# Accelerating Algorithmic Quantum and Classical Simulations by Corrected Product Formulas

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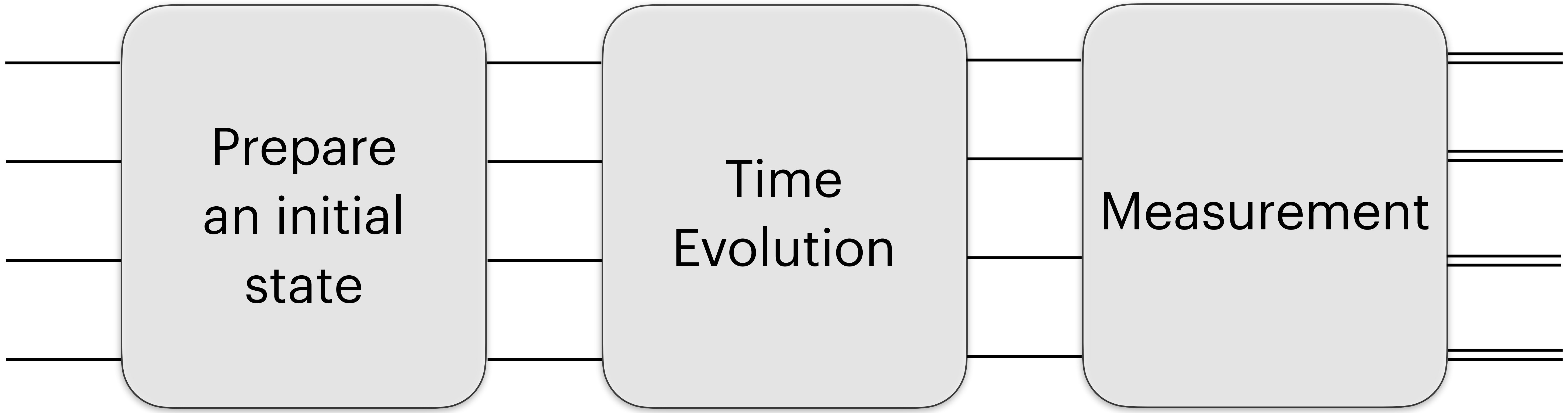
October 9, 2025 — Institut Quantique

arXiv:2409.08265

# Algorithmic quantum simulation

… the most natural application of quantum computers!




**Hamiltonian simulation problem**

**Given:** Description of $H$
Evolution time $t$
Error tolerance $\varepsilon$

**Task:** Construct U by a sequence of "gates" such that

$$\| e^{-iHt} - U \| \leq \varepsilon$$

**Goal:** Develop a resource-efficient simulation…

… ideally with a minimal cost as a function of $t$, $\varepsilon$ and parameters of $H$.

# Hamiltonian simulation as an algorithmic primitive

- **Measurement as Hamiltonian simulation**

[Knill, Ortiz, Somma; 07]

$$\langle\psi|\mathbf{M}|\psi\rangle \approx -\operatorname{Im}\left(\langle\psi|e^{-i\mathbf{M}t}|\psi\rangle\right)/t$$

- **Quantum linear algebra**

[Harrow, Hassidim, Lloyd; 09]
[Childs, Kothari, Somma; 17]
...

$f(A) =$ combination of Hamiltonian evolutions

Reduction in resource requirements $\longrightarrow$ scalable quantum simulation!

# Approaches for Hamiltonian simulation

- Product formulas — the original approach!

## Universal Quantum Simulators

SETH LLOYD Authors Info & Affiliations

*SCIENCE* • 23 Aug 1996 • Vol 273, Issue 5278 • pp. 1073-1078 • DOI: 10.1126/science.273.5278.1073

Feynman's 1982 conjecture, that quantum computers can be programmed to simulate any local quantum system, is shown to be correct.

Home > Communications in Mathematical Physics > Article

## Efficient Quantum Algorithms for Simulating Sparse Hamiltonians

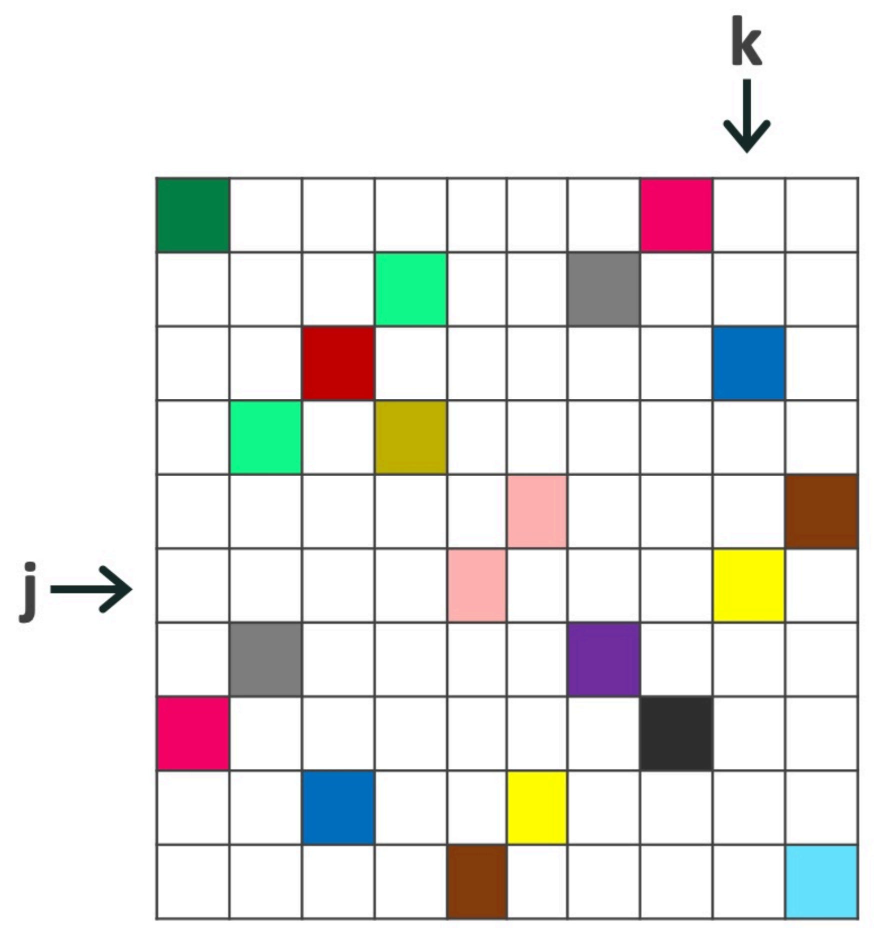
Published: 14 December 2006

Volume 270, pages 359–371, (2007)

Dominic W. Berry, Graeme Ahokas, Richard Cleve & Barry C. Sanders

- Local Hamiltonians
- Cost: $\mathcal{O}(t^2/\varepsilon)$

- Sparse Hamiltonians
- Cost: $\mathcal{O}(t^{1+1/2k}/\varepsilon^{1/2k})$
- No fast-forwarding! $\Omega(t)$




Sparse Hamiltonian

# Approaches for Hamiltonian simulation

- Product formulas (PFs)
- Quantum walk [Berry, Childs; 12]

$$\mathcal{O}(t/\sqrt{\varepsilon})$$

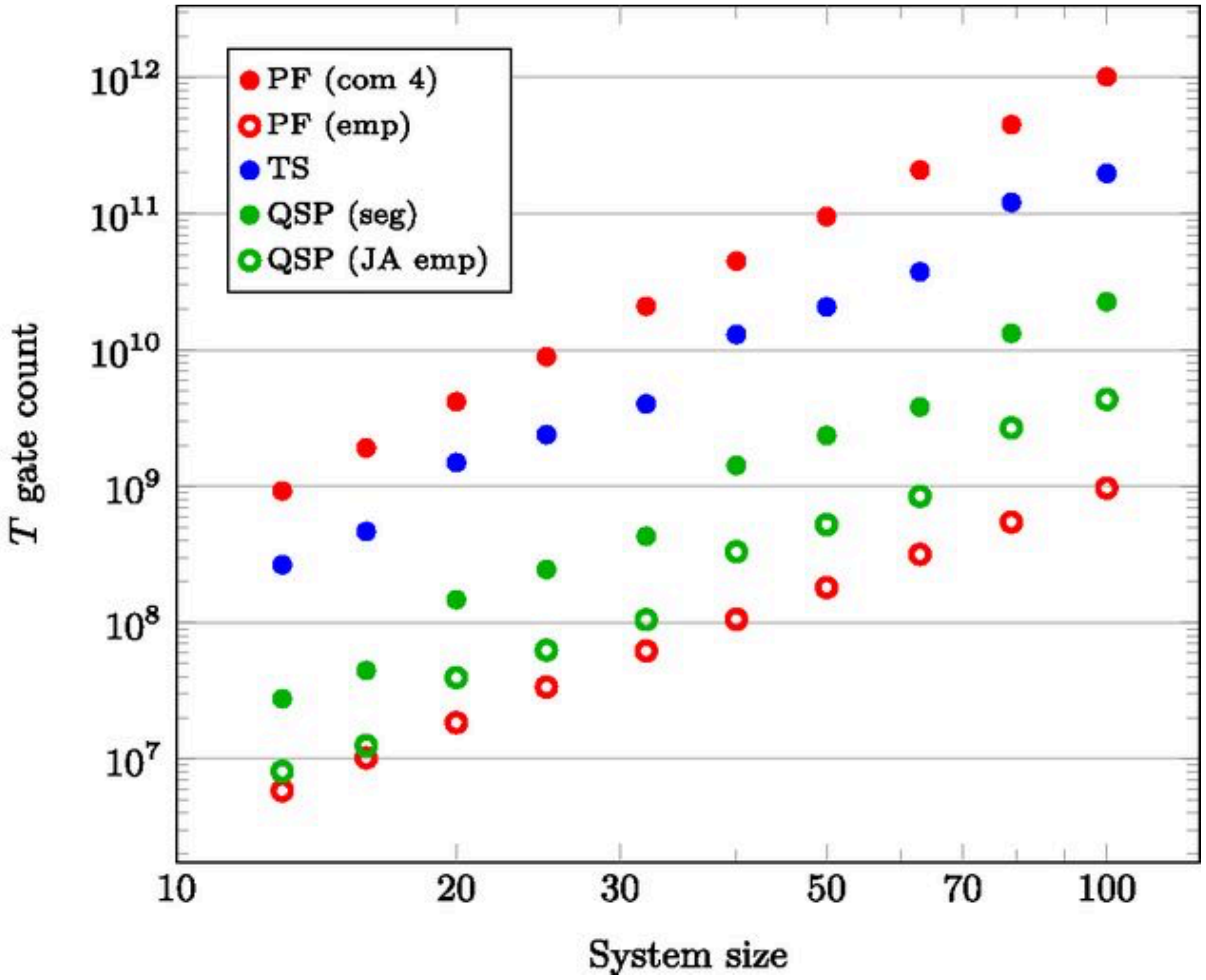
- Truncated Taylor series (TS) (Linear combination of unitaries) [Berry, Childs, Cleve, Kothari, Somma; 12]

