Three simple tricks for better Trotterization

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Discrete time evolution

- Real time evolution

$$|\psi(t)\rangle = \mathrm{e}^{-\mathrm{i}\,Ht}\,|\psi(0)\rangle$$

Discrete time evolution

- Real time evolution
- Imaginary time evolution

$$|\psi_0\rangle = \lim_{\tau\to\infty} \mathrm{e}^{-H\tau}\,|\psi\rangle$$

Discrete time evolution

- Real time evolution
- Imaginary time evolution
- Symplectic integration

$$\dot{x} = \frac{\partial H}{\partial p}$$
$$\dot{p} = -\frac{\partial H}{\partial x}$$

Discrete time evolution

- Real time evolution
- Imaginary time evolution
- Symplectic integration

$$\dot{x} = \frac{\partial H}{\partial p}$$

$$\dot{p} = -\frac{\partial H}{\partial x}$$

$$\Leftrightarrow \begin{pmatrix} x(t) \\ p(t) \end{pmatrix} = \mathrm{e}^{t\left(\frac{\partial H}{\partial p}\frac{\partial}{\partial x} - \frac{\partial H}{\partial x}\frac{\partial}{\partial p}\right)} \begin{pmatrix} x(0) \\ p(0) \end{pmatrix}$$

Suzuki-Trotter decomposition

[Suzuki *CommunMathPhys* **51** (1976); Trotter *ProcAMS* **4** (1959)]

$$H = \sum_{i}^{\Lambda} A_i \,, \quad [A_i, A_j] \neq 0$$

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$$U(h) = \mathrm{e}^{\mathrm{i}\, A_1 h}\, \mathrm{e}^{\mathrm{i}\, A_2 h} \cdots \mathrm{e}^{\mathrm{i}\, A_\Lambda h} + \mathcal{O}\left(h^2\right)$$

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$$U(h) = \mathrm{e}^{\mathrm{i}\, A_1 h/2}\, \mathrm{e}^{\mathrm{i}\, A_2 h/2} \dots \mathrm{e}^{\mathrm{i}\, A_\Lambda h/2}\, \mathrm{e}^{\mathrm{i}\, A_\Lambda h/2} \dots \mathrm{e}^{\mathrm{i}\, A_2 h/2}\, \mathrm{e}^{\mathrm{i}\, A_1 h/2} + \mathcal{O}\left(h^3\right)$$

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$$\vdots$$

Error estimation and efficiency [Omelyan et al. *CPC* **146** (2002), *CPC* **151** (2003)]

$$\mathrm{e}^{(A+B)h+\mathcal{O}_1\,h+\mathcal{O}_3\,h^3+\mathcal{O}_5\,h^5+\cdots} = \mathrm{e}^{Aa_1h}\,\mathrm{e}^{Bb_1h}\cdots\mathrm{e}^{Bb_qh}\,\mathrm{e}^{Aa_{q+1}h}$$

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$$\mathcal{O}_1 = (\nu-1)A + (\sigma-1)B, \quad \nu = \sum_i a_i, \sigma = \sum_i b_i$$

Error estimation and efficiency [Omelyan et al. *CPC* **146** (2002), *CPC* **151** (2003)]

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$$\mathcal{O}_1 = (\nu-1)A + (\sigma-1)B, \quad \nu = \textstyle\sum_i a_i, \sigma = \sum_i b_i$$

$$\mathcal{O}_3 = \alpha[A,[A,B]] + \beta[B,[A,B]]$$

Error estimation and efficiency [Omelyan et al. *CPC* **146** (2002), *CPC* **151** (2003)]

$$\mathrm{e}^{(A+B)h+\mathcal{O}_1\,h+\mathcal{O}_3\,h^3+\mathcal{O}_5\,h^5+\cdots} = \mathrm{e}^{Aa_1h}\,\mathrm{e}^{Bb_1h}\cdots\mathrm{e}^{Bb_qh}\,\mathrm{e}^{Aa_{q+1}h}$$

$$\begin{aligned}
\mathcal{O}_1 &= (\nu-1)A+(\sigma-1)B, \quad \nu=\textstyle\sum_i a_i,\, \sigma=\sum_i b_i \\
\mathcal{O}_3 &= \alpha[A,[A,B]]+\beta[B,[A,B]] \\
\mathcal{O}_5 &= \gamma_1[A,[A,[A,[A,B]]]]+\gamma_2[A,[A,[B,[A,B]]]] \\
&\quad+\gamma_3[B,[A,[A,[A,B]]]]+\gamma_4[B,[B,[B,[A,B]]]] \\
&\quad+\gamma_5[B,[B,[A,[A,B]]]]+\gamma_6[A,[B,[B,[A,B]]]]
\end{aligned}$$

