poles.

Three new algorithms: Interpolation at Chebyshev points, modified AAA–Lawson and BRASIL.

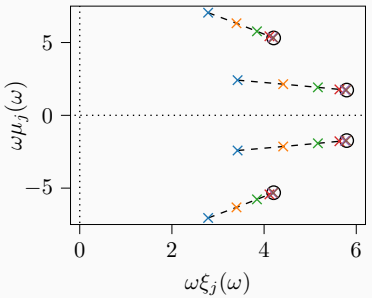
Superlinear convergence, A-stability, Time-symmetry

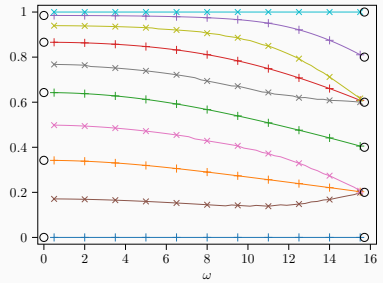


convergence rates



Poles





interpolation nodes

equioscillation points

Jawecki & S 2023. *Unitary rational best approximations to the exponential function*, submitted.

How to compute the matrix exponential?

C. Moler & C. V. Loan, *Nineteen Dubious Ways to Compute the Exponential of a Matrix, Twenty-Five Years Later*, SIAM Review (2003).

	Asymptotic $z \to 0$	Approximate e^z on spectrum $z \in [a, b] \subseteq \sigma(A)$	Iterative Use A and u_0
Polynomial	Taylor $\sum_{k=0}^{n} \frac{z^k}{k!}$	Chebyshev $J_0(\mathrm{i}) + 2\sum_{k=1}^{n} \mathrm{i}^k J_k(-\mathrm{i})\, T_k(z)$	Lanczos
Rational	Padé $\frac{1+\frac{1}{2}z+\frac{1}{12}z^2}{1-\frac{1}{2}z+\frac{1}{12}z^2}$	unitary best approximations	Rational Krylov

Other techniques: Diagonalisation & Spectral methods, Scaling and Squaring, Splitting

AAA [NST 18], AAA–Lawson [NT 20], their unitary modifications [JS 23], and three new algorithms [JS *submitted*].

- Jawecki & S. 2023. *Unitarity of some barycentric rational approximants*, IMA J. Num. Anal.
- Jawecki & S. 2023. *Unitary rational best approximations to the exponential function*, submitted.
- Jawecki & S., in preparation.

Outline

Hamiltonian Simulation

$$\mathrm{i}\partial_t \psi \;=\; \mathrm{H}(\psi, t)\,\psi, \qquad \psi(t) \in \mathscr{H}.$$

1. Linear

$$\partial_t u = A u$$

2. **Driven**

$$\partial_t u = A(t) u$$

3. Non-linear

$$\partial_t u = A u + N(u)$$

Driven systems

The solution to $u'(t) = A(t)u(t)$ can be approximated by

- Autonomisation (Sanz-Serna & Portillo 1996), if $A(t) = B(t) + C$

$$u_{n+1} = \left(\prod_{k=1}^{s} \mathrm{e}^{b_k h B(\tau_k)} \mathrm{e}^{c_k h C} \right) u_n, \qquad \tau_{k+1} = \tau_k + c_k h, \quad \tau_0 = t_n,$$

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- Commutator-free (Alvermann & Fehske 2011)

$$\exp(\Theta) \approx \exp\left(\sum_{k=1}^{n} c_{1k} h\, A(t_k) \right) \ldots \exp\left(\sum_{k=1}^{n} c_{pk} h\, A(t_k) \right).$$

Blanes, Casas & Thalhammer 2017, Rational extension (S. Maslovskaya, Offen, Ober-Blöbaum, S. & Wembe 2024, Commutator-free Cayley methods, *submitted*)

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- Magnus expansion (Magnus 1954)

$$u(h) = \exp\left(\Theta(h)\right) u_0, \qquad \Theta(h) = \int_0^h A(\xi)\,\mathrm{d}\xi - \tfrac{1}{2} \int_0^h \int_0^\xi [A(\zeta), A(\xi)]\,\mathrm{d}\zeta\,\mathrm{d}\xi + \mathcal{O}\left(h^5\right)$$

Magnus–Krylov (Kormann, Holmgren & Karlsson 2008, Iserles, Kropielnicka, & S. 2018, SINUM), Magnus–Zassenhaus (IKS 2016, Proc. Roy. Soc. A, IKS 2019a, J. Comput. Phys.), Magnus–Splittings for laser–matter (IKS 2019a, Comput. Phys. Commun., S. 2019c, J. Chem. Phys.)