$$\mathcal{O}\left(t\frac{\log(t/\varepsilon)}{\log\log(t/\varepsilon)}\right)$$

- Quantum signal processing (QSP) [Low, Chuang; 17]

$$\mathcal{O}\left(t+\frac{\log(1/\varepsilon)}{\log\log(1/\varepsilon)}\right)$$

... and many others!




Plot from: [Childs, Maslov, Nam, Ross, Su; 18]

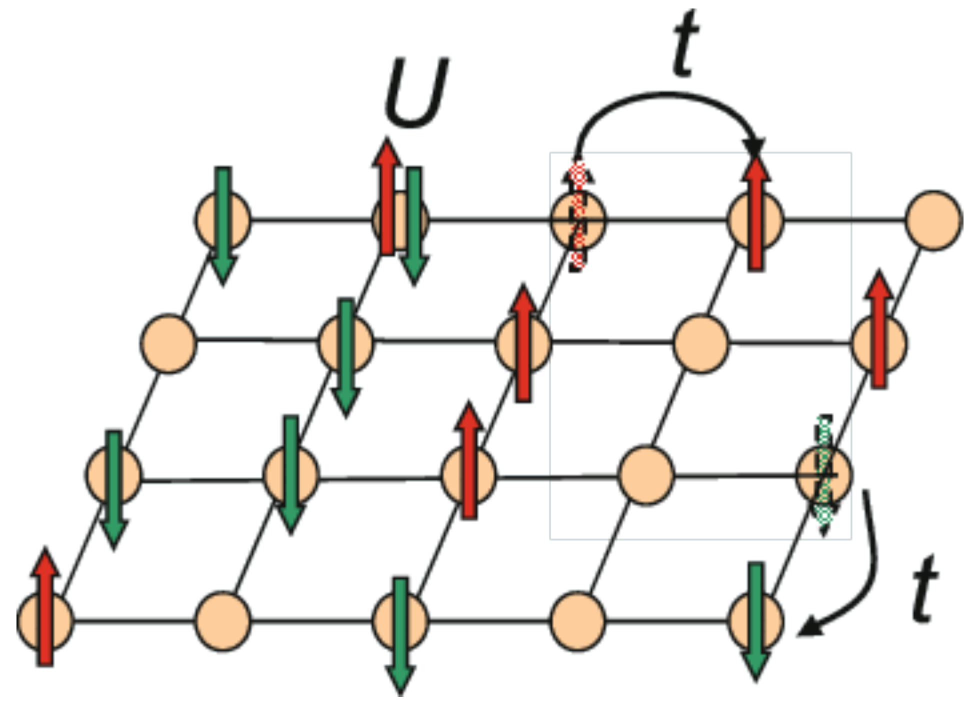
# Setup and assumptions

$$H = \sum_j H_j = A + \alpha B$$

Partitions with similar norm: $\|A\| \approx \|B\|$

Perturbed systems $\alpha \ll 1$

Non-perturbed systems $\alpha = 1$




Lattice Hamiltonians, e.g., Hubbard model

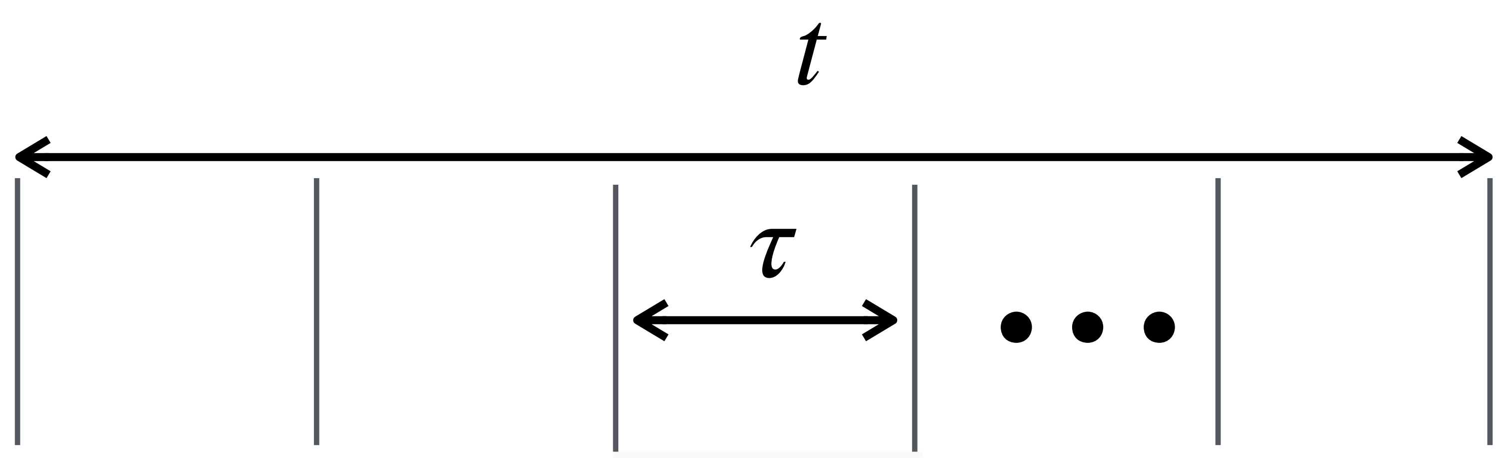
$$H = \underbrace{-t_{\text{hop}} \sum_{j,\sigma} (c^\dagger_{j,\sigma} c_{j+1,\sigma} + c^\dagger_{j+1,\sigma} c_{j,\sigma})}_{\text{kinetic (hopping) term}} + \underbrace{U_{\text{int}} \sum_j n_{j,\uparrow} n_{j,\downarrow}}_{\text{potential term}}$$