Error estimation and efficiency [Omelyan et al. *CPC* **146** (2002), *CPC* **151** (2003)]

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$$\begin{aligned}\mathcal{O}_5 &= \gamma_1[A,[A,[A,[A,B]]]]+\gamma_2[A,[A,[B,[A,B]]]] \\ &\quad+\gamma_3[B,[A,[A,[A,B]]]]+\gamma_4[B,[B,[B,[A,B]]]] \\ &\quad+\gamma_5[B,[B,[A,[A,B]]]]+\gamma_6[A,[B,[B,[A,B]]]]\end{aligned}$$

$$\mathrm{Eff}_2 = \frac{1}{q^2\sqrt{|\alpha|^2+|\beta|^2}}$$

Error estimation and efficiency [Omelyan et al. *CPC* **146** (2002), *CPC* **151** (2003)]

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$$\begin{aligned}\mathcal{O}_5 = {} & \gamma_1[A,[A,[A,[A,B]]]] + \gamma_2[A,[A,[B,[A,B]]]] \\ & + \gamma_3[B,[A,[A,[A,B]]]] + \gamma_4[B,[B,[B,[A,B]]]] \\ & + \gamma_5[B,[B,[A,[A,B]]]] + \gamma_6[A,[B,[B,[A,B]]]]\end{aligned}$$

$$\mathrm{Eff}_2 = \frac{1}{q^2\sqrt{|\alpha|^2+|\beta|^2}}$$

$$\mathrm{Eff}_4 = \frac{1}{q^4\sqrt{\sum_{j=1}^{6}|\gamma_j|^2}}$$

Decompositions into 2 operators

$$\mathrm{e}^{(A+B)h+\mathcal{O}\left(h^{n+1}\right)} = \mathrm{e}^{Aa_1h}\,\mathrm{e}^{Bb_1h}\,\mathrm{e}^{Aa_2h}\cdots\mathrm{e}^{Bb_qh}\,\mathrm{e}^{Aa_{q+1}h}$$

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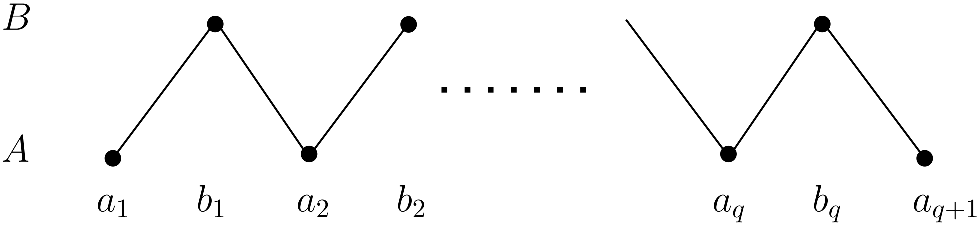

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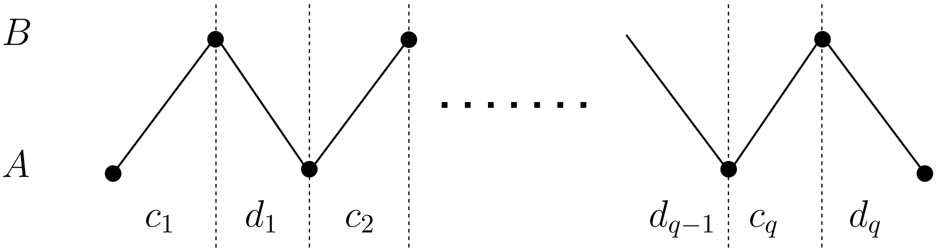
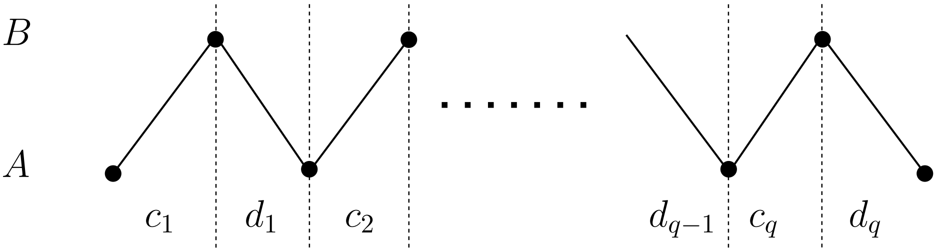
$$\mathrm{e}^{(A+B)h+\mathcal{O}\left(h^{n+1}\right)} = \mathrm{e}^{Aa_1h}\,\mathrm{e}^{Bb_1h}\,\mathrm{e}^{Aa_2h}\cdots\mathrm{e}^{Bb_qh}\,\mathrm{e}^{Aa_{q+1}h}$$



