Toward Efficient Trotter-Suzuki Schemes for Long-Time Quantum Dynamics

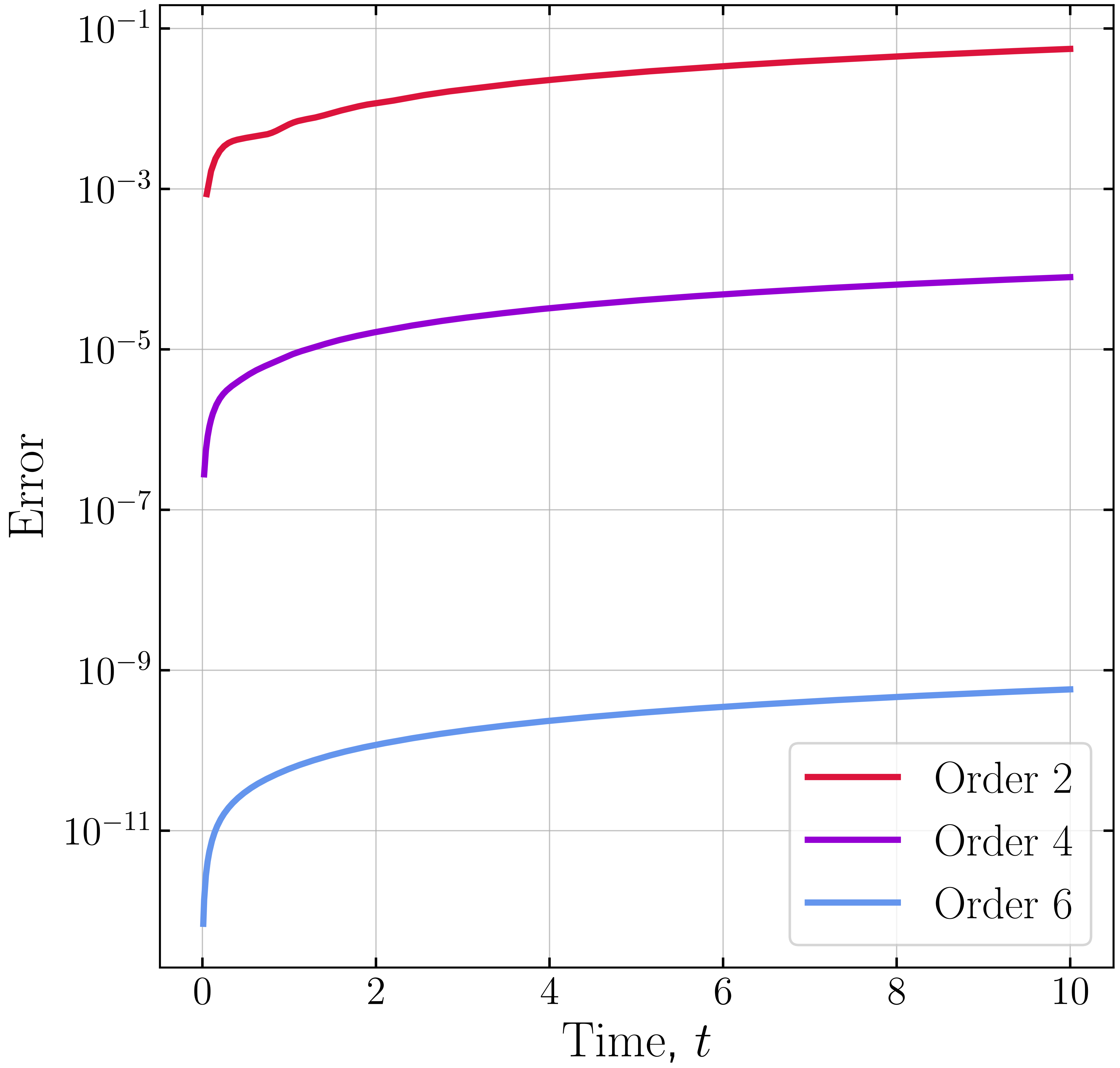
Marko Maležič, Johann Ostmeyer

3.9.2025

Trento ECT*, Hamiltonian LGT workshop

Motivation

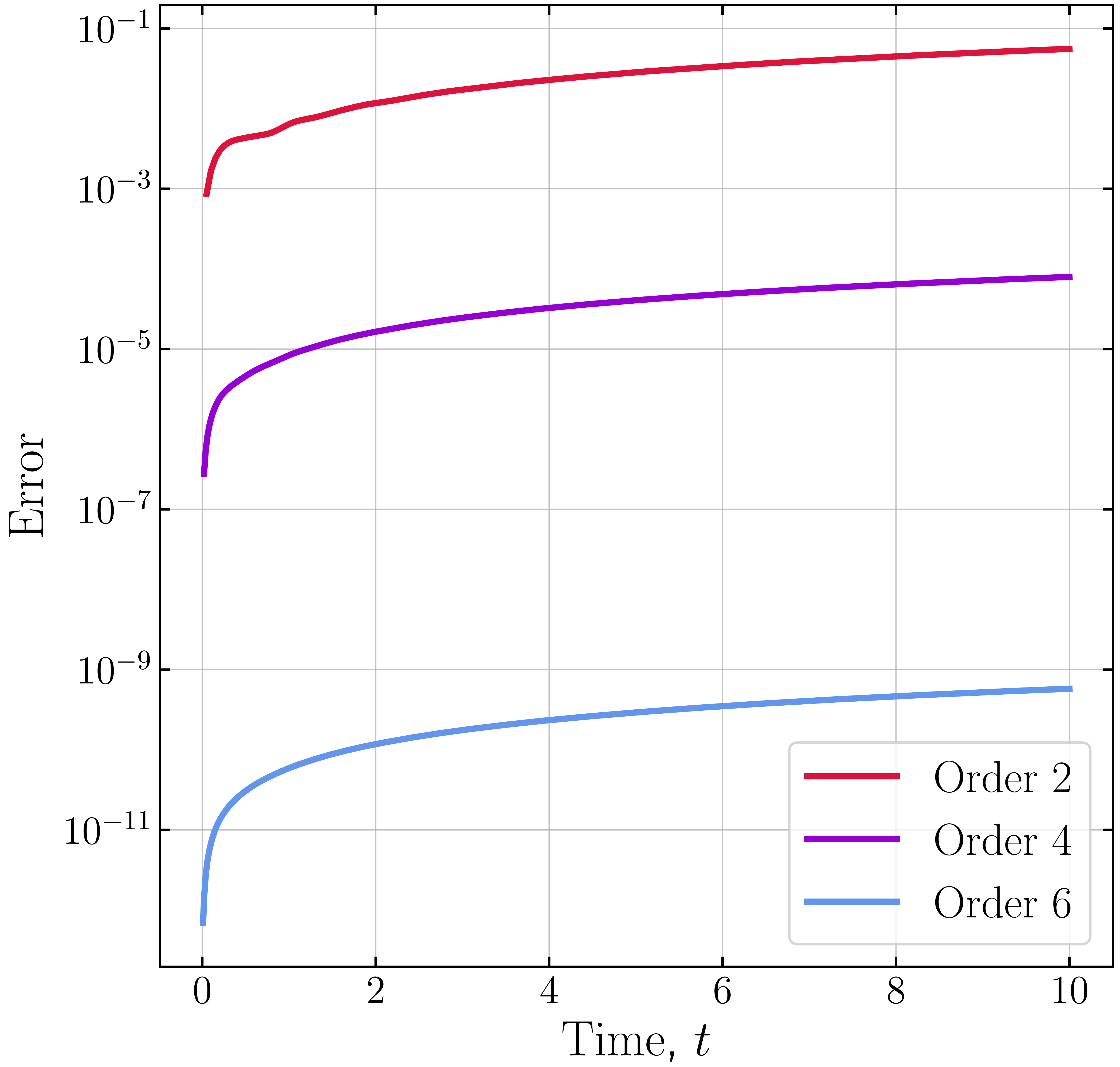
- Accurate long-time quantum simulations are challenging in complex systems
- Limits on access to observables and ground state properties
- Accumulation of errors in time both on classical and quantum hardware



Motivation

- Quantum computers also face hardware problems, e.g. Decoherence and gate depth
- Improving theoretical methods could reduce simulation error
- Time evolution operator:

$$U(t) = e^{-iHt} \approx [S_n(h)]^{t/h}$$

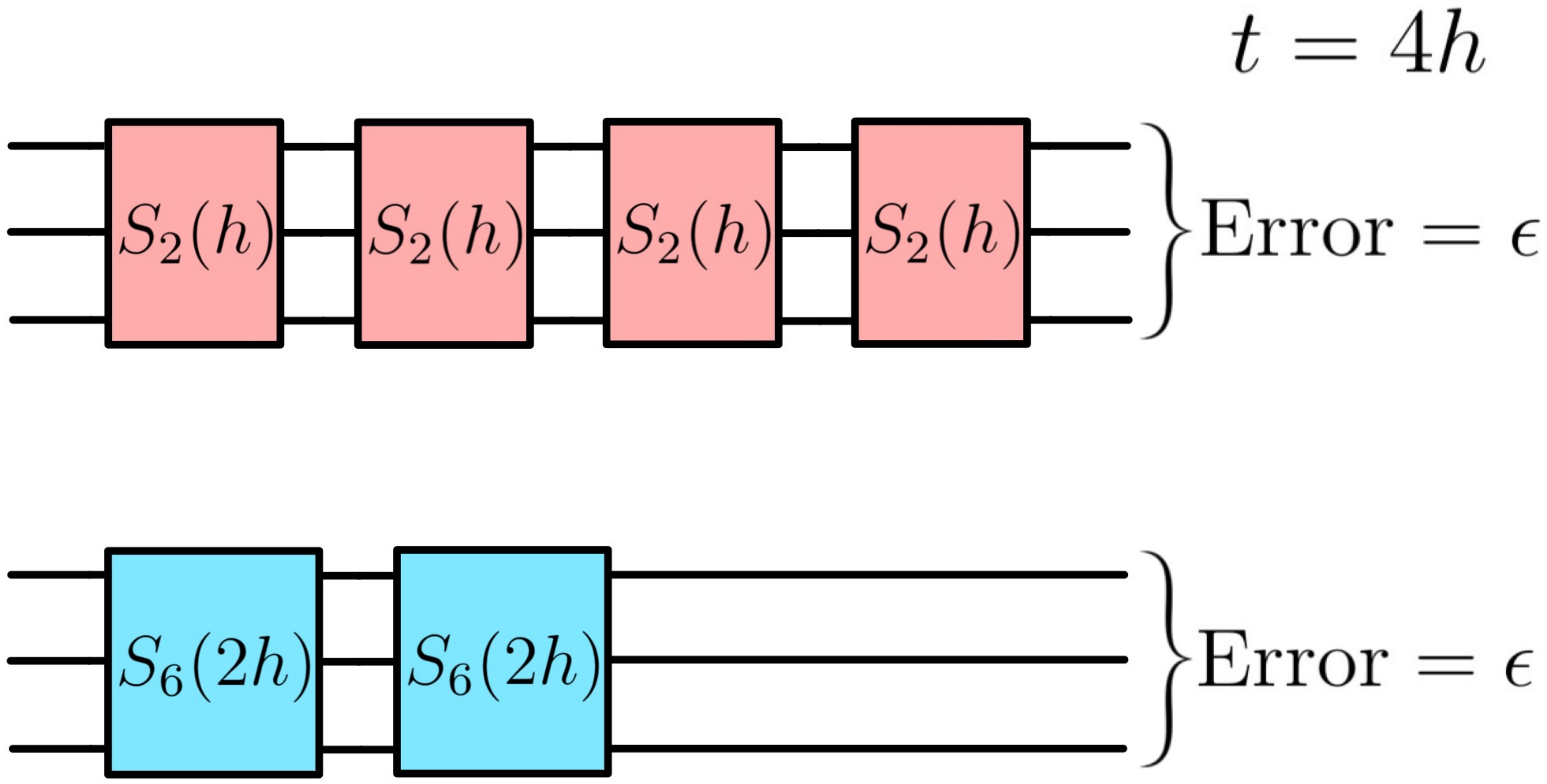


Motivation

- Quantum computers also face hardware problems, e.g. Decoherence and gate depth
- Improving theoretical methods could reduce simulation error
- Time evolution operator:

$$U(t) = e^{-iHt} \approx [S_n(h)]^{t/h}$$

Efficiency

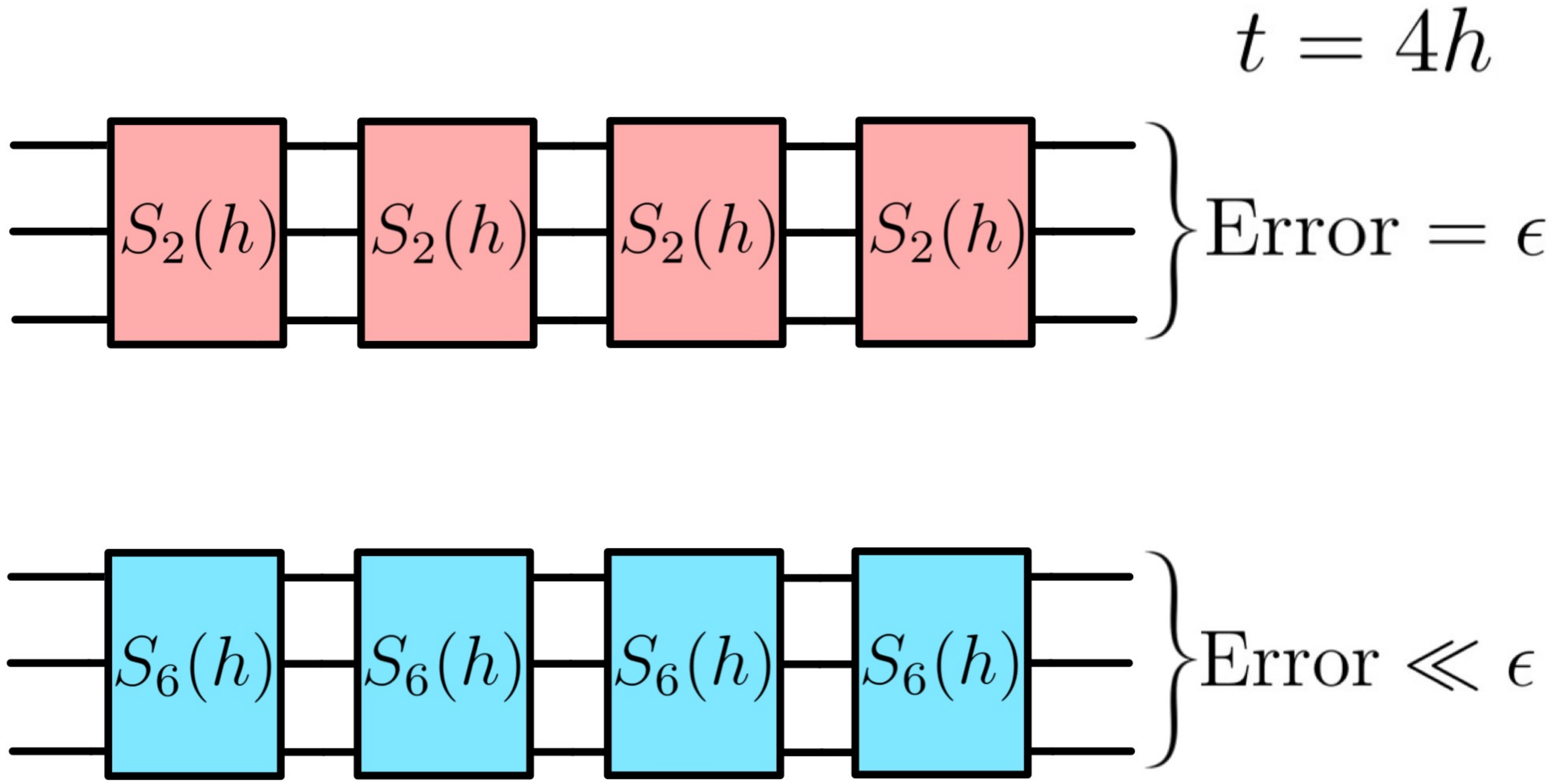


Motivation

- Quantum computers also face hardware problems, e.g. Decoherence and gate depth
- Improving theoretical methods could reduce simulation error
- Time evolution operator:

$$U(t) = e^{-iHt} \approx [S_n(h)]^{t/h}$$

Accuracy



Trotter-Suzuki decompositions

Time evolution

- Schrödinger equation: $i\frac{\partial}{\partial t}|\psi(t)\rangle = H|\psi(t)\rangle$
- Solved by the time evolution operator $U(t) = e^{-iHt}$: $|\psi(t)\rangle = U(t)|\psi(0)\rangle$
- Imaginary time evolution $(t = -i\tau)$: $|\psi(0)\rangle = \lim_{\tau\to\infty} e^{-H\tau}|\psi(0)\rangle$

Trotter-Suzuki decompositions

Time evolution

- Schrödinger equation: $i\frac{\partial}{\partial t}|\psi(t)\rangle = H|\psi(t)\rangle$
- Solved by the time evolution operator $U(t) = e^{-iHt}$: $|\psi(t)\rangle = U(t)|\psi(0)\rangle$
- Imaginary time evolution $(t = -i\tau)$: $|\psi(0)\rangle = \lim_{\tau\to\infty} e^{-H\tau}|\psi(0)\rangle$
- Analytical solutions possible for simple, small and symmetric systems
- Exact diagonalization possible for small systems (e.g. spin chains with $L \lesssim 20$)
- Exchange scalability for a discretization error using Trotterizations

$$\boxed{U(t) \approx [S_n(h)]^{t/h}}$$

Trotter-Suzuki decompositions

Baker-Campbell-Hausdorf formula

- Hamiltonian with two terms: $H = A + B$
- BCH formula: $e^{Ah}e^{Bh} = e^{(A+B)h + \frac{h^2}{2}[A,B] - \frac{h^3}{24}[A,[A,B]] + \frac{h^3}{12}[B,[B,A]] + \mathcal{O}(h^4)}$

Trotter-Suzuki decompositions

Baker-Campbell-Hausdorf formula

- Hamiltonian with two terms: $H = A + B$
- BCH formula: $e^{Ah}e^{Bh} = e^{(A+B)h + \frac{h^2}{2}[A,B] - \frac{h^3}{24}[A,[A,B]] + \frac{h^3}{12}[B,[B,A]] + \mathcal{O}(h^4)}$
- Non-commuting case: $e^{Ah}e^{Bh} = e^{(A+B)h + \mathcal{O}(h^2)}$ - Order $n = 1$
- Leapfrog (Verlet) scheme: $e^{\frac{A}{2}h}e^{Bh}e^{\frac{A}{2}h} = e^{(A+B)h + \mathcal{O}(h^3)}$ - Order $n = 2$
- Symmetric schemes lead to even orders without much cost

Trotter-Suzuki decompositions

Scheme construction

- Construction of higher order decompositions $(n \geq 4)$
- Suzuki and Yoshida methods - Construction using lower order schemes
- Both methods fail to find maximally efficient schemes