Weak coupling: $U_{\text{int}} \ll t_{\text{hop}}$

Strong coupling: $t_{\text{hop}} \ll U_{\text{int}}$

Generic Hamiltonians of the form $H = T + V$ $\quad \|V\| \ll \|T\|$

# Product formulas (PFs)




$\tau = t/r$

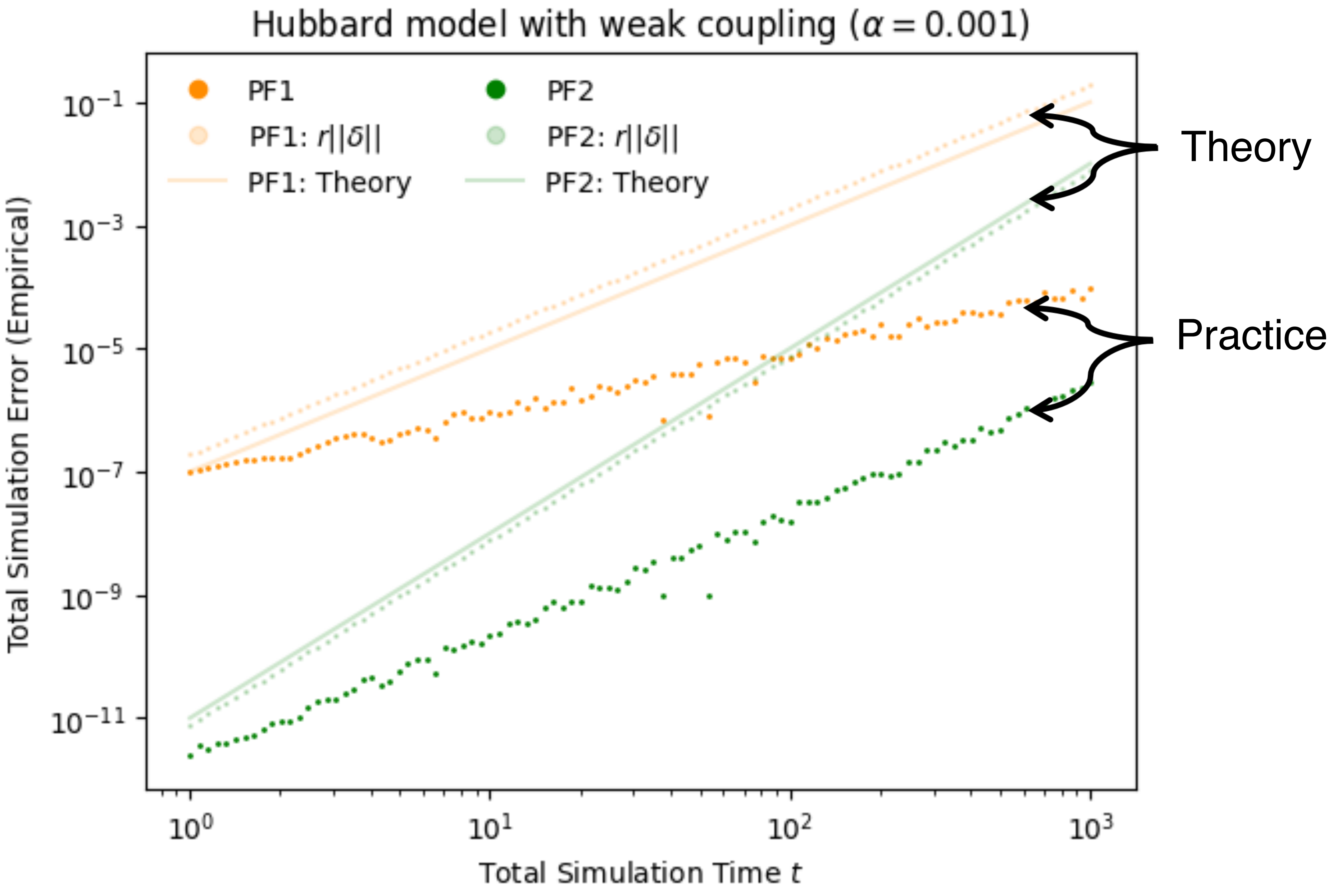
$e^{-iH\tau}$

| | | Step error | Total error |
|---|---|---|---|
| $S_1(\tau) =$ | $e^{-iA\tau}\, e^{-i\alpha B\tau}$ | $\mathcal{O}(\alpha\tau^2)$ | $r\,\mathcal{O}(\alpha\tau^2) \longrightarrow r = \mathcal{O}(\alpha t^2/\varepsilon)$ |
| $S_2(\tau) =$ | $e^{-iA\frac{\tau}{2}}\, e^{-i\alpha B\tau}\, e^{-iA\frac{\tau}{2}}$ | $\mathcal{O}(\alpha\tau^3)$ | $r = \mathcal{O}(\sqrt{\alpha/\varepsilon}\, t^{3/2})$ |
| $S_4(\tau) =$ | $S_2(\tau_2)\, S_2(\tau_2)\, S_2(\tau_2')\, S_2(\tau_2)\, S_2(\tau_2)$ | $\mathcal{O}(\alpha\tau^5)$ | $\vdots$ |
| $S_{2k}(\tau) =$ | $\left[S_{2k-2}(\tau_k)\right]^2 S_{2k-2}(\tau_k')\left[S_{2k-2}(\tau_k)\right]^2$ | $\mathcal{O}(\alpha\tau^{2k+1})$ | $r = \mathcal{O}((\alpha/\varepsilon)^{1/2k}\, t^{1+1/2k})$ |

[Suzuki; 92]

# Appealing features of product formulas

- Perform much better in practice




Large gap between errors in theory and practice!

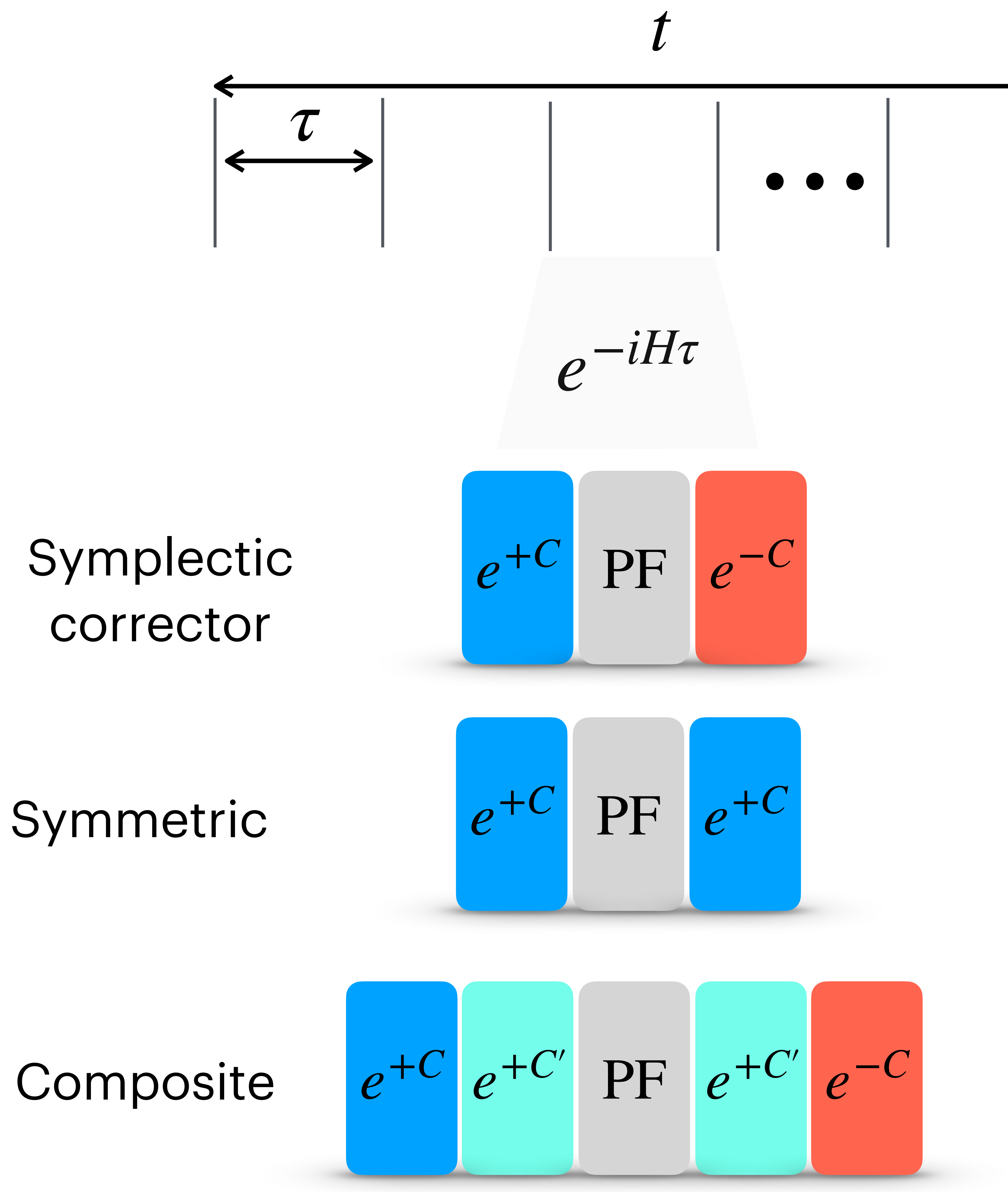
- No need for ancilla qubits
- No complicated oracles

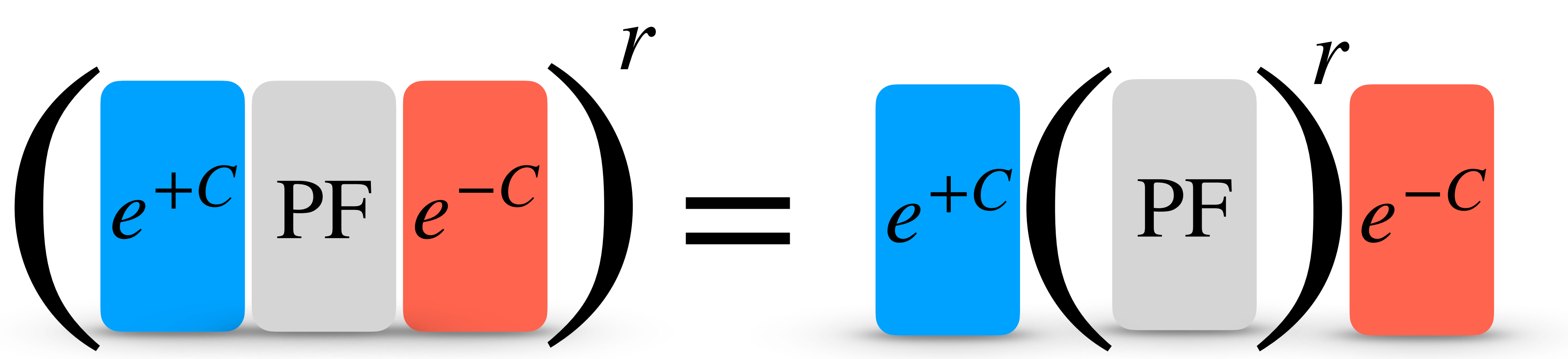
$$e^{-iH\tau} \approx e^{-iA\frac{\tau}{2}} e^{-i\alpha B\tau} e^{-iA\frac{\tau}{2}}$$

