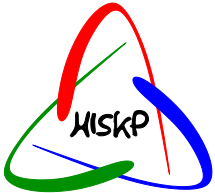


A04: Optimising Higher-Order Trotter Methods

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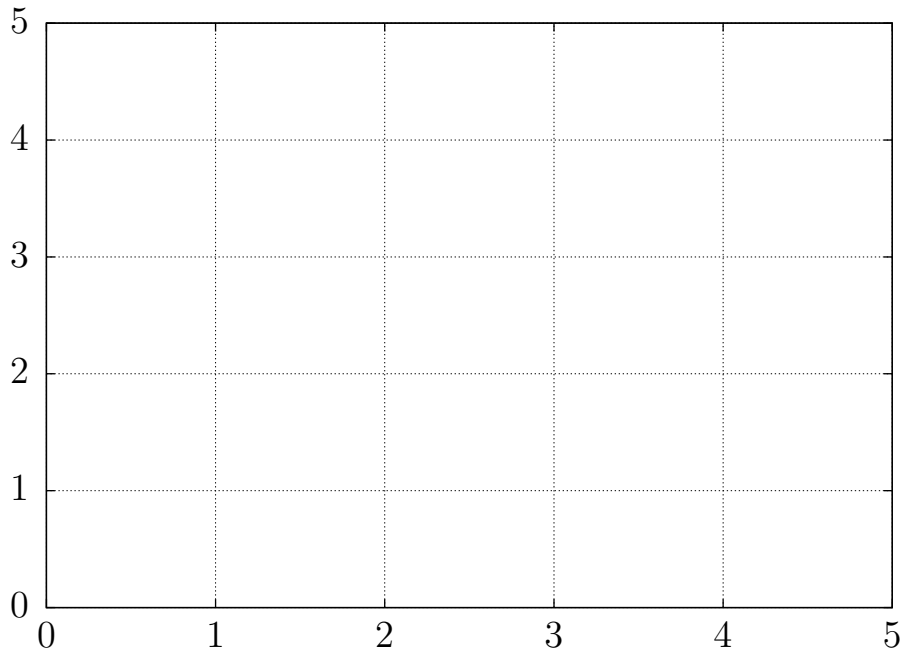


Schrödinger equation and time evolution

$$i \frac{\partial}{\partial t} |\psi\rangle = H |\psi\rangle \quad (\hbar = 1)$$

Schrödinger equation and time evolution

$$\begin{aligned} \mathrm{i} \frac{\partial}{\partial t} |\psi\rangle &= H |\psi\rangle & (\hbar = 1) \\ \Rightarrow |\psi(t)\rangle &= \mathrm{e}^{-\mathrm{i} H t} |\psi(0)\rangle \end{aligned}$$



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

$$e^{(A+B)h + \mathcal{O}_1 h + \mathcal{O}_3 h^3 + \mathcal{O}_5 h^5 + \dots} = e^{Aa_1 h} e^{Bb_1 h} \dots e^{Bb_q h} e^{Aa_{q+1} h}$$

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

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

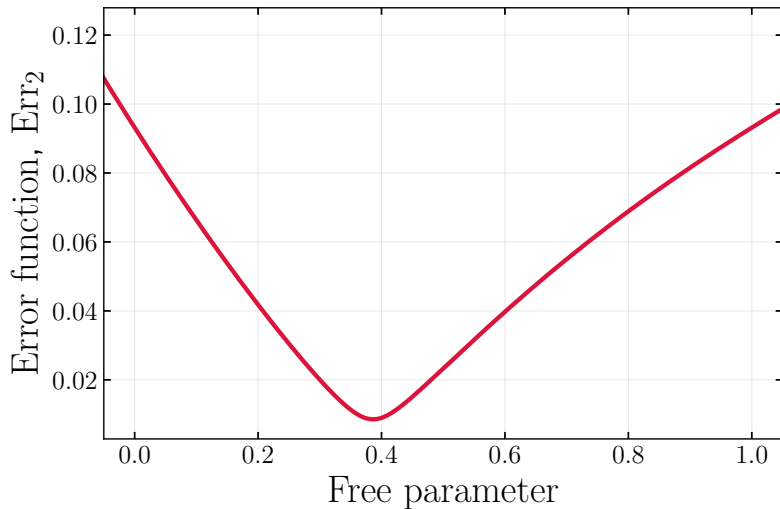
$$\begin{aligned} \mathcal{O}_5 = & \gamma_1[A, [A, [A, [A, B]]]] + \gamma_2[A, [A, [B, [A, B]]]] \\ & + \gamma_3[B, [A, [A, [A, B]]]] + \gamma_4[B, [B, [B, [A, B]]]] \\ & + \gamma_5[B, [B, [A, [A, B]]]] + \gamma_6[A, [B, [B, [A, B]]]] \end{aligned}$$