Trotter-Suzuki decompositions

Scheme construction

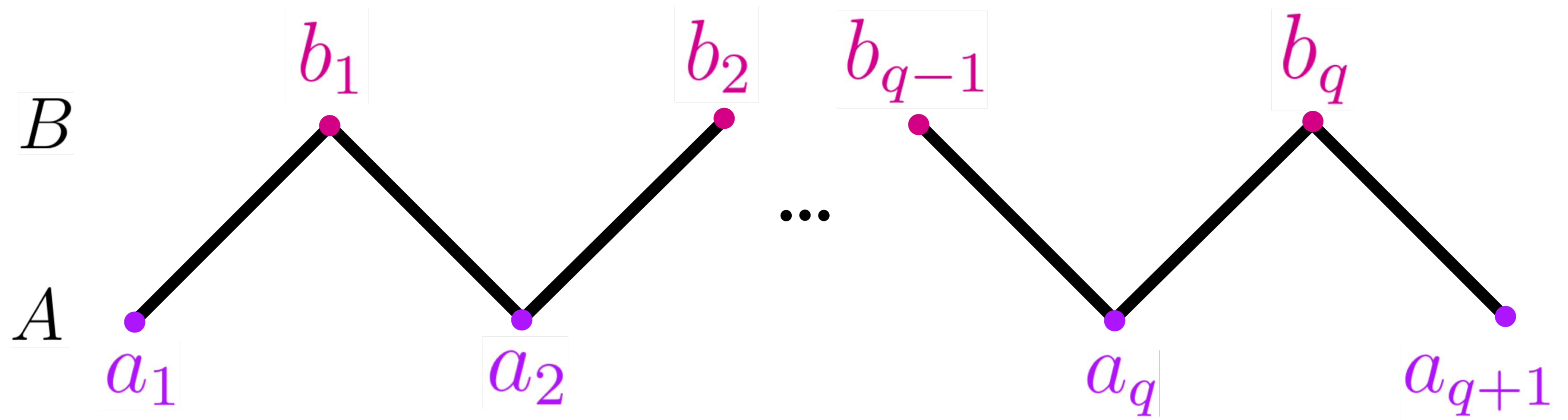
- Construction of higher order decompositions $(n \geq 4)$
- Omelyan's method - Construction from scratch
- Assume symmetric (not necessarily real) parameters $(a_1 = a_{q+1},\ b_1 = b_q)$

$$e^{(A+B)h+O_1h+O_3h^3+O_5h^5} = e^{a_1Ah}e^{b_1Bh}\cdots e^{b_qBh}e^{a_{q+1}Ah}$$

- Notation: - Stage, $e^{a_iA_ih}$

  - Ramp (up, down)

  - No. cycles q



Trotter-Suzuki decompositions

Omelyan's method

- Assume symmetric (not necessarily real) parameters $(a_1 = a_{q+1},\ b_1 = b_q)$

$$e^{(A+B)h+O_1h+O_3h^3+O_5h^5} = e^{a_1 Ah} e^{b_1 Bh} \cdots e^{b_q Bh} e^{a_{q+1} Ah}$$

- Valid if, $\nu = \sigma = 1$ which is guaranteed by:

$$\sum_i a_i = \sum_i b_i = 1$$

$$O_1 = (\nu - 1)A + (\sigma - 1)B,$$

$$O_3 = \alpha C_1 + \beta C_2, \quad C_1 = [A, [A, B]], \quad C_2 = [B, [B, A]],$$

$$O_5 = \sum_{k=1}^{6} \gamma_k D_k, \quad D_1 = [A, [A, [A, [A, B]]]], \quad D_2 = [A, [A, [B, [A, B]]]],$$

$$D_3 = [B, [A, [A, [A, B]]]], \quad D_4 = [A, [B, [B, [B, A]]]],$$

$$D_5 = [B, [B, [A, [B, A]]]], \quad D_6 = [B, [B, [B, [B, A]]]].$$

Trotter-Suzuki decompositions

Omelyan's method

- Assume symmetric (not necessarily real) parameters $(a_1 = a_{q+1},\ b_1 = b_q)$

$$e^{(A+B)h+O_1h+O_3h^3+O_5h^5} = e^{a_1Ah}e^{b_1Bh}\cdots e^{b_qBh}e^{a_{q+1}Ah}$$

- Order $n = 4$ satisfied by:

$$\alpha(a_i, b_i) = \beta_i(a_i, b_i) = 0$$

- Order $n = 6$ satisfied by:

$$\gamma_j(a_i, b_i) = 0$$

$$O_1 = (\nu - 1)A + (\sigma - 1)B,$$

$$O_3 = \alpha C_1 + \beta C_2, \quad C_1 = [A,[A,B]], \quad C_2 = [B,[B,A]],$$

$$O_5 = \sum_{k=1}^{6} \gamma_k D_k, \quad D_1 = [A,[A,[A,[A,B]]]], \quad D_2 = [A,[A,[B,[A,B]]]],$$

$$D_3 = [B,[A,[A,[A,B]]]], \quad D_4 = [A,[B,[B,[B,A]]]],$$

$$D_5 = [B,[B,[A,[B,A]]]], \quad D_6 = [B,[B,[B,[B,A]]]].$$

Trotter-Suzuki decompositions

Omelyan's method

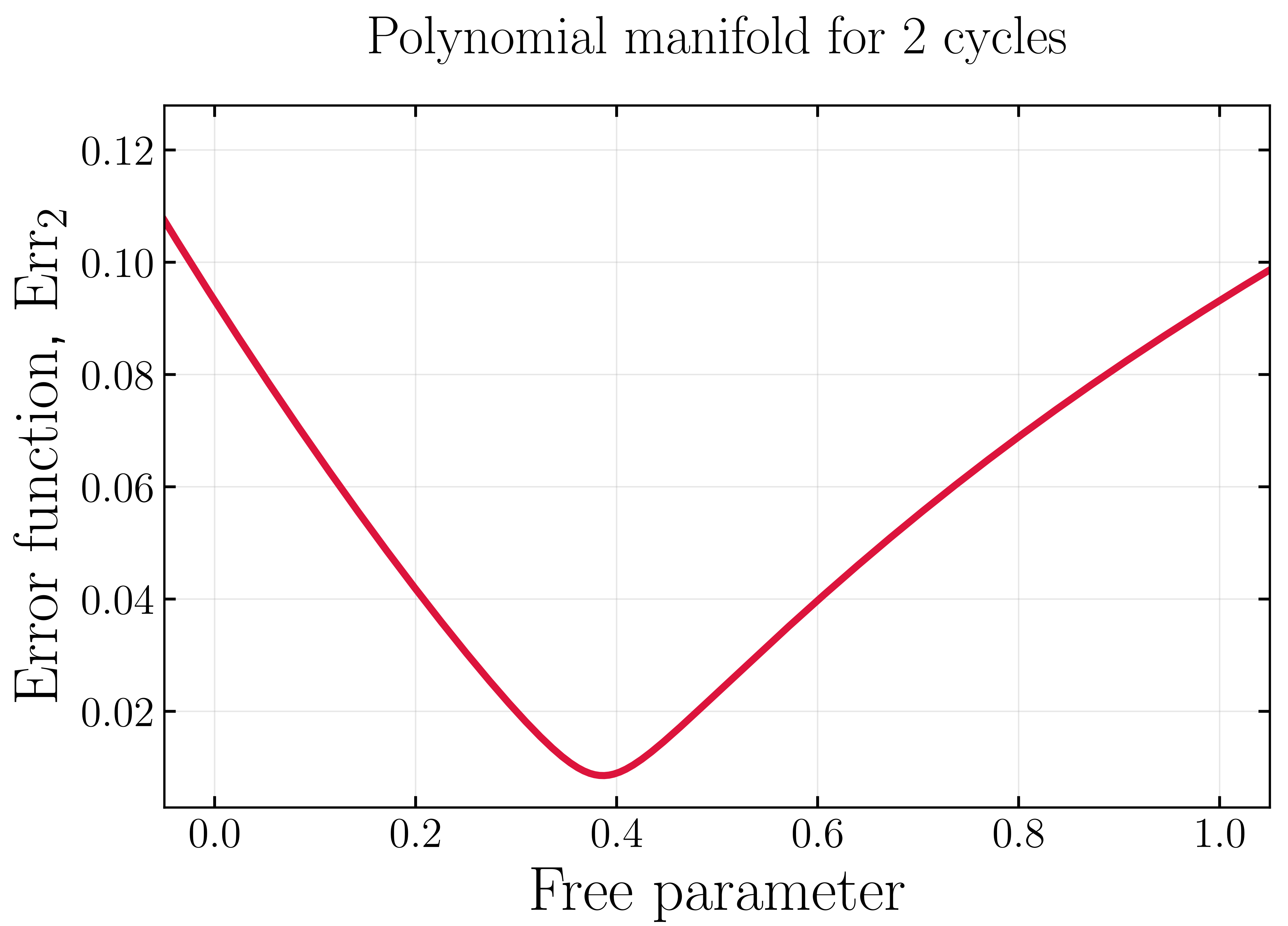
- "A decomposition is efficient if its leading order errors are small compared to the no. cycles q it requires"
- Error definition: $\mathrm{Err}_2(a_i, b_i) = \sqrt{|\alpha|^2 + |\beta|^2}$, $\mathrm{Err}_4(a_i, b_i) = \sqrt{\sum_{i=1}^{6} |\gamma_i|^2}$,

  where we assume orthogonality of the basis
- Efficiency definition: $\mathrm{Eff}_2 = \dfrac{1}{q^2 \mathrm{Err}_2}$, $\mathrm{Eff}_4 = \dfrac{1}{q^4 \mathrm{Err}_4}$