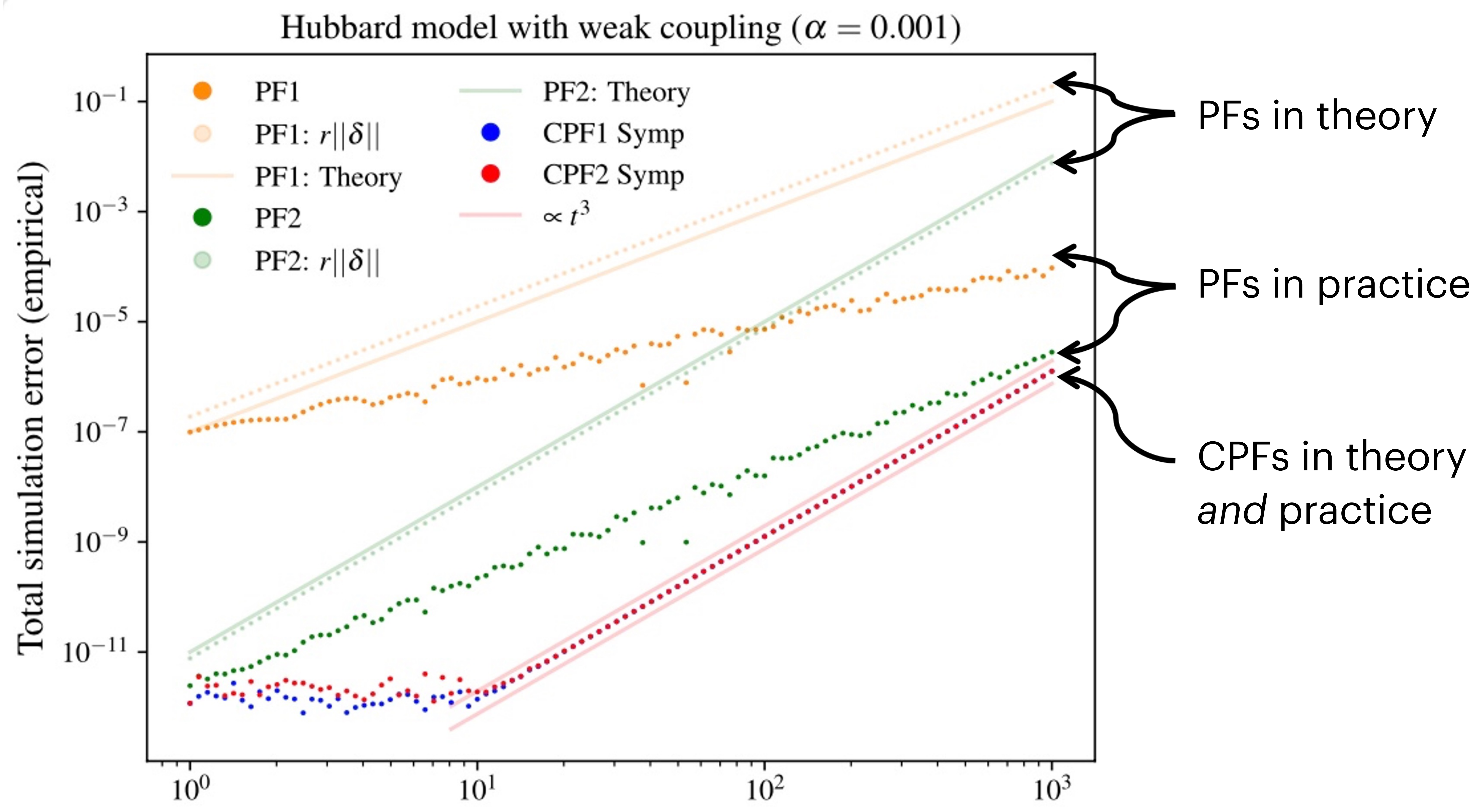
**Corrected product formulas:**

remove the gap and have the same features!

# Corrected product formulas (CPFs)




**CPFs remove the gap and have the same features of PFs!**

# A symplectic corrector for PF2

$$\mathrm{e}^{\frac{\lambda}{2}A}\mathrm{e}^{\lambda\alpha B}\mathrm{e}^{\frac{\lambda}{2}A} = \exp\left(\lambda H + \sum_{j=1}^{\infty}\lambda^{2j+1}E_{2j+1}\right)$$

Third-order term:

$$E_3 = -\frac{1}{24}[A,[A,\alpha B]] + \frac{1}{12}[\alpha B,[\alpha B, A]]$$

$$K \equiv \lambda H + \sum_{j=1}^{\infty}\frac{B_{2j}(1/2)}{2j!}\lambda^{2j+1}\,\mathrm{ad}_A^{2j}(\alpha B)$$

$B_j(x)$ : Bernoulli polynomial

$$\mathrm{e}^{+C}\mathrm{e}^{K}\mathrm{e}^{-C} = \mathrm{e}^{K'}$$

$$K' = \mathrm{e}^{\mathrm{ad}_C}K = K + [C,K] + \cdots$$

$$\mathrm{ad}_A(B) := [A,B]$$

$$C = \sum_{j=1}^{k}\frac{B_{2j}(1/2)}{(2j)!}\lambda^{2j}\,\mathrm{ad}_A^{2j-1}(B)$$

Error: $\mathcal{O}(\alpha\tau^3) \to \mathcal{O}(\alpha^2\tau^3 + \tau^{2k+3})$

# of steps: $r \to \sqrt{\alpha}\, r$

# Corrected product formulas

Low-order formulas are used in practice

| Product Formula | Error Bound for Non-corrected PF | Correctors | Error Bound for Corrected PF |
|---|---|---|---|
| PF1 | $\mathcal{O}(\alpha\lvert\lambda\rvert^2)$ | $C_{\text{symp}} = \frac{\lambda}{2}\alpha B$ | $\mathcal{O}\left(\alpha\lvert\lambda\rvert^3\right)$ |
| | | $C_{\text{symp}} = \frac{\lambda}{2}\alpha B + \frac{\lambda^2}{12}\text{ad}_A(\alpha B)$ | $\mathcal{O}\left(\alpha^2\lvert\lambda\rvert^3 + \alpha\lvert\lambda\rvert^4\right)$ |
| | | $C_{\text{sym}} = -\frac{\lambda^2}{4}\text{ad}_A(\alpha B) - \frac{\lambda^3}{12}\text{ad}^2_{\alpha B}(A)$ | $\mathcal{O}\left(\alpha\lvert\lambda\rvert^3\right)$ |
| | | $C_{\text{com}} = C_{\text{symp}} \circ C_{\text{sym}}$ with $C_{\text{symp}} = \frac{\lambda^2}{12}\text{ad}_A(\alpha B)$ | $\mathcal{O}(\alpha\lvert\lambda\rvert^4)$ |
| PF2 | $\mathcal{O}\left(\alpha\lvert\lambda\rvert^3\right)$ | $C_{\text{symp}} = -\frac{\lambda^2}{24}\text{ad}_A(\alpha B)$ | $\mathcal{O}\left(\alpha^2\lvert\lambda\rvert^3 + \alpha\lvert\lambda\rvert^5\right)$ |
| | | $C_{\text{com}} = C_{\text{sym}} \circ C_{\text{symp}}$ with $C_{\text{sym}} = -\frac{\lambda^3}{48}\text{ad}^2_{\alpha B}(A)$ | $\mathcal{O}\left(\alpha\lvert\lambda\rvert^5\right)$ |
| | | $C_{\text{symp}} = \sum_{j=1}^{k} \frac{B_{2j}(\frac{1}{2})}{(2j)!}\lambda^{2j}\text{ad}_A^{2j-1}(\alpha B)$ | $\mathcal{O}\left(\alpha^2\lvert\lambda\rvert^3 + \alpha\lvert\lambda\rvert^{2k+3}\right)$ |
| PF4 | $\mathcal{O}\left(\alpha\lvert\lambda\rvert^5\right)$ | $C_{\text{symp}} = c\lambda^4\text{ad}^3_A(\alpha B)$ with $c$ a known constant | $\mathcal{O}\left(\alpha^2\lvert\lambda\rvert^5\right)$ |

# Corrected product formulas

- Suzuki's product formulas

| | | Error | |
|---|---|---|---|
| PF2$k$ | $S_{2k}(\lambda) := [S_{2k-2}(p_k\lambda)]^2 S_{2k-2}((1-4p_k)\lambda)[S_{2k-2}(p_k\lambda)]^2$ | $\mathcal{O}\left(\alpha\lvert\lambda\rvert^{2k+1}\right)$ | |
| CPF2$k$ | $S^c_{2k}(\lambda) := \left[S^c_{2k-2}(a_k\lambda)\right]^2 S^c_{2k-2}((1-4a_k)\lambda)\left[S^c_{2k-2}(a_k\lambda)\right]^2$ | $\mathcal{O}\left(\alpha^2\lvert\lambda\rvert^{2k+1}\right)$ | Symplectic |
| | | $\mathcal{O}\left(\alpha\lvert\lambda\rvert^{2k+3}\right)$ | Composite |