Decompositions into 2 operators

$$\mathrm{e}^{(A+B)h+\mathcal{O}\left(h^{n+1}\right)} = \mathrm{e}^{Aa_1h}\,\mathrm{e}^{Bb_1h}\,\mathrm{e}^{Aa_2h}\cdots\mathrm{e}^{Bb_qh}\,\mathrm{e}^{Aa_{q+1}h}$$
$$= \mathrm{e}^{Ac_1h}\,\mathrm{e}^{Bc_1h}\,\mathrm{e}^{Bd_1h}\,\mathrm{e}^{Ad_1h}\cdots\mathrm{e}^{Bd_qh}\,\mathrm{e}^{Ad_qh}$$

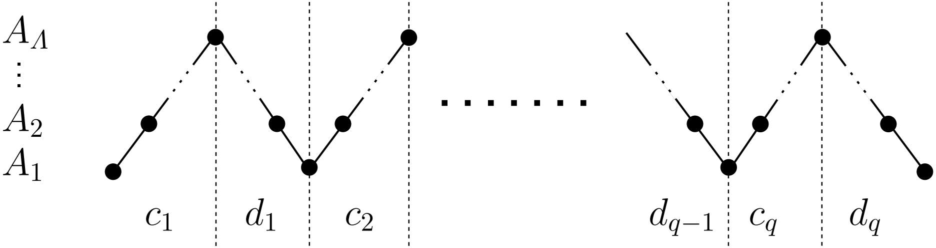


$$c_1 = a_1\,, \qquad d_1 = b_1 - c_1\,,$$
$$c_2 = a_2 - d_1\,, \qquad d_2 = b_2 - c_2\,,$$
$$\vdots \qquad \vdots$$

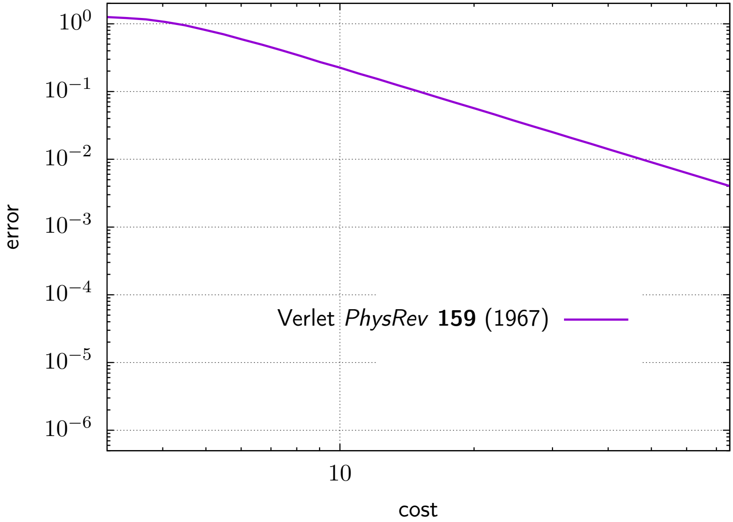
Decompositions into $\varLambda$ operators [JO *JPhysA* **56** (2023)]

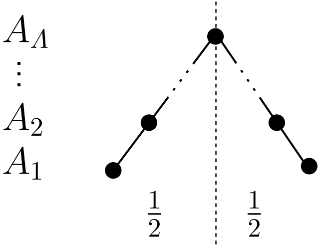
$$\mathrm{e}^{h\sum_{k=1}^{\varLambda} A_k + \mathcal{O}\left(h^{n+1}\right)}$$

$$= \left(\prod_{k=1}^{\varLambda} \mathrm{e}^{A_k c_1 h}\right)\left(\prod_{k=\varLambda}^{1} \mathrm{e}^{A_k d_1 h}\right)\cdots\left(\prod_{k=1}^{\varLambda} \mathrm{e}^{A_k c_q h}\right)\left(\prod_{k=\varLambda}^{1} \mathrm{e}^{A_k d_q h}\right)$$