Trotter-Suzuki decompositions

Omelyan's method

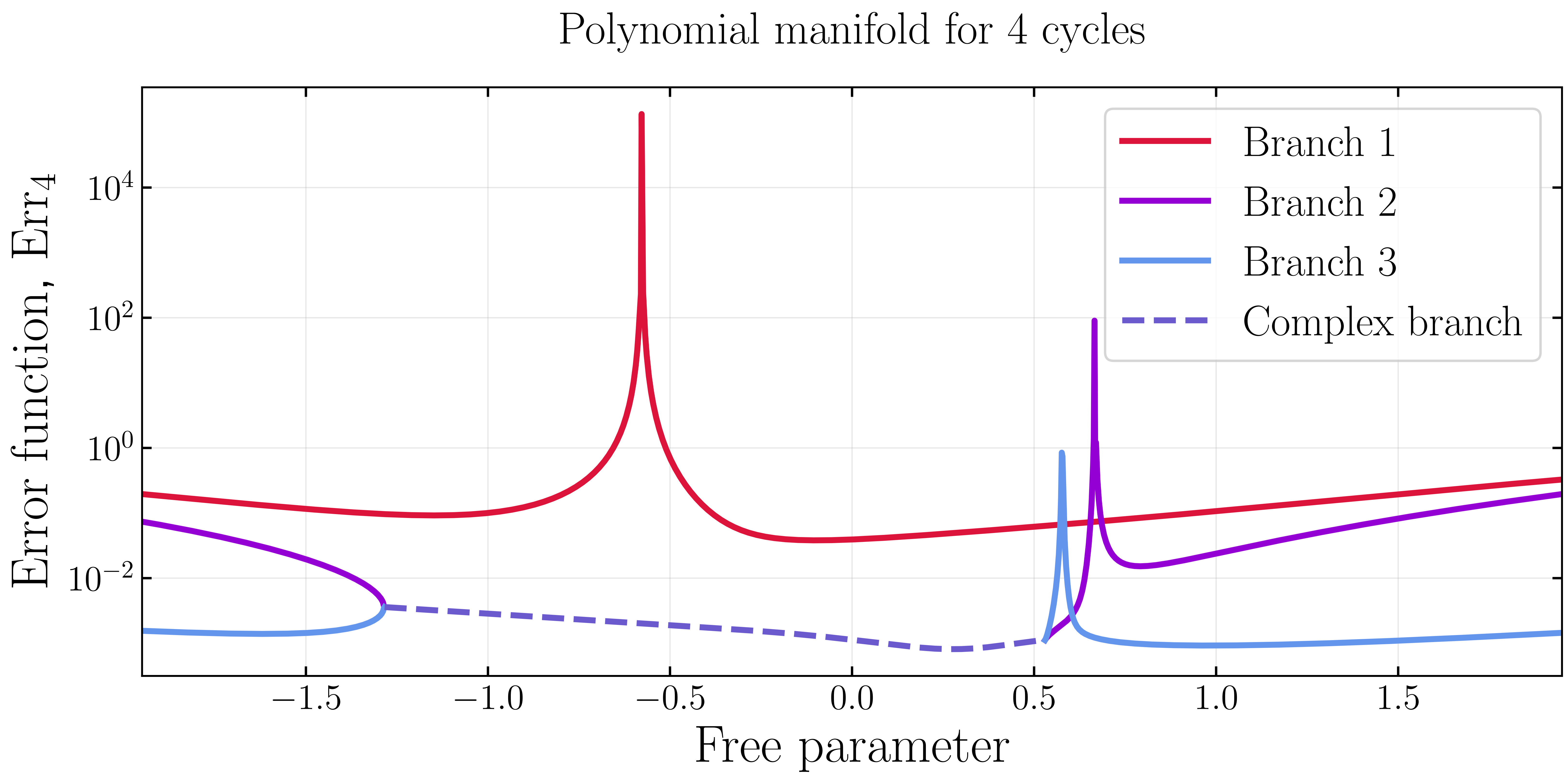
- With increased order and no. cycles the error manifold complexity rises



Trotter-Suzuki decompositions

Omelyan's method

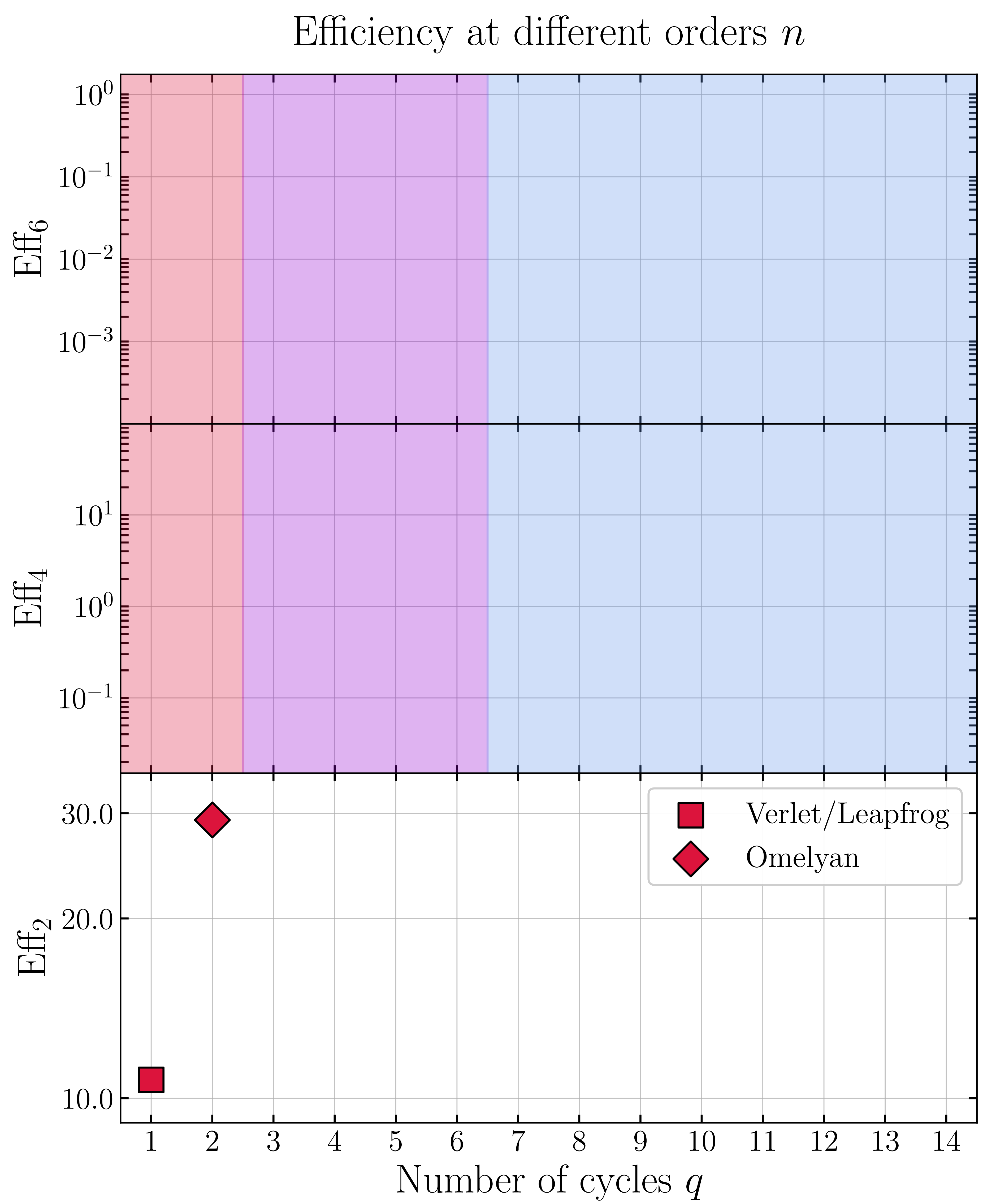
- With increased order and no. cycles the error manifold complexity rises