- Yoshida's product formulas (YPFs)

$$S_m(\lambda) = \left(\prod_{j=m}^{1} S_2(w_j\lambda)\right) S_2(w_0\lambda) \left(\prod_{j=1}^{m} S_2(w_j\lambda)\right)$$

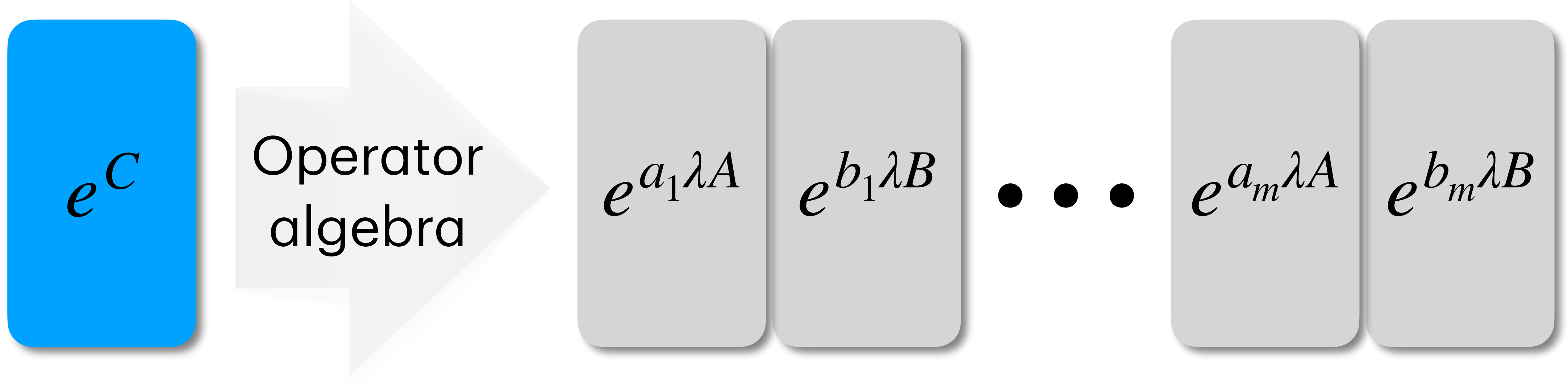
$\{\omega_j\}$: solutions of nonlinear equations

| Product Formula | Error Bound for Non-corrected YPF | Correctors | Error Bound for Corrected YPF |
|---|---|---|---|
| YPF6 | $\mathcal{O}\left(\alpha\lvert\lambda\rvert^7\right)$ | $C_{\text{symp}} = c\lambda^6 \text{ad}_A^5(\alpha B)$ | $\mathcal{O}\left(\alpha^2\lvert\lambda\rvert^7 + \alpha\lvert\lambda\rvert^9\right)$ |
| YPF8 | $\mathcal{O}\left(\alpha\lvert\lambda\rvert^9\right)$ | $C_{\text{symp}} = c\lambda^8 \text{ad}_A^7(\alpha B)$ | $\mathcal{O}\left(\alpha^2\lvert\lambda\rvert^9 + \alpha\lvert\lambda\rvert^{11}\right)$ |
| YPF2$k$, $k = 3, 4, 5$ | $\mathcal{O}\left(\alpha\lvert\lambda\rvert^{2k+1}\right)$ | $C_{\text{symp}} = \sum_{j=1}^{k} \frac{B_{2j}(1/2)}{(2j)!}(w_\ell\lambda)^{2j}\text{ad}_A^{2j-1}(\alpha B)$ | $\mathcal{O}\left(\alpha^2\lvert\lambda\rvert^{2k+1} + \alpha\lvert\lambda\rvert^{2k+3}\right)$ |

# Compilation for correctors

$$e^C = \prod_j e^{a_j \lambda A} e^{b_j \lambda B} + E_{\text{comp}}$$

- For some $a_j, b_j \in \mathbb{R}$ .
- We want $E_{\text{comp}} \leq E_{\text{CPF}}$ .




Compilation error and cost

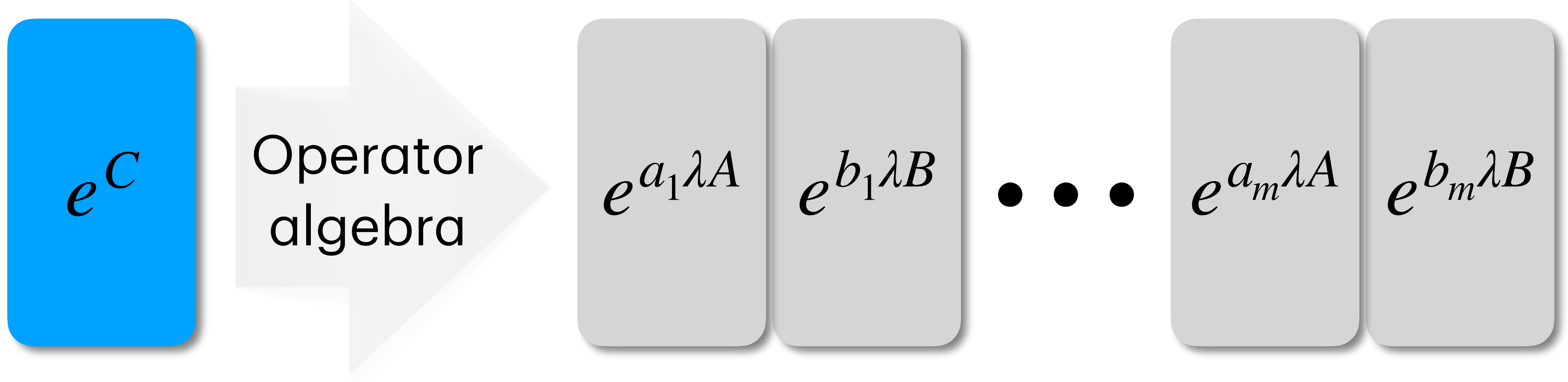
| Corrector | Error | Cost |
|---|---|---|
| $C = c_2\lambda^2 \mathrm{ad}_A(B) + c_3\lambda^3 \mathrm{ad}_B^2(A)$ | $\mathcal{O}(\lambda^4)$ | 5 |
| $C = c_2\lambda^2 \mathrm{ad}_A(B)$ | $\mathcal{O}(\lambda^4)$ | 6 |
| $C = c_3\lambda^3 \mathrm{ad}_B^2(A)$ | $\mathcal{O}(\|\lambda\|^5)$ | 9 |
| $C = c_1\lambda B + c_2\lambda^2 \mathrm{ad}_A(B)$ | $\mathcal{O}(\lambda^4)$ | 7 |
| $C = \sum_{j=1}^{k} \frac{B_{2j}(1/2)}{(2j)!} \lambda^{2j} \mathrm{ad}_A^{2j-1}(\alpha B)$ | $\mathcal{O}(\alpha^3\|\lambda\|^3)$ | $10k$ |

**Compilations have applications beyond CPFs**

- Simulate time evolution for nested commutators
- Generate circuits to implement complicated U on a hardware with limited native gates

# Compilation for correctors

$$C = \sum_{j=1}^{k} \frac{B_{2j}(1/2)}{(2j)!} \lambda^{2j} \, \mathrm{ad}_A^{2j-1}(B)$$




$$\begin{bmatrix} a_0 & a_1 & \cdots & a_{k-1} \\ a_0^3 & a_1^3 & \cdots & a_{k-1}^3 \\ \vdots & \vdots & \ddots & \vdots \\ a_0^{2k-1} & a_1^{2k-1} & \cdots & a_{k-1}^{2k-1} \end{bmatrix} \begin{bmatrix} b_0 \\ b_1 \\ \vdots \\ b_{k-1} \end{bmatrix} = \frac{1}{8} \begin{bmatrix} B_2\left(\frac{1}{2}\right) \\ \frac{1}{2} B_4\left(\frac{1}{2}\right) \\ \vdots \\ \frac{1}{k} B_{2k}\left(\frac{1}{2}\right) \end{bmatrix}$$