$$\text{Err}_2 = \sqrt{|\alpha|^2 + |\beta|^2}$$

$$\text{Err}_4 = \sqrt{\sum_{j=1}^6 |\gamma_j|^2}$$

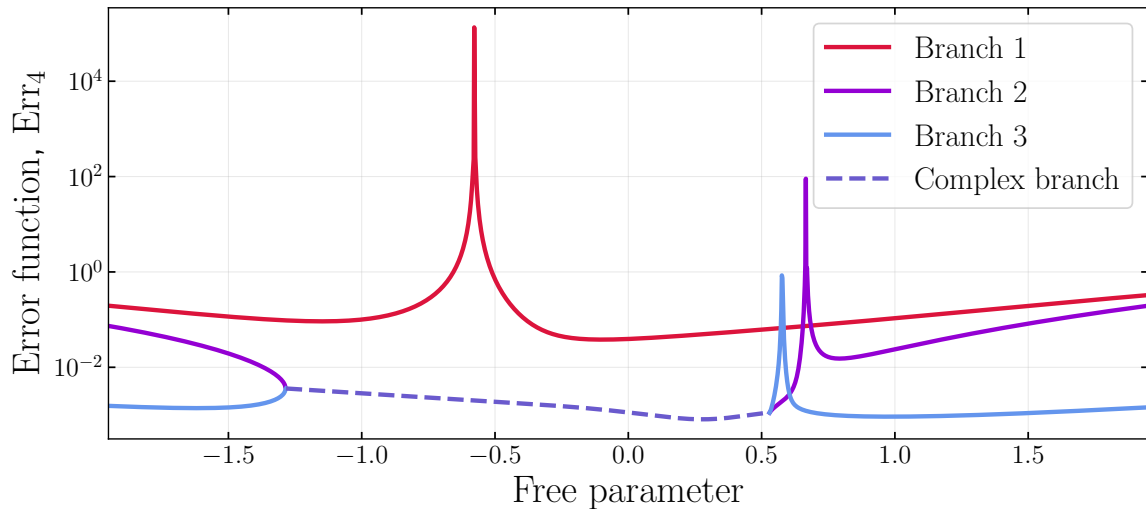
The minimisation problem

Polynomial manifold for 2 cycles



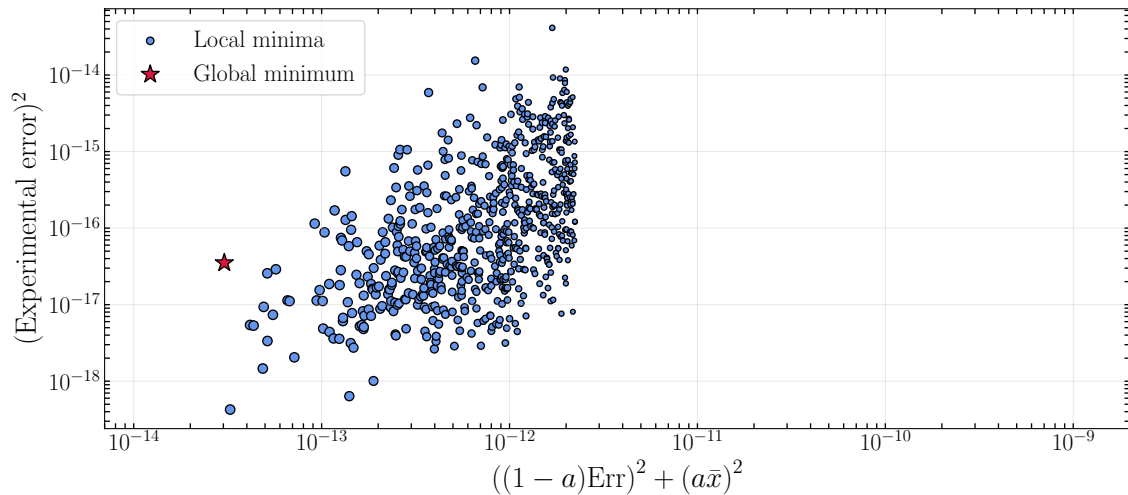
The minimisation problem

Polynomial manifold for 4 cycles