Efficiency results

Order 2

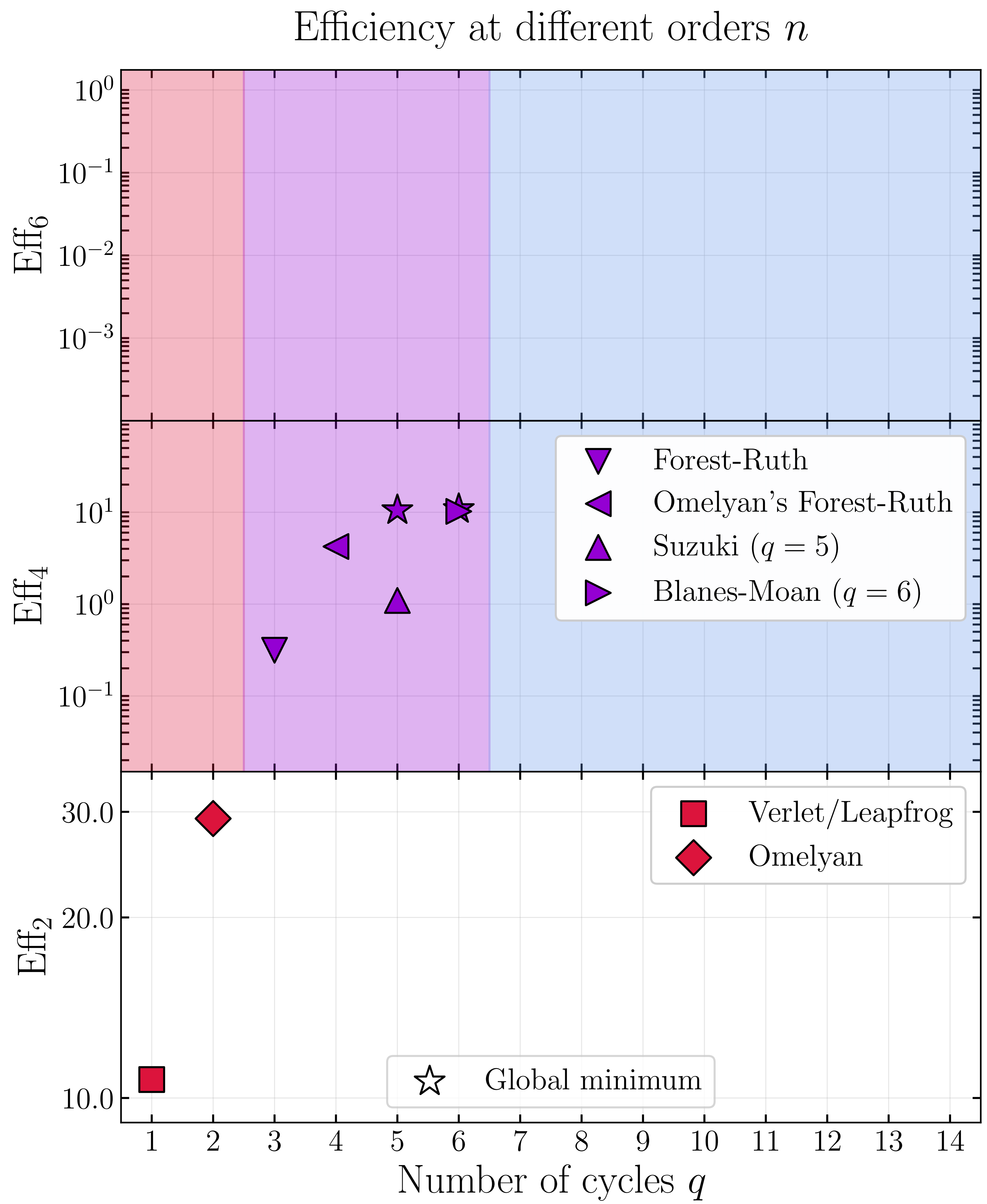
- Verlet or Leapfrog scheme $(q = 1)$
  - Simple, yet performs very well
  - Valid, if high precision is not desired
- Omelyan's scheme $(q = 2)$
  - One free parameter to optimize
  - Comparable to Leapfrog



Efficiency results

Order 4

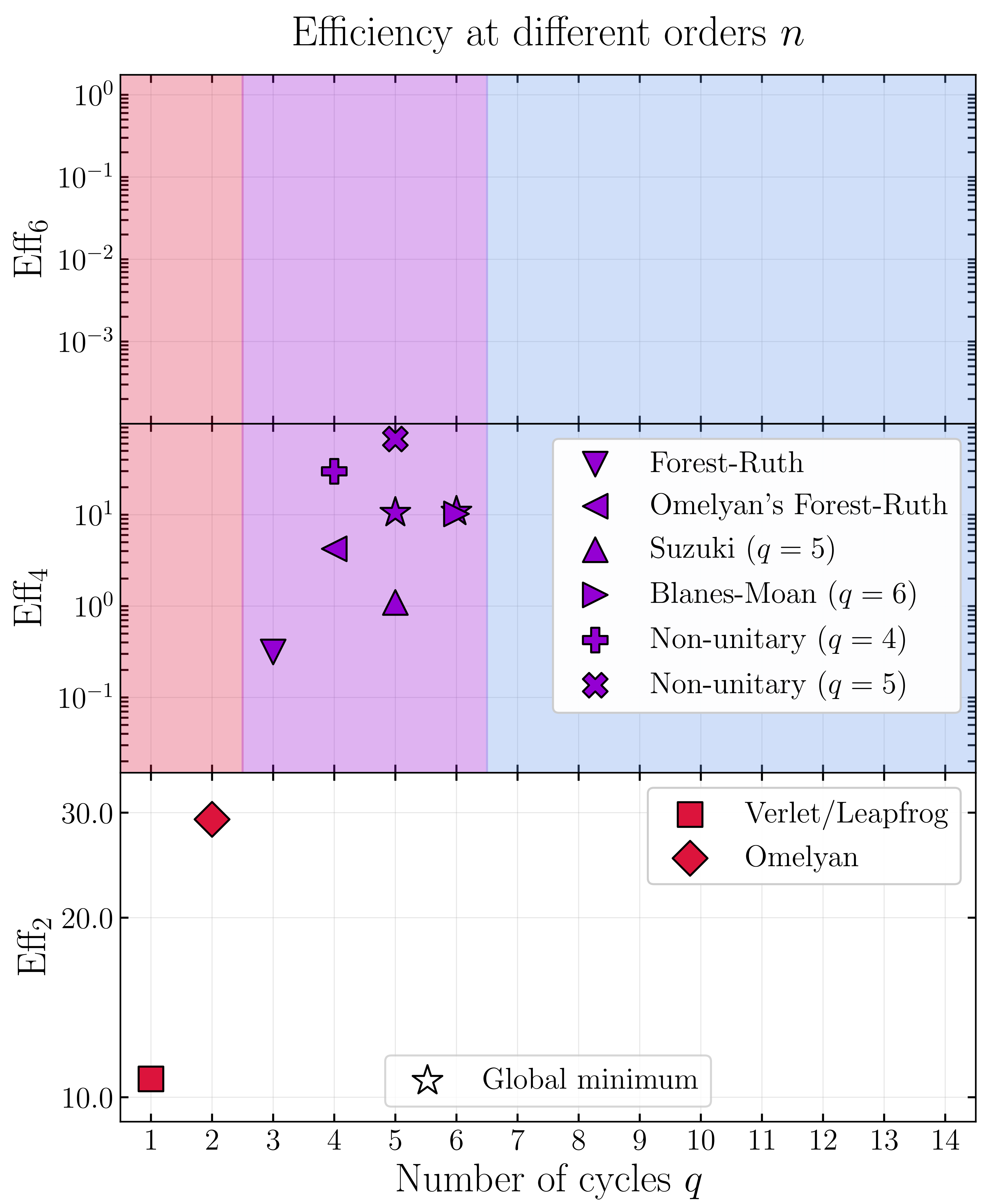
- Forest-Ruth scheme $(q = 3)$
  - Poor performance
- Omelyan's Forest-Ruth scheme $(q = 4)$
  - One free parameter
- Suzuki's scheme $(q = 5)$
  - Favourable error accumulation
- Blanes-Moan $(q = 6)$
  - Highly efficient order 4 scheme



Efficiency results

Order 4

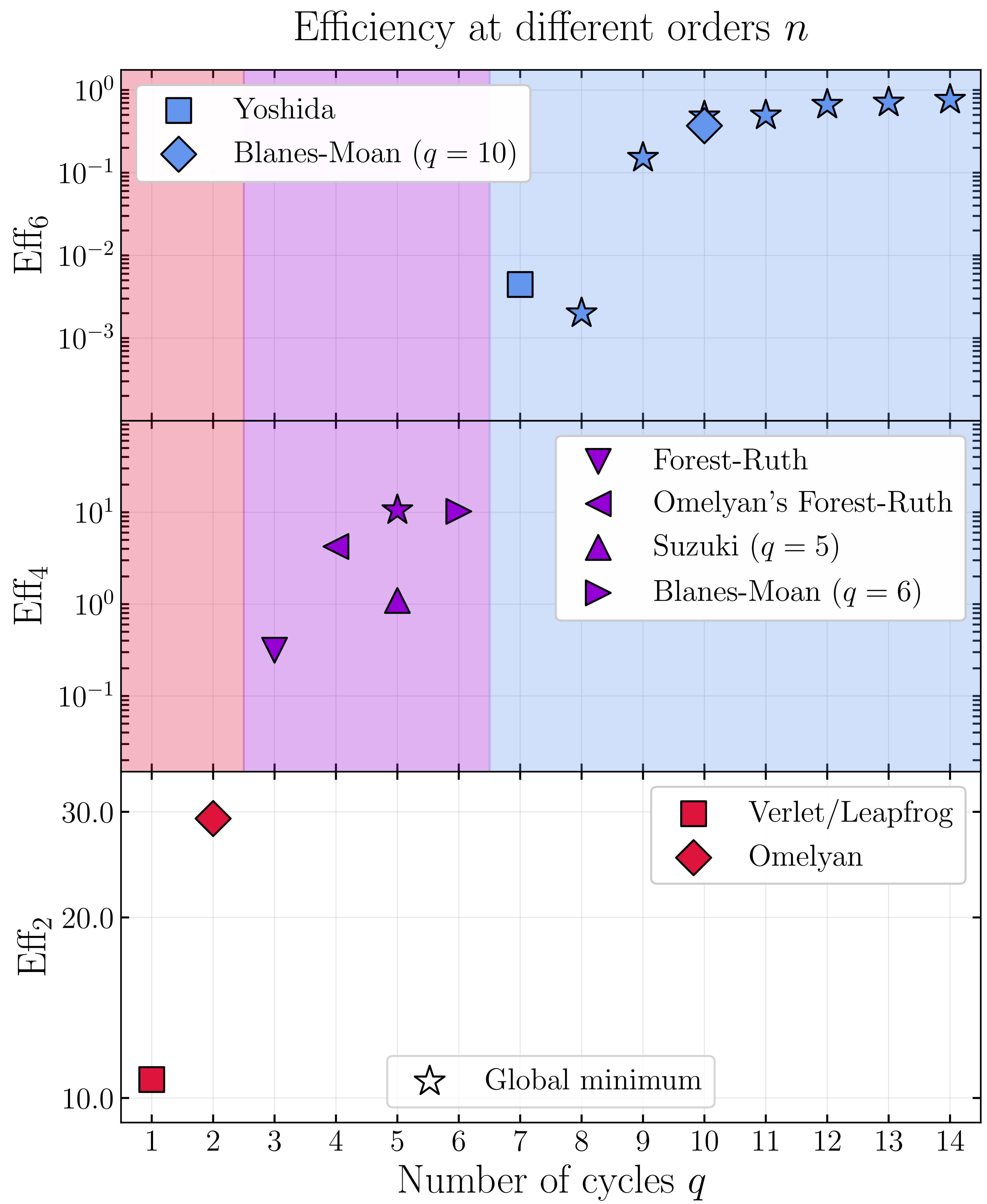
- Forest-Ruth scheme $(q = 3)$
  - Poor performance
- Omelyan's Forest-Ruth scheme $(q = 4)$
  - One free parameter
- Suzuki's scheme $(q = 5)$
  - Favourable error accumulation
- Blanes-Moan $(q = 6)$
  - Highly efficient order 4 scheme