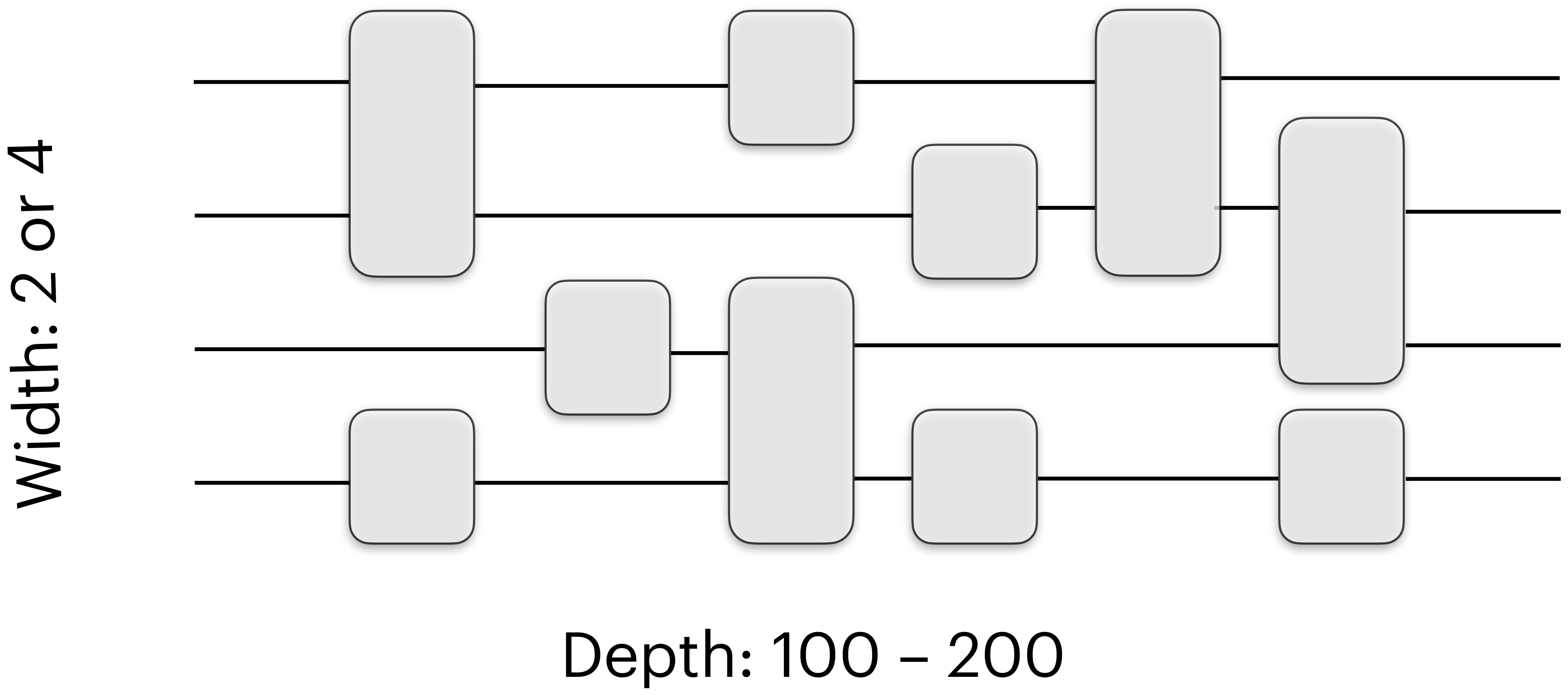
Vandermonde system

| $k=1$ | $k=2$ | $k=3$ | $k=4$ | $k=5$ |
|---|---|---|---|---|
| $b_0 = \frac{-1}{96}$ | $b_0 = \frac{-167}{11520}$ | $b_0 = \frac{-64457}{3870720}$ | $b_0 = \frac{-16705243}{928972800}$ | $b_0 = \frac{-1543769039}{81749606400}$ |
| | $b_1 = \frac{47}{23040}$ | $b_1 = \frac{3643}{967680}$ | $b_1 = \frac{4732843}{928972800}$ | $b_1 = \frac{10431823}{1703116800}$ |
| | | $b_2 = \frac{-1669}{3870720}$ | $b_2 = \frac{-103343}{103219200}$ | $b_2 = \frac{-28718033}{18166579200}$ |
| | | | $b_3 = \frac{176509}{1857945600}$ | $b_3 = \frac{8177231}{30656102400}$ |
| | | | | $b_4 = \frac{-2105933}{98099527680}$ |

$$a_j = j + 1$$

# Quantum hardware implementations

- Correctors provide improvement — even in the presence of hardware noise!
- Simple system: Ising model
- Circuits with small width but large depth (maximum reliable circuit depth for hardware)