Benchmarking the Heisenberg model

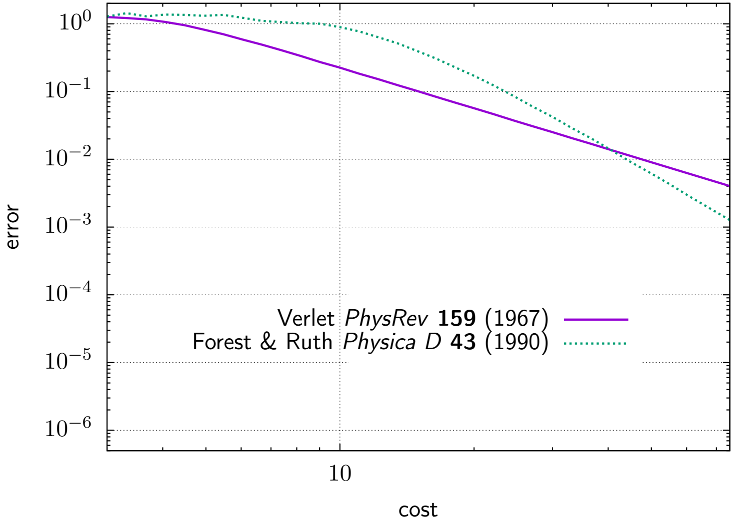


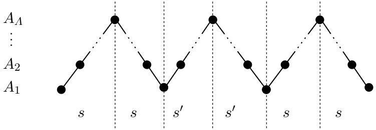


order $= 2$,

cycles $= 1$

Benchmarking the Heisenberg model





$$s = \frac{1}{2(2 - \sqrt[3]{2})}$$

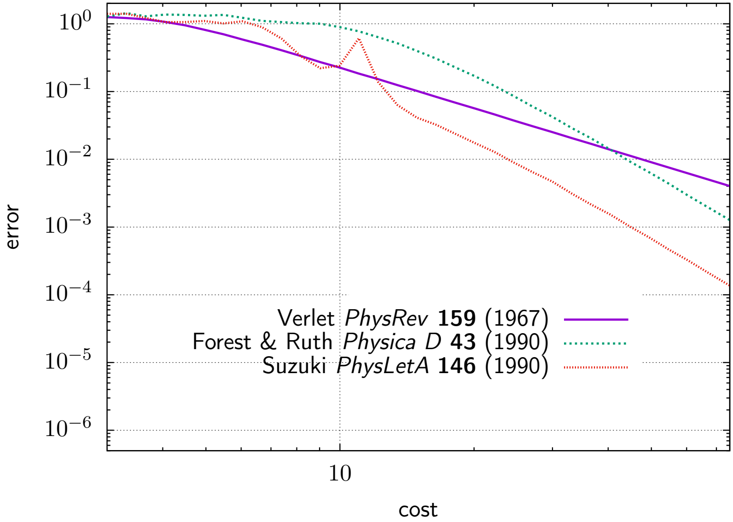
$$s' = \frac{1}{2} - 2s$$

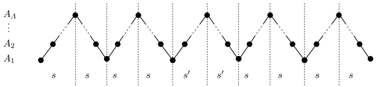
$$\text{order} = 4\,,$$

$$\text{cycles} = 3\,,$$

$$\mathrm{Eff}_4 = 0.315$$

Benchmarking the Heisenberg model





$$s = \frac{1}{2(4 - \sqrt[3]{4})}$$

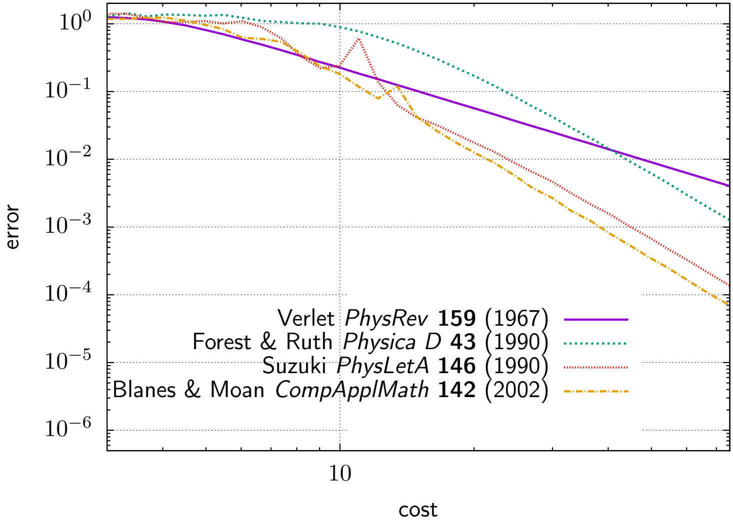
$$s' = \frac{1}{2} - 4s$$

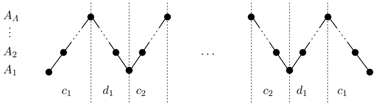
$$\text{order} = 4\,,$$

$$\text{cycles} = 5\,,$$

$$\text{Eff}_4 = 1.10$$

Benchmarking the Heisenberg model

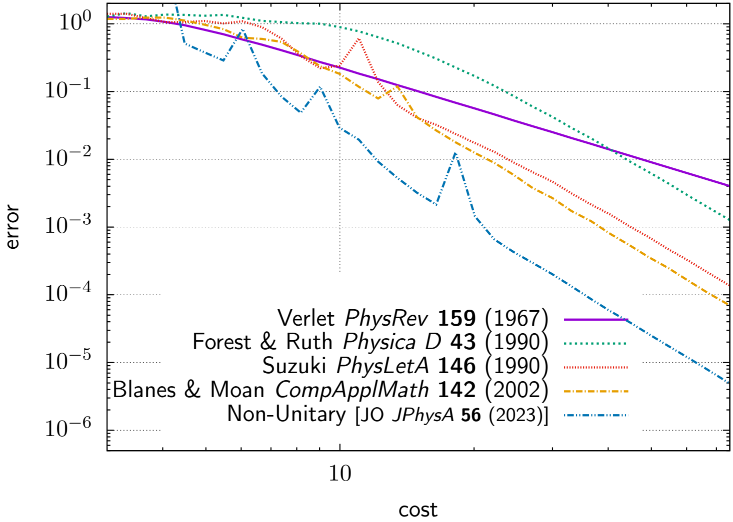


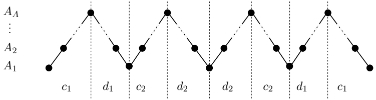


$$c_1 \approx 0.08 \quad d_1 \approx 0.13$$