Efficiency results

Order 6

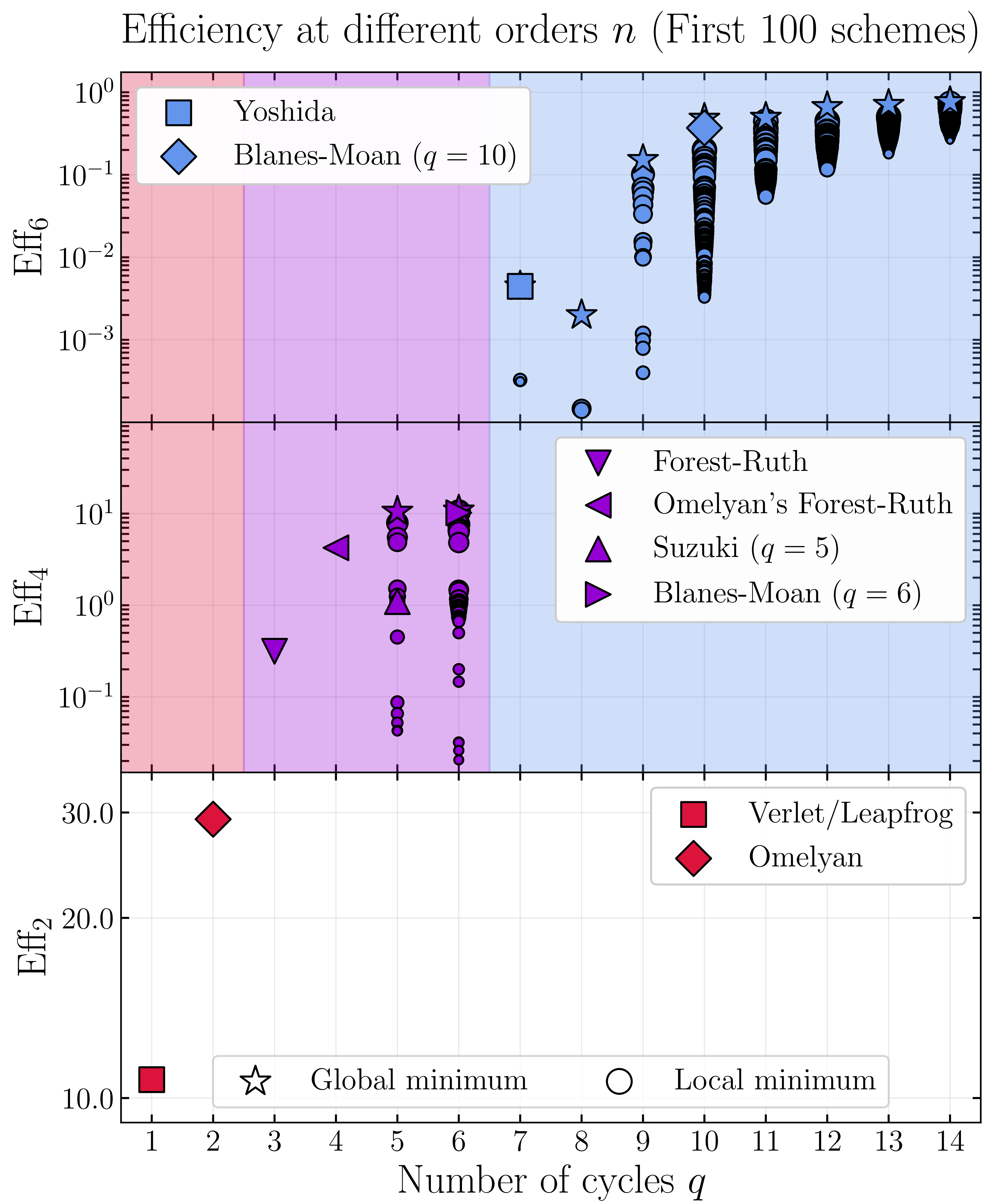
- Yoshida $(q = 7)$
  - Unusual scheme $(n_p = 8, n_c = 10)$
  - Extremely poor efficiency
- Blanes-Moan $(q = 10)$
  - One of the best order 6 schemes
- New found schemes
  - Improvement over the known schemes



Efficiency results

Order 6

- Yoshida $(q = 7)$
  - Unusual scheme $(n_p = 8, n_c = 10)$
  - Extremely poor efficiency
- Blanes-Moan $(q = 10)$
  - One of the best order 6 schemes
- New found schemes
  - Improvement over the known schemes
  - Also explored the local minima



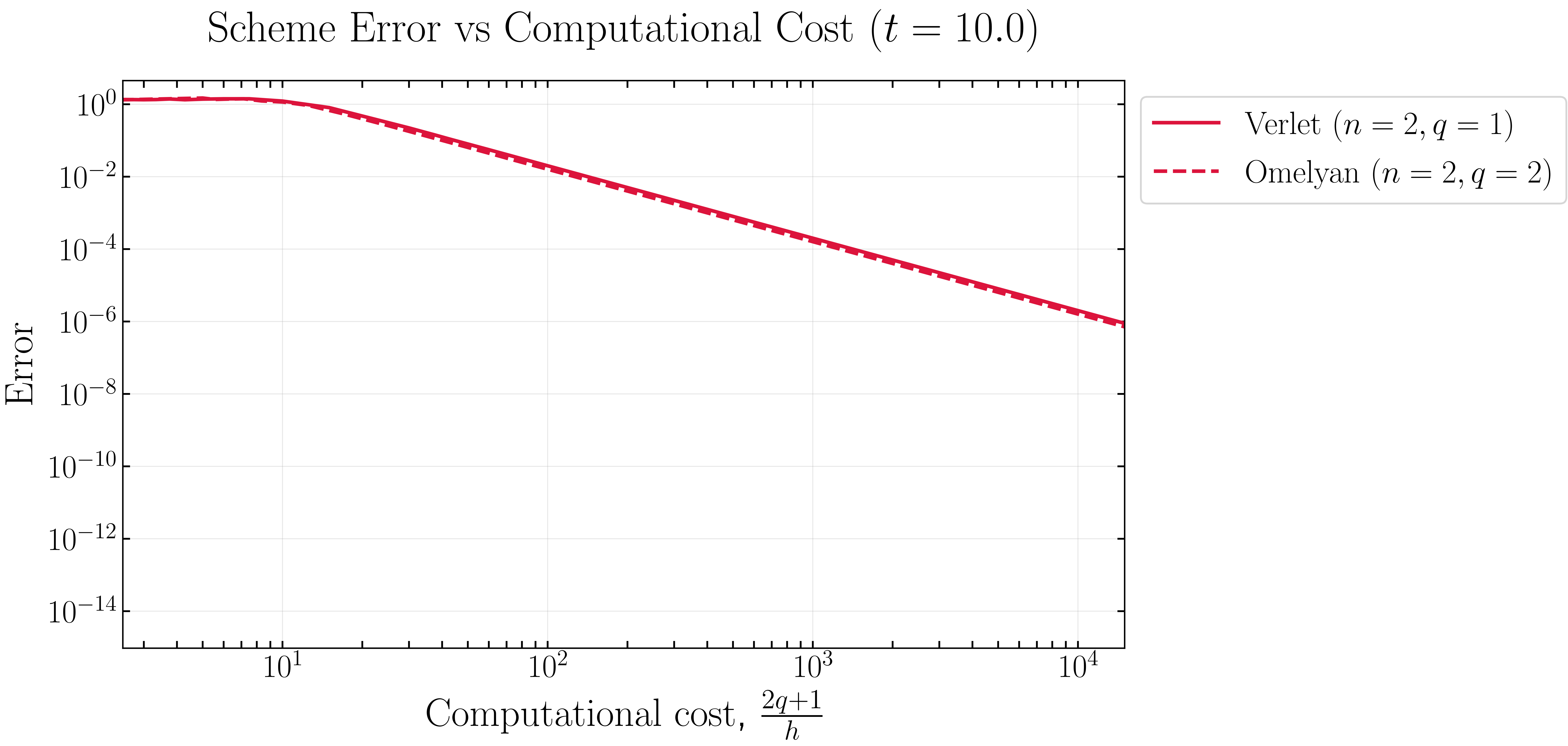
Numerical experiments

- The Heisenberg XXZ model: $H = \sum_{i=1}^{L} \left(J^x \sigma_i^x \sigma_{i+1}^x + J^y \sigma_i^y \sigma_{i+1}^y + J^z \sigma_i^z \sigma_{i+1}^z + h_i \sigma_i^z \right)$, $J^\alpha = 1$
- Correspondence with quantum computers (local gates)
- Periodic spin chain of length $L = 6$
- Estimate error using the Frobenius norm:

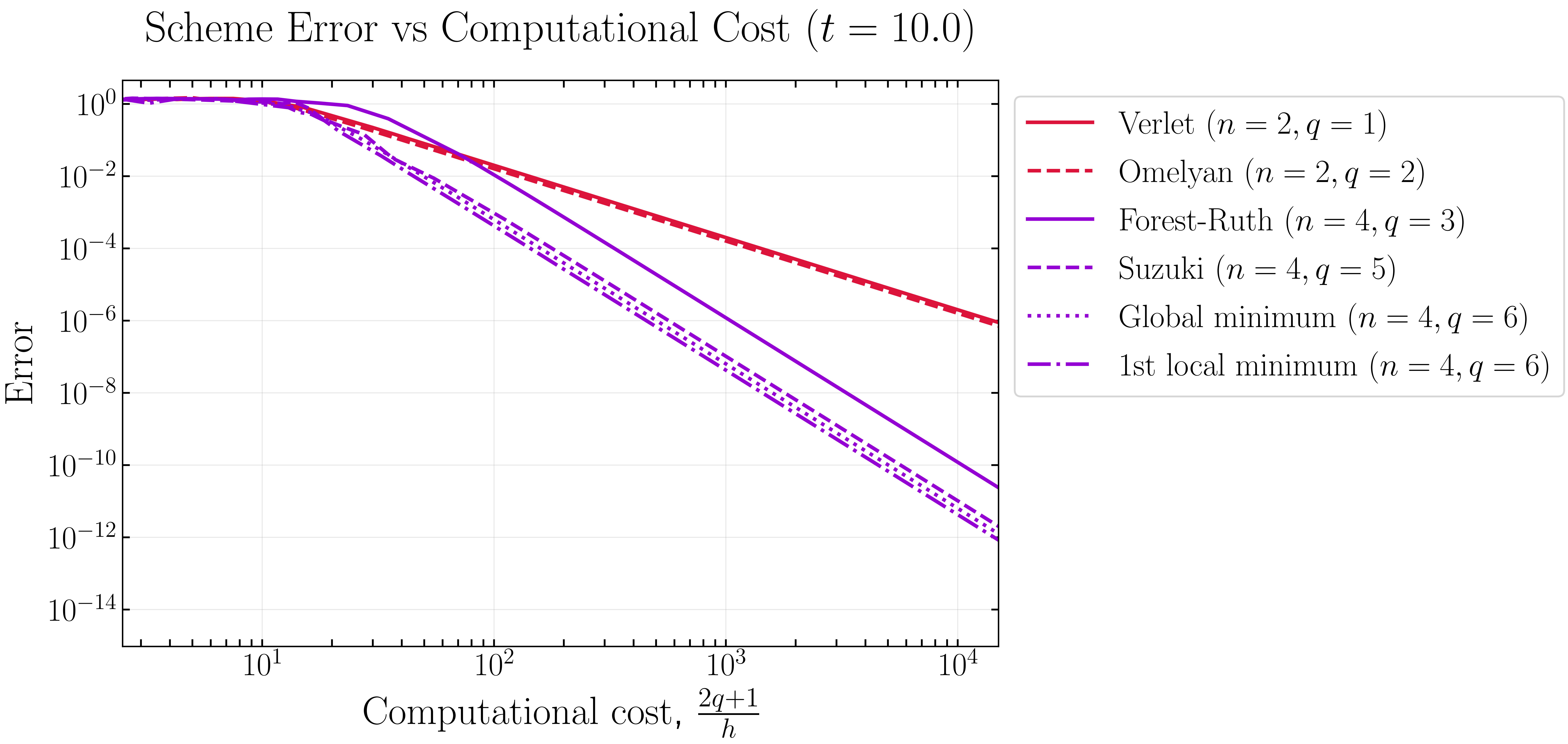
$$\mathrm{Error}(t) = \left\| U(t) - S(h)^{t/h} \right\|_F \, , \quad U(t) \approx [S(h)]^{t/h}$$