Is Magnus expansion DoA for quantum algorithms?

$$A(t) = -\mathrm{i}\mathrm{H}(t), \quad \mathrm{H}(t) = \sum_{k=1}^{n} \sum_{\alpha \in \{X,Y,Z\}} \mathrm{e}_k^{\alpha}(t)\, \alpha_k + \frac{1}{2} \sum_{j,k=1}^{n} \sum_{\alpha,\beta \in \{X,Y,Z\}} C_{j,k}^{\alpha,\beta}\, \alpha_j\, \beta_k$$

A has $\mathcal{O}(|C|) = \mathcal{O}\left(n^2\right)$ terms. Does $\int_0^h \int_0^{\xi} [A(\zeta), A(\xi)]\, \mathrm{d}\zeta\, \mathrm{d}\xi$ have $\mathcal{O}\left(|C|^2\right) = \mathcal{O}\left(n^4\right)$ terms?

Instead, other approaches were developed: Dyson series (Kieferova et al. 2019), time-ordered operators (Watkins et al. 2022), L1 norm scaling (Berry et al. 2020), permutation expansion (Chen et al. 2021), slowly varying Hamiltonians (Haah et al. 2021), interaction picture (Low & Wiebe 2018), Floquet approach (Mizuta et al. 2023), Schrödingerization (Jin, Liu, Yu 2022)

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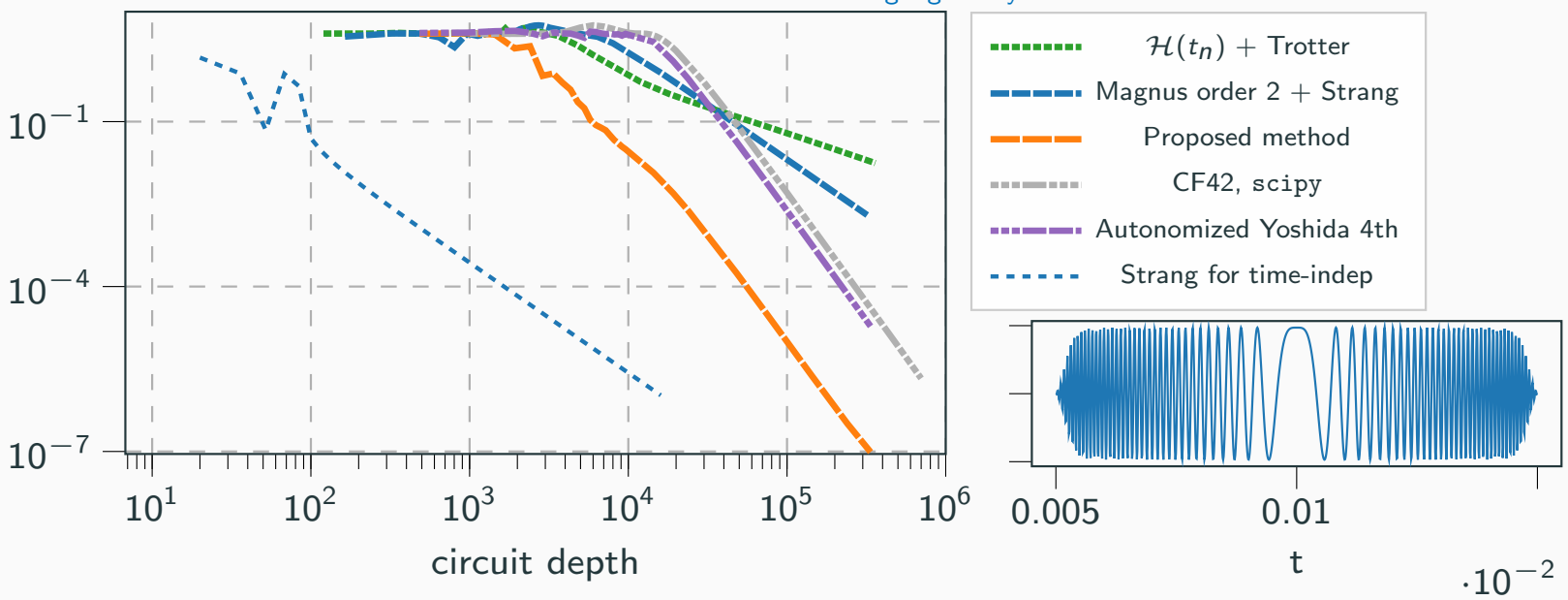
$$\mathrm{e}^{\mathrm{i}\frac{2}{h}\mathbf{u}^{\top}\mathbb{S}} \underbrace{\mathrm{e}^{-\mathrm{i}\check{\mathbf{r}}^{\top}\mathbb{S} - \mathrm{i}\frac{h}{2}\mathbb{S}^{\top} C\, \mathbb{S}}}_{\text{reuse 4th order Trotterised circuit}} \underbrace{\mathrm{e}^{-\mathrm{i}\frac{2}{h}\mathbf{u}^{\top}\mathbb{S}}}_{\text{two single-gate layers}} = \mathrm{e}^{\Theta_2} + \mathcal{O}\left(h^5\right)$$