$$c_2 \approx 0.22 \quad d_2 \approx -0.36$$
$$c_3 \approx 0.32 \quad d_3 \approx 0.11$$

$$\text{order} = 4\,,$$
$$\text{cycles} = 6\,,$$
$$\mathrm{Eff}_4 = 10.2$$

Benchmarking the Heisenberg model





$$c_1 \approx 0.10 + 0.02\,\mathrm{i}$$

$$d_1 \approx 0.15 + 0.07\,\mathrm{i}$$

$$c_2 \approx 0.14 + 0.07\,\mathrm{i}$$

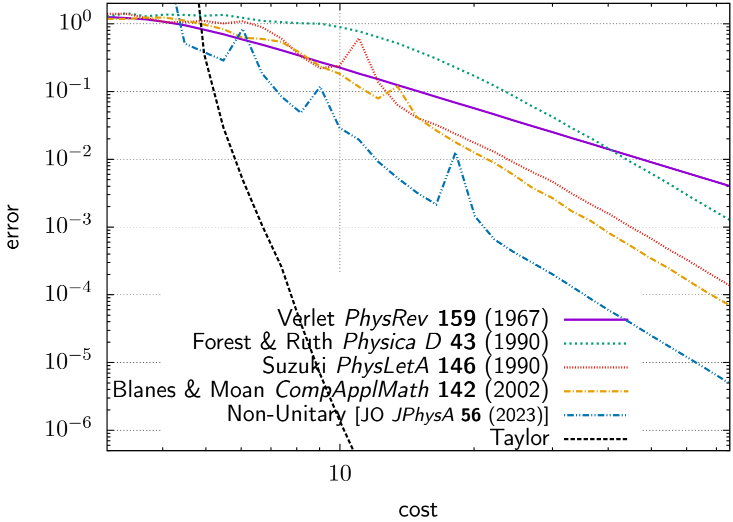
$$d_2 \approx 0.11 - 0.16\,\mathrm{i}$$

$$\text{order} = 4\,,$$

$$\text{cycles} = 4\,,$$

$$\mathrm{Eff}_4 = 29.9$$

Benchmarking the Heisenberg model

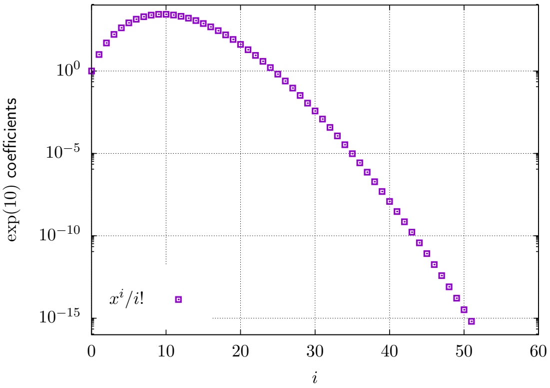


$$e^{Hh} = \lim_{k\to\infty} \sum_{i=0}^{k} \frac{(Hh)^i}{i!}$$

$$\left| \frac{(\lambda_{\mathrm{max}}(H)h)^k}{(k+1)!} \right| < \varepsilon$$

Taylor series factorisation

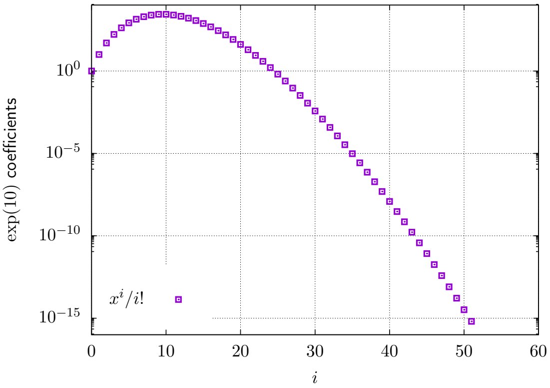
$$e^{Hh} = \sum_{i=0}^{k} \frac{(Hh)^i}{i!} + \mathcal{O}\left(h^{k+1}\right)$$