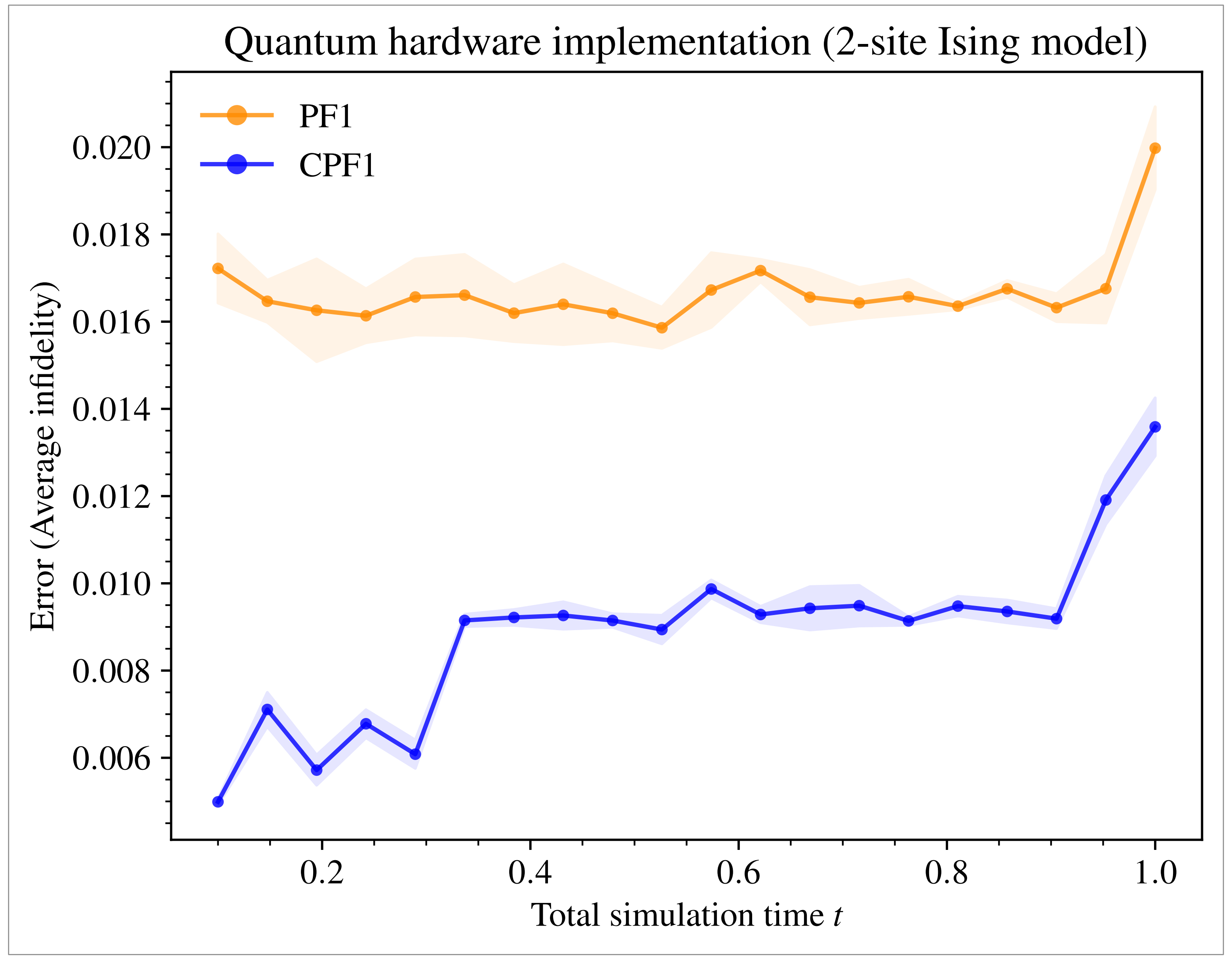


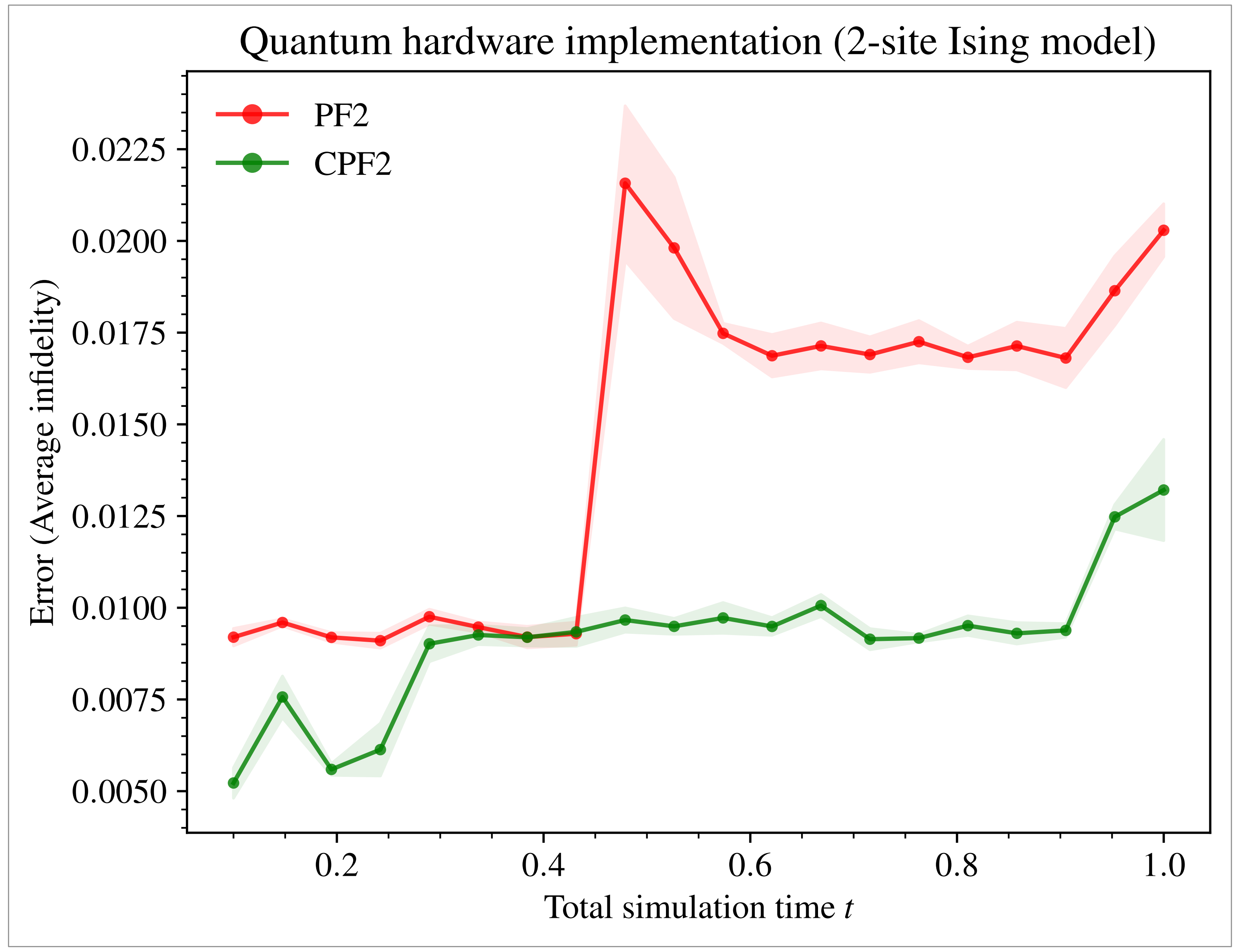

- Error metric:

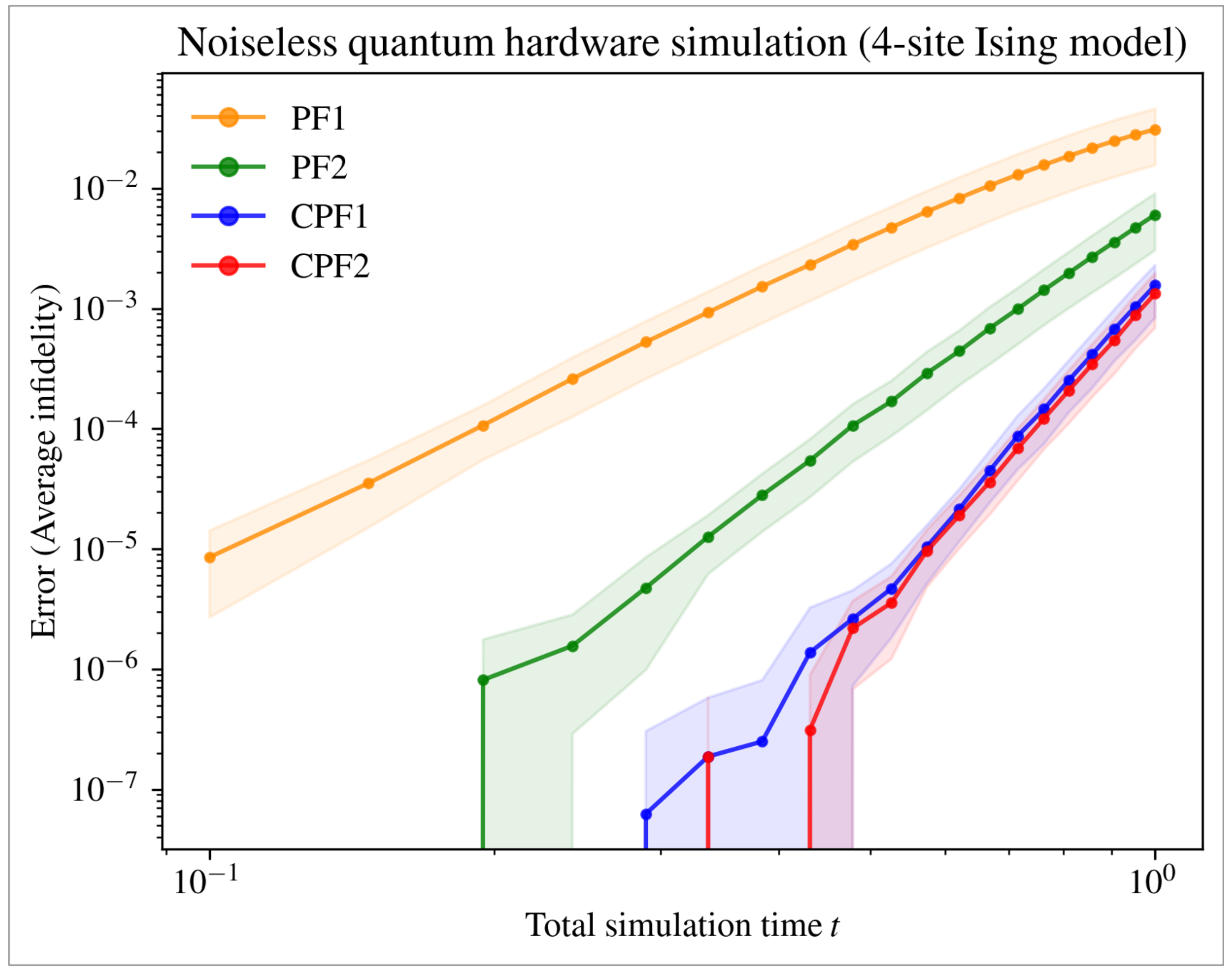
$$\text{Average infidelity} = \mathbb{E}_{\{|x\rangle\}}\left[1 - \left|\langle x|\, U_{\text{exact}}^{\dagger} U_{\text{approx}}\, |x\rangle\right|^2\right]$$

# Quantum hardware implementations

- Correctors $$C_{\text{symp}}^{\text{PF1}} = -\frac{\mathrm{i}}{2}\alpha\tau B - \frac{1}{12}\alpha\tau^2[A,B], \quad C_{\text{symp}}^{\text{PF2}} = \frac{1}{24}\alpha\tau^2[A,B]$$




IBM 127-qubit quantum hardware

Hardware simulator (127-qubit)

# Conclusions

- Product formulas —> a competitive approach for Hamiltonian simulation in practice.
- CPFs fills the gap between theoretical error bounds and empirical error of PFs.
- Compilation for correctors is the key part of CPFs.
- Useful algorithmic tool for quantum computers with limited resources.
- CPFs could also be used in classical simulations, similar to PFs.

# Future directions

- Construct better correctors (ideally symplectic) for high-order product formulas.
- Explore performance of CPFs in more practical settings: fixed input states or observables.

# Thank you!

Natural Sciences and Engineering Research Council of Canada

Conseil de recherches en sciences naturelles et en génie du Canada

# Yoshida-based product formulas

$$S^{(m)}(\lambda) = \left( \prod_{j=1}^{m} S_2(w_{m-j+1}\lambda) \right) S_2(w_0\lambda) \left( \prod_{j=1}^{m} S_2(w_j\lambda) \right)$$

| Product Formula | Error Bound for Non-corrected YPF | Correctors | Error Bound for Corrected YPF |
|---|---|---|---|
| YPF6 | $\mathcal{O}\left(\alpha\lvert\lambda\rvert^7\right)$ | $C_{\text{symp}} = c\lambda^6 \text{ad}_A^5(\alpha B)$ with $c$ in Eq. (82). | $\mathcal{O}\left(\alpha^2\lvert\lambda\rvert^7 + \alpha\lvert\lambda\rvert^9\right)$ |
| YPF8 | $\mathcal{O}\left(\alpha\lvert\lambda\rvert^9\right)$ | $C_{\text{symp}} = c\lambda^8 \text{ad}_A^7(\alpha B)$ with $c$ in Eq. (86). | $\mathcal{O}\left(\alpha^2\lvert\lambda\rvert^9 + \alpha\lvert\lambda\rvert^{11}\right)$ |
| YPF2$k$<br>$k = 3, 4, 5$ | $\mathcal{O}\left(\alpha\lvert\lambda\rvert^{2k+1}\right)$ | $C_{\text{symp}} = \sum_{j=1}^{k} \frac{B_{2j}(1/2)}{(2j)!}(w_\ell\lambda)^{2j} \text{ad}_A^{2j-1}(\alpha B)$<br>used in base case $S_2^c(w_\ell\lambda)$ in Eq. (89) | $\mathcal{O}\left(\alpha^2\lvert\lambda\rvert^{2k+1} + \alpha\lvert\lambda\rvert^{2k+3}\right)$ |