Chen, Foroozandeh, Budd & S. 2023. submitted

related: 2 controls Ikeda, Abrar, Chuang & Sugiura 2023, Quantum., commutator-free Casares, Zini & Arrazola

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- Autonomisation (Sanz-Serna & Portillo 1996), if $A(u, t) = Lu + g(u, t)u$

$$u^{[k+1]} = \mathrm{e}^{b_k h L} \mathrm{e}^{c_k h g(u^{[k]}, \tau_k)} u^{[k]}, \qquad \tau_{k+1} = \tau_k + b_k h, \quad \tau_0 = t_n,$$
$$u_{n+1} = u^{[s]}, \qquad u^{[0]} = u_n$$

Related: dilation techniques such as Schrödingerization (Jin, Liu, Yu 2022)

- Exponential Integrators (Hochbruck & Ostermann 2000), $A(u) = Lu + g(u)u$,

$$u_{n+1} = \mathrm{e}^{hL} u_n + L^{-1}(\mathrm{e}^{hL} - I) g(u_n) u_n$$

not a geometric integrator

- Iterative linearisations

$$u^{[k+1]}(h) = \exp\left(\Theta^{[k]}(h)\right) u^{[k]},$$

$$\Theta^{[k]}(h) = \int_0^h A(u^{[k]}(\xi), \xi)\, \mathrm{d}\xi - \tfrac{1}{2} \int_0^h \int_0^\xi \left[A(u^{[k]}(\zeta), \zeta), A(u^{[k]}(\xi), \xi)\right] \mathrm{d}\zeta\, \mathrm{d}\xi + \mathcal{O}\left(h^5\right).$$

$$u_{n+1} = u^{[3]}, \qquad u^{[0]} = u_n$$

Chen, Iserles, Kropielnicka, & S. 2024, Computation of some dispersive equations through their iterated linearisation, *submitted*.

Takeaways

Hamiltonian Simulation is central to quantum computing

- early candidate for quantum supremacy
- has real-world applications
- is a building block for many quantum algorithms

Correspondence between Classical and Quantum algorithms

- Qubitization
  - achieves additive complexity, based on Chebyshev approximation
  - does not conserve unitarity, norm and energy; may have stability issues
- Unitary rational approximations (Padé, AAA, best approximation,...)
  - faster convergence, extremely stable, conserve unitarity, norm and energy
  - currently no quantum algorithm
- Machine learned Trotterisations (splittings)
  - convergence guarantees, conserve unitarity, norm and modified energy
  - allow long time-steps, low error constants
  - can they help create optimized cricuits?
  - can we do this in an unsupervised way?
- Magnus based methods work well for driven spin systems