Taylor series factorisation

$$e^{Hh} = \sum_{i=0}^{k} \frac{(Hh)^i}{i!} + \mathcal{O}\left(h^{k+1}\right)$$

$$\sum_{i=0}^{n} \frac{(Hh)^i}{i!} = \prod_{i=1}^{n} \left(1 + a_i^n Hh\right)$$



Taylor series factorisation

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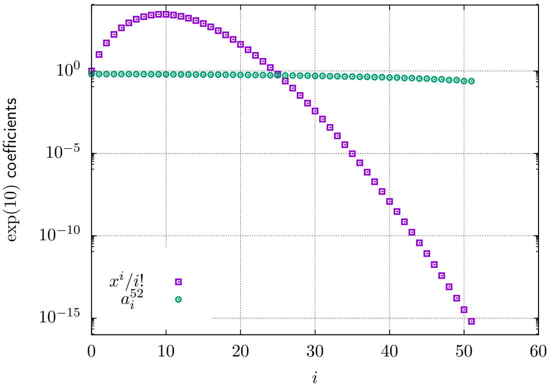
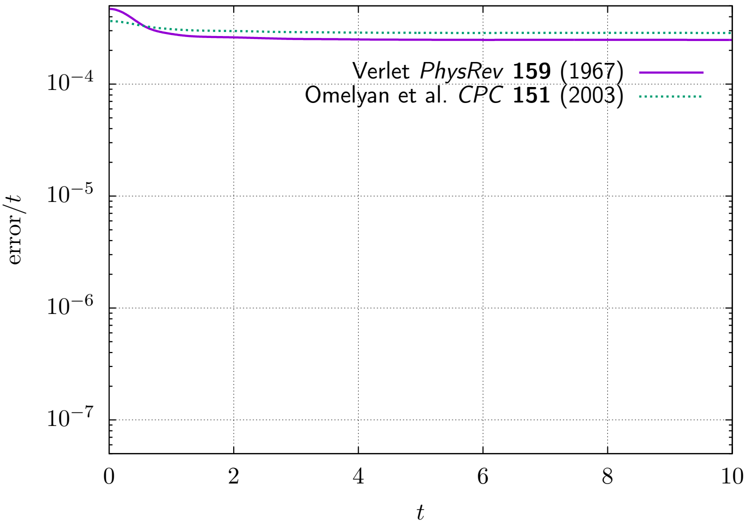
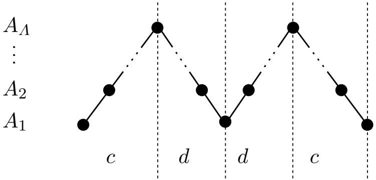