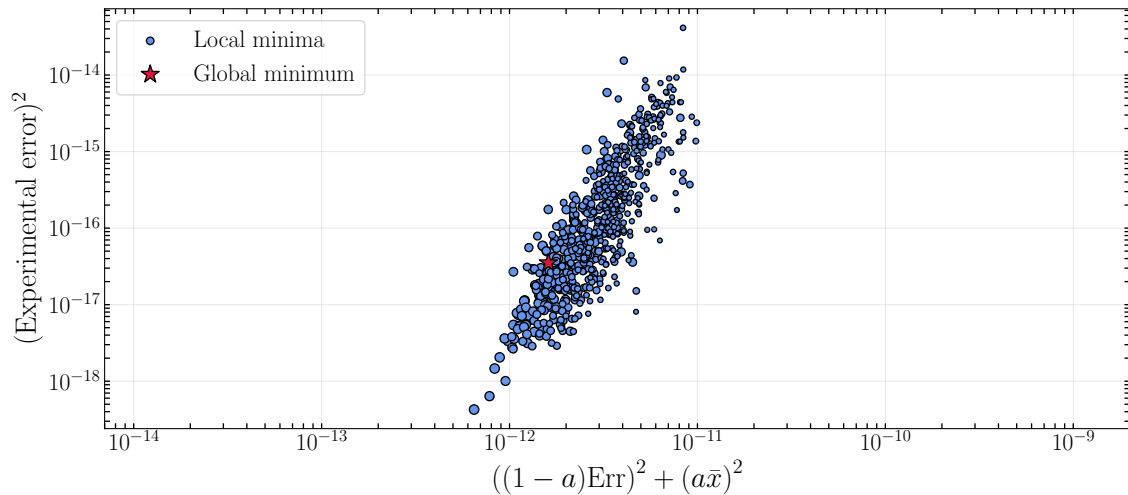
Comparing local minima

Error comparison at 14 cycles, $a = 0.000 \times 10^0$

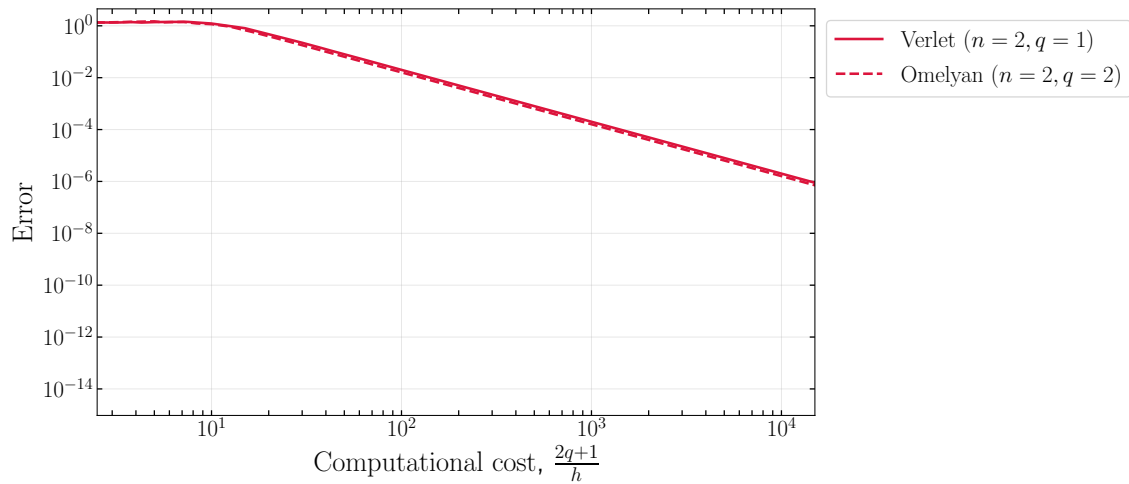


Comparing local minima

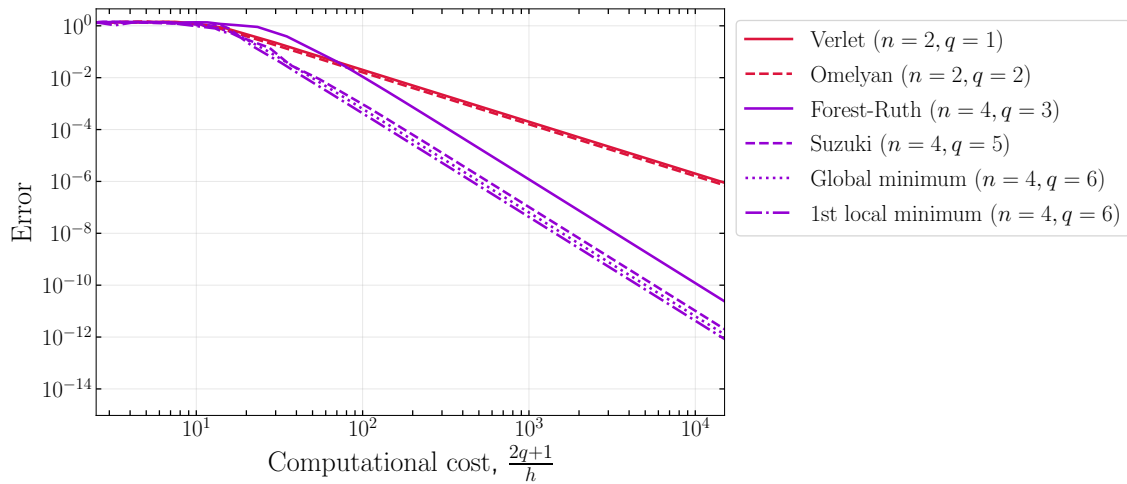
Error comparison at 14 cycles, $a = 1.000 \times 10^{-6}$



Benchmarks



Benchmarks



Benchmarks