# Hardware implementation

$$\text{Average infidelity} = \mathbb{E}_{\{|x\rangle\}}\left[1 - \left|\langle x| U^{\dagger}_{\text{exact}} U_{\text{approx}} |x\rangle\right|^2\right]$$

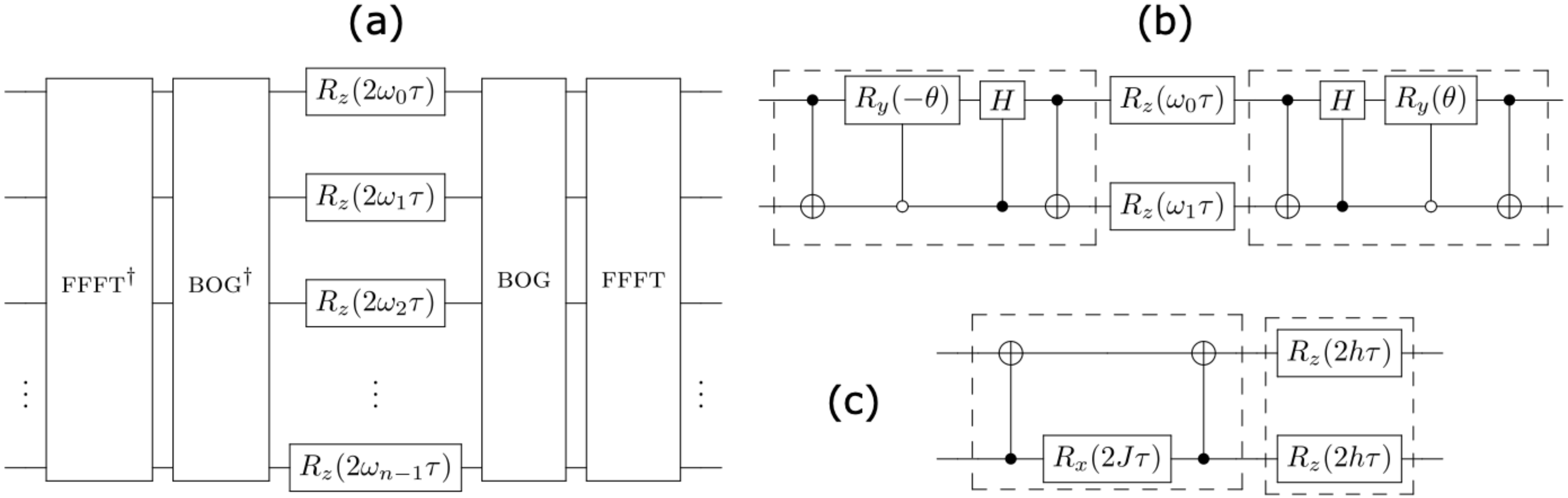



Figure 5: Quantum circuits for the Ising model. (a) Circuit for exact evolution of $n$-site model by fast fermionic Fourier transform (FFFT) and Bogoliubov transform (BOG). (b) Tailored circuit for the 2-site model. Gates inside the (left) right dashed box implement the (inverse) unitary that diagonalizes the Hamiltonian. (c) Circuit for PF1 with gates in the left (right) box implementing the evolution by the interaction (external field) term.

# Hardware implementation

| Size | timesteps | Optimization level for circuits | PF1 (Infid) | PF2 (Infid) | CPF1 (Infid) | CPF2 (Infid) | Exact evolution |
|---|---|---|---|---|---|---|---|
| 2 | 10 | Level 1 | 91 (138) | 91 (138) | 154 (200) | 145 (192) | 49 |
| | | Level 2 | 12 (12) | 12 (12) | 12 (12) | 12 (12) | 12 |
| | | Level 3 | 12 (12) | 12 (12) | 12 (12) | 12 (12) | 12 |
| 4 | 1 | Level 1 | 34 (263) | 34 (263) | 296 (526) | 232(461) | 231 |
| | | Level 2 | 48 (130) | 46 (129) | 389 (473) | 309 (393) | 77 |
| | | Level 3 | 48 (111) | 46 (110) | 389 (454) | 309 (374) | 57 |

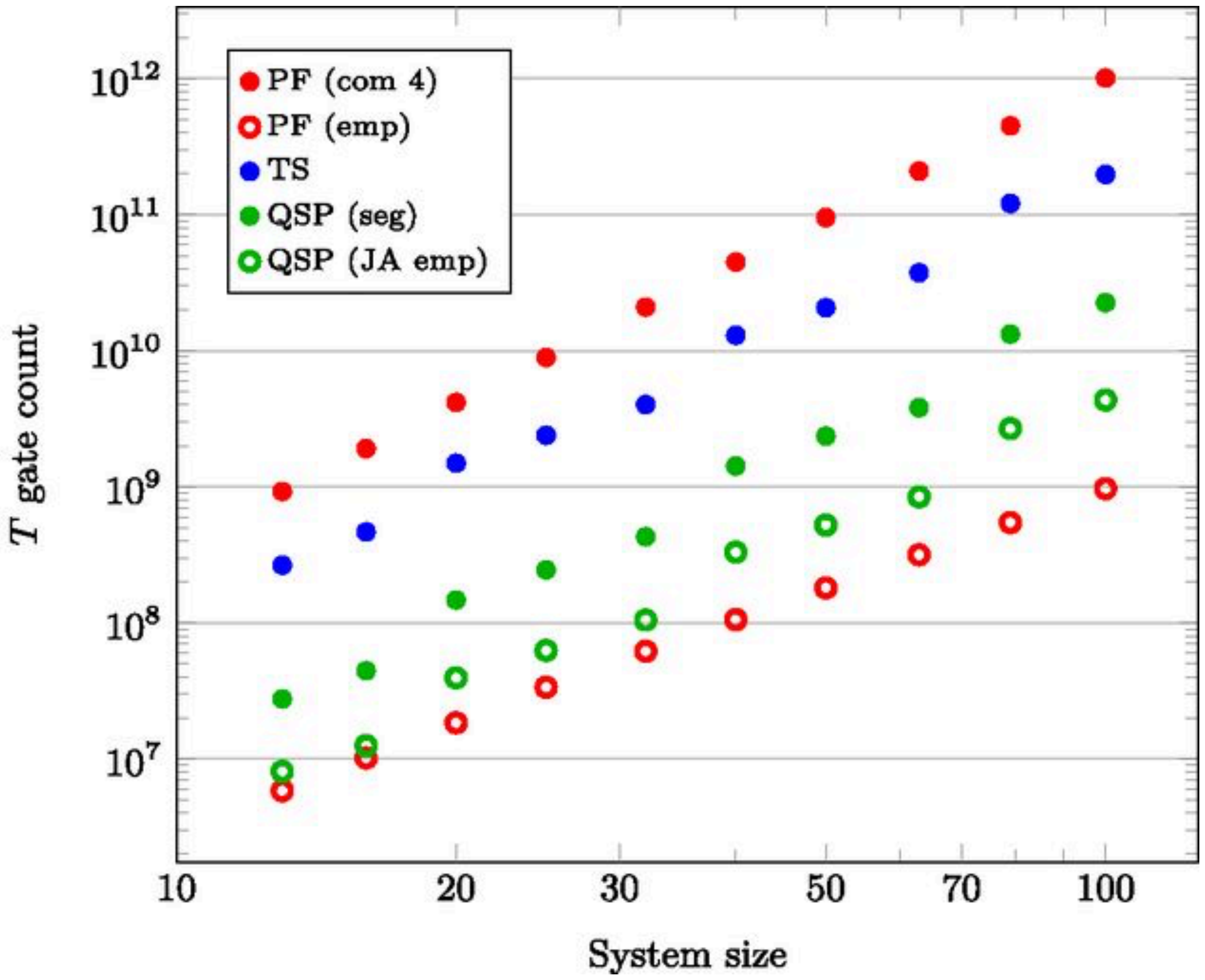
Table 5: Depth of the circuits transpiled to the native gates of `ibm_quebec` QPU for the exact evolution, the approximate evolutions by corrected and standard product formulas, and the average infidelity (Infid) circuits for the 2- and 4-site Ising model used for hardware experiments in Fig. 4. Duration of each timestep is $\tau = 0.1$, and the total evolution time for $r$ steps is $r \times \tau$. Transpiled circuits are optimized using Qiskit's compiler at different optimization levels: Level 1 provides a light optimization, Level 2 provides a medium optimization, and Level 3 provides a heavy optimization [51]. Level-3 optimization is used for hardware experiments in Fig. 4.

# Backup: system and algorithm specification

**System:** Nearest-neighbor Heisenberg model with a random magnetic field in the Z direction

$$\sum_{j=1}^{n} (\vec{\sigma}_j \cdot \vec{\sigma}_{j+1} + h_j \sigma_j^z)$$

- Periodic boundary conditions imposed.
- Random $h_j \in [-1,1]$
- Gate count in simulations are obtained by
  - $t = n$
  - $\varepsilon = 10^{-3}$
- Focus on the system-size dependence of quantum simulation algorithms.




**PF algorithm:** PF4 with commutator scaling bound; Better of PF4 & PF6 with empirical error

**QSP algorithm:** segmented version with analytic error bound and the nonsegmented version with empirical Jacobi–Anger error bound