Error accumulation





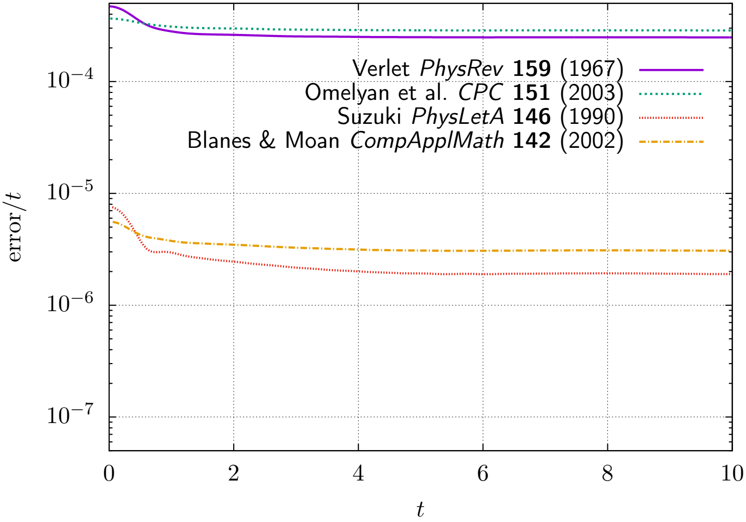
$$c \approx 0.193$$

$$d \approx 0.407$$

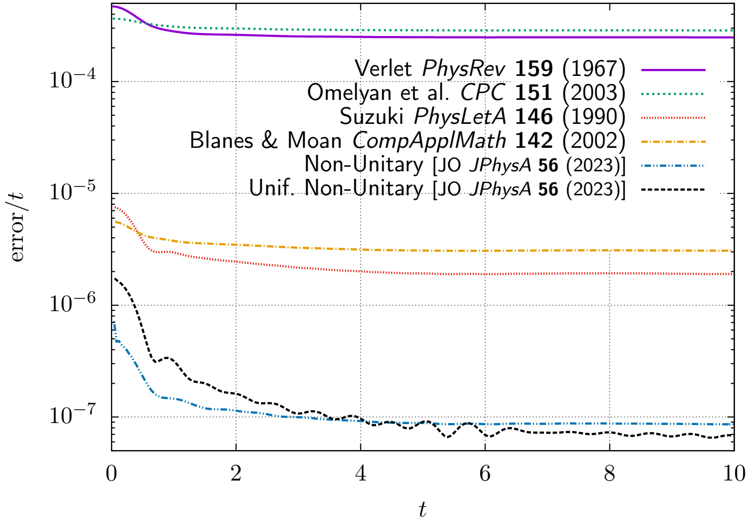
$$\text{order} = 2\,,$$

$$\text{cycles} = 2$$

Error accumulation

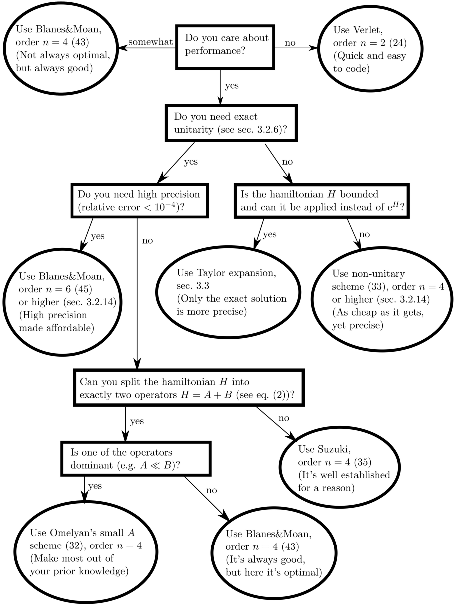


Error accumulation



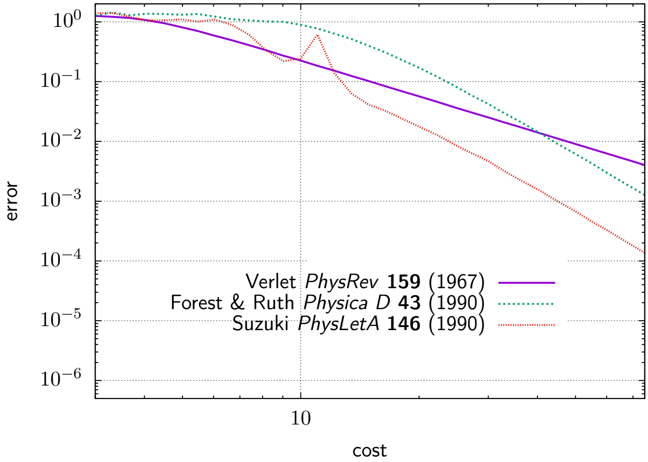
$$c_1 = 0.1 + 0.025\,\mathrm{i}$$
$$d_1 = 0.1 + 0.025\,\mathrm{i}$$
$$c_2 = 0.1 - 0.066\,\mathrm{i}$$
$$d_2 = 0.1 - 0.066\,\mathrm{i}$$
$$c_3 = 0.1 + 0.082\,\mathrm{i}$$
$$\text{order} = 4\,,$$
$$\text{cycles} = 5\,,$$
$$\mathrm{Eff}_4 = 6.38$$

How to choose... [JO *JPhysA* **56** (2023)]



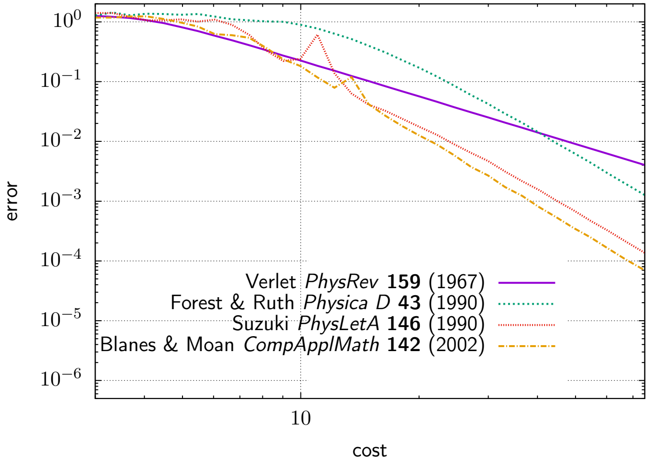
Three simple tricks for better Trotterization

Three simple tricks for better Trotterization



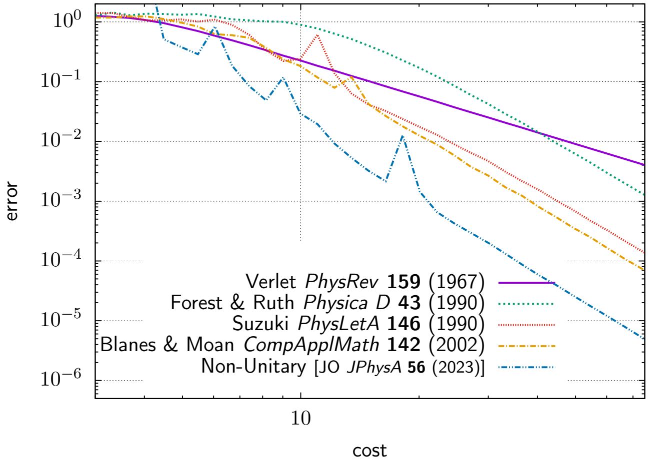
0. Don't use Forest & Ruth.

Three simple tricks for better Trotterization



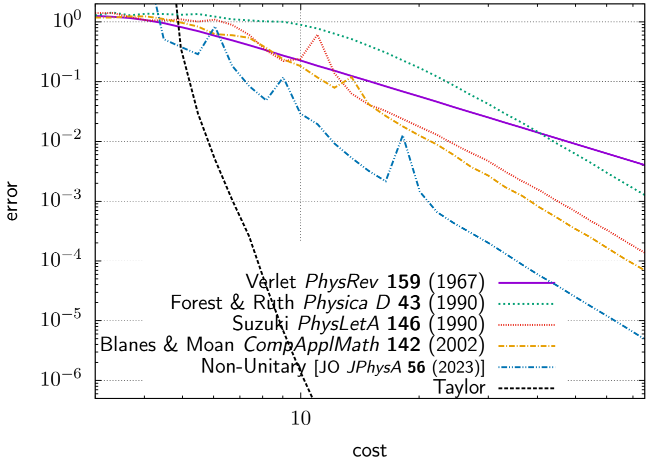
0. Don't use Forest & Ruth.
1. Use 2-operator methods for Λ operators.

Three simple tricks for better Trotterization



0. Don't use Forest & Ruth.
1. Use 2-operator methods for Λ operators.
2. Use complex coefficients.

Three simple tricks for better Trotterization



0. Don't use Forest & Ruth.
1. Use 2-operator methods for Λ operators.
2. Use complex coefficients.
3. Use Taylor expansion.

Bibliography I

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Heisenberg model and error estimation

$$
\begin{aligned}
H &= \sum_{i=1}^{L} \left(\sigma_i^x \sigma_{i+1}^x + \sigma_i^y \sigma_{i+1}^y + \sigma_i^z \sigma_{i+1}^z + h_i \sigma_i^z \right) \ , \\
U(t) &\equiv \mathrm{e}^{\mathrm{i}\, Ht} \\
&= U(h)^{t/h} \\
&= S(h)^{t/h} + \mathcal{O}\left(h^n\right) \ , \\
S(h) &= \mathrm{e}^{\mathrm{i}\, H_1^x c_1 h} \mathrm{e}^{\mathrm{i}\, H_1^y c_1 h} \mathrm{e}^{\mathrm{i}\, H_1^z c_1 h} \mathrm{e}^{\mathrm{i}\, H_2^x c_1 h} \mathrm{e}^{\mathrm{i}\, H_2^y c_1 h} \mathrm{e}^{\mathrm{i}\, H_2^z c_1 h} \dots \mathrm{e}^{\mathrm{i}\, H_1^z d_q 1 h} \mathrm{e}^{\mathrm{i}\, H_1^y d_q h} \mathrm{e}^{\mathrm{i}\, H_1^x d_q h} , \\
\mathrm{error} &= \frac{1}{\sqrt{N}} \left\| U(t) - S(h)^{t/h} \right\|_{\mathsf{F}} \\
&= \frac{1}{\sqrt{N}} \sqrt{\sum_v \left| U(t) \cdot v - S(h)^{t/h} \cdot v \right|^2}
\end{aligned}
$$