Evolve until time $t = 10.0$, using some time step h

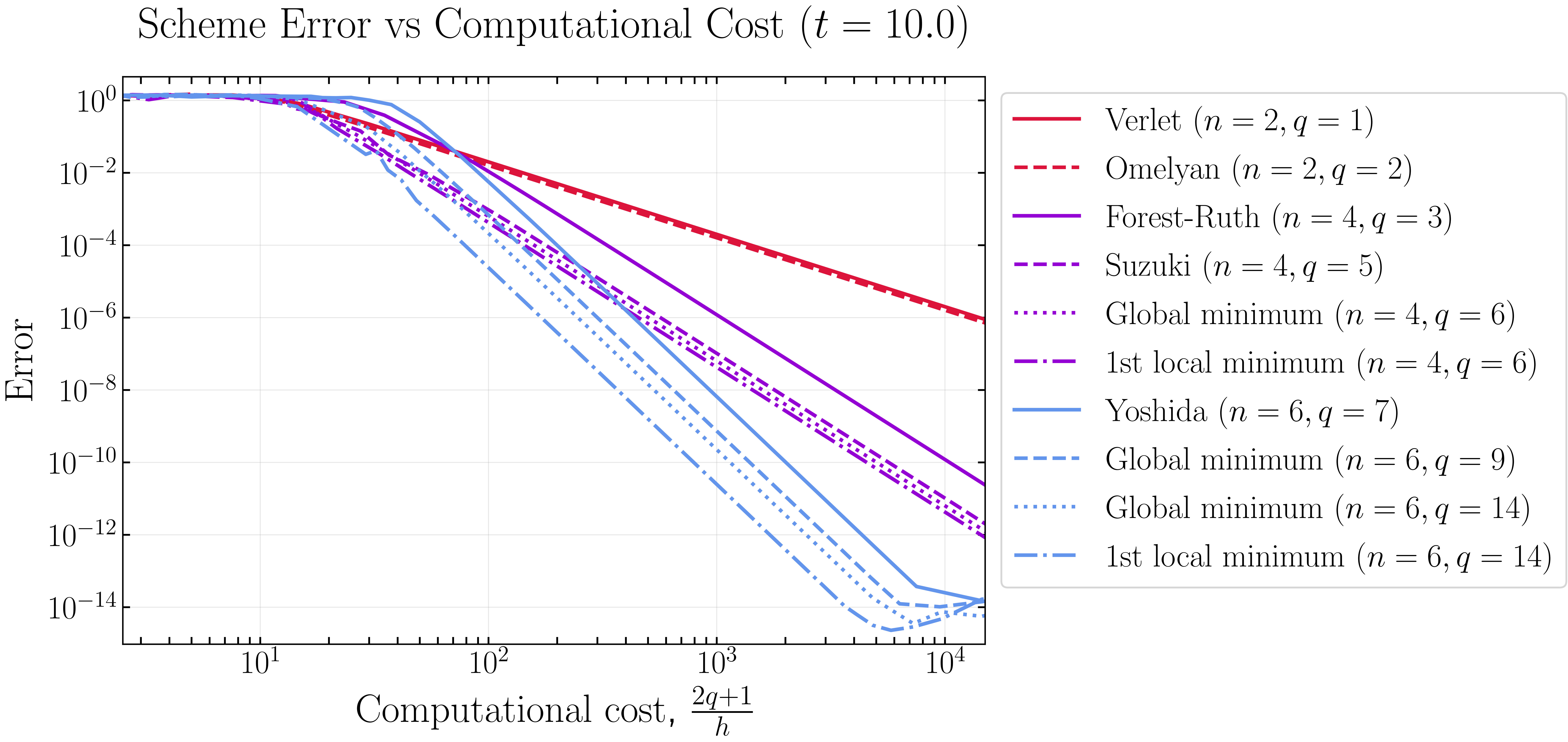
Numerical experiments



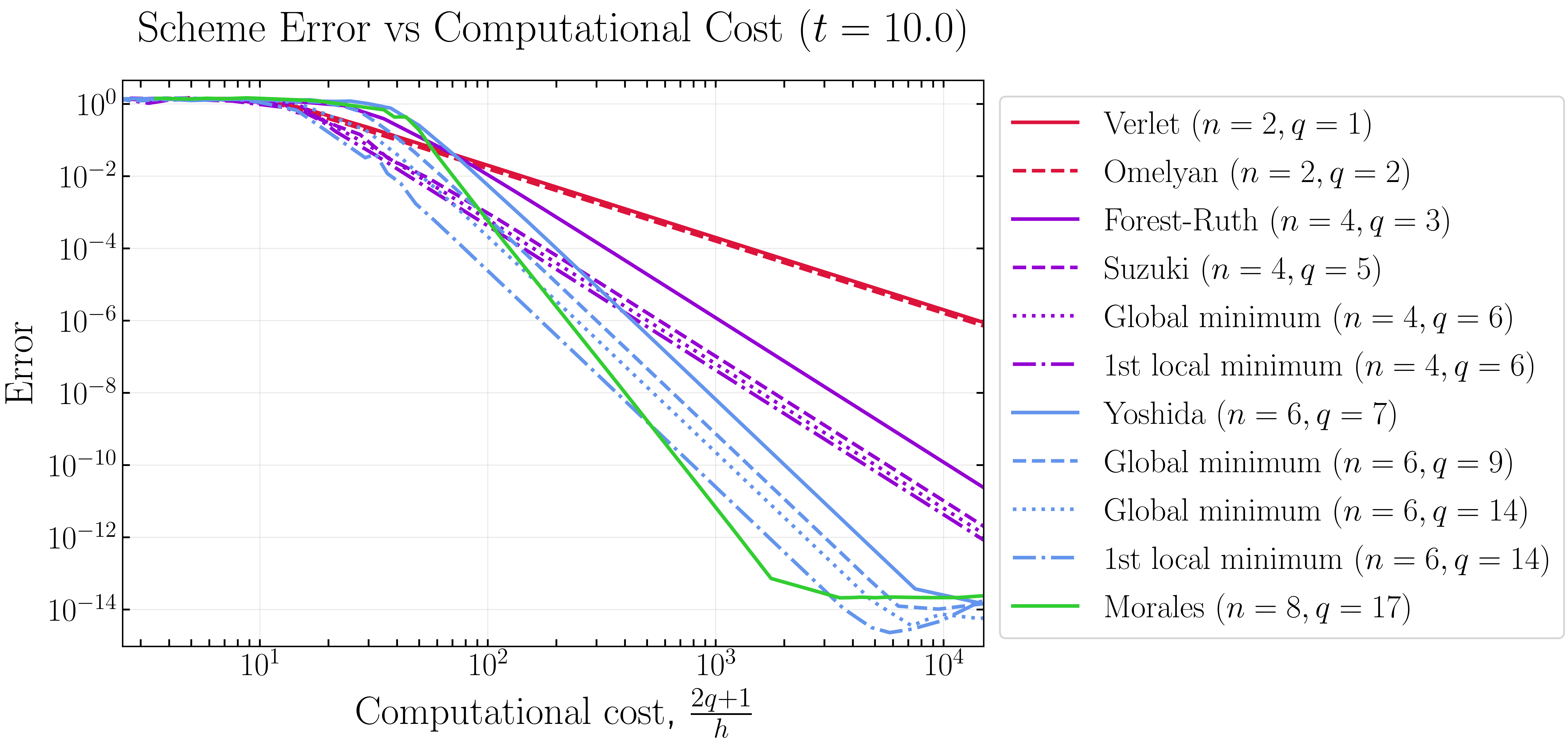
Numerical experiments



Numerical experiments



Numerical experiments



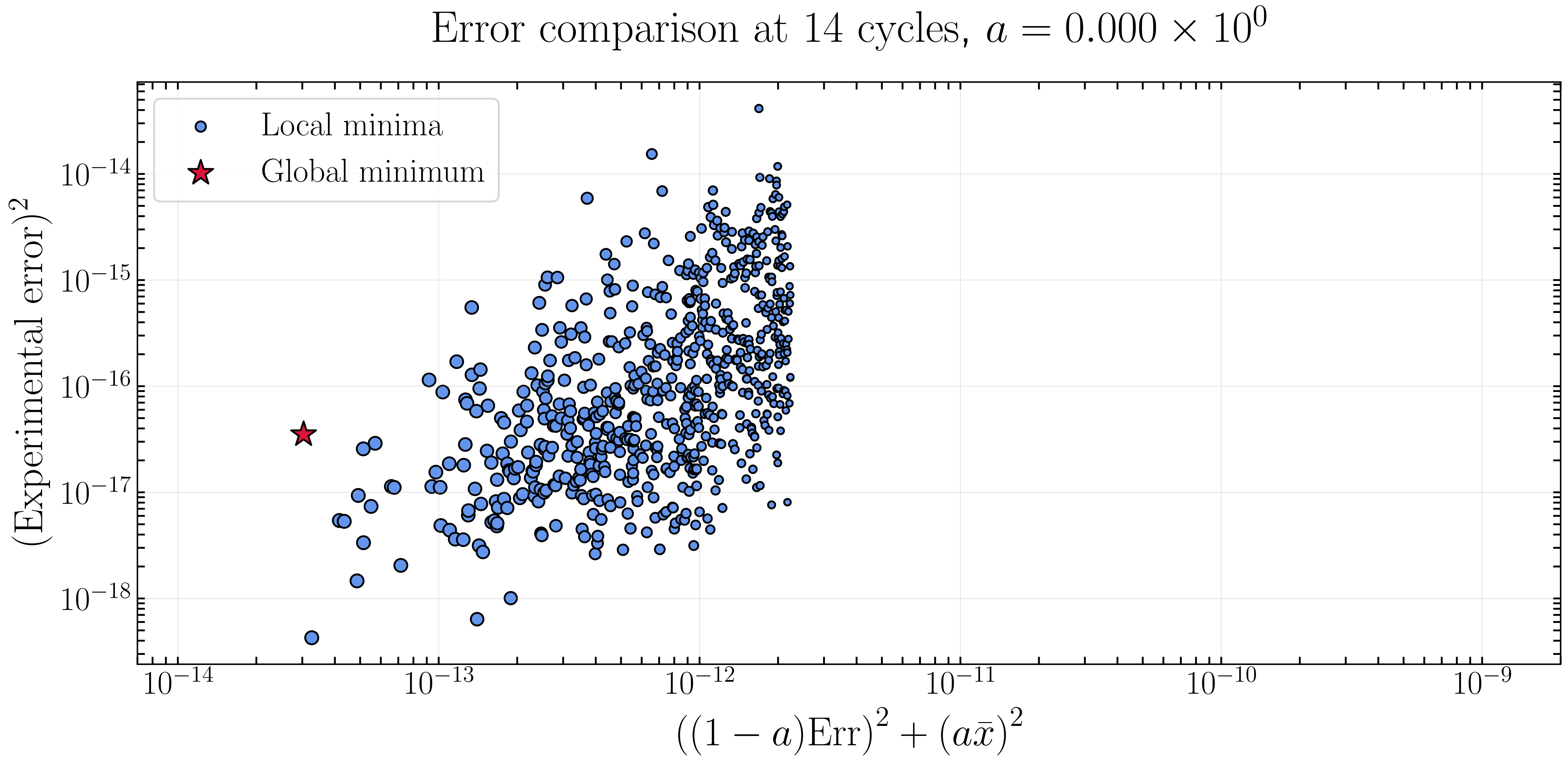
Numerical experiments

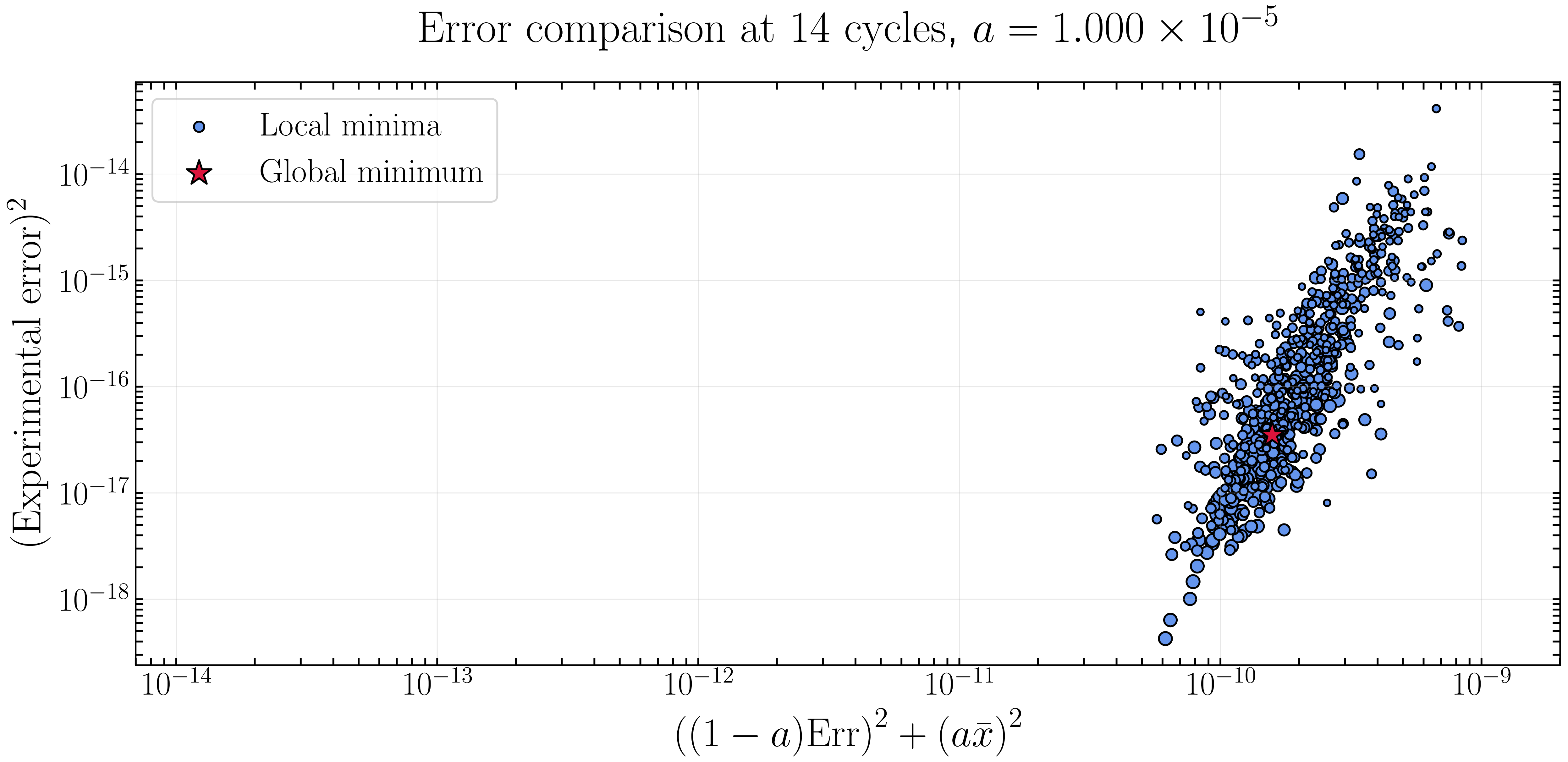
- Correspondence between the experimental and theoretical error is not exact
- Investigate the properties of the parameters (a_i, b_i)
- Optimally: All parameters are exactly the same: $a_i = b_i = x_{\text{opt.}}, \quad x_{\text{opt.}} = \frac{1}{q}$
- Add a term to the theoretical error function:

$$((1-a)\text{Err})^2 + (a\bar{x})^2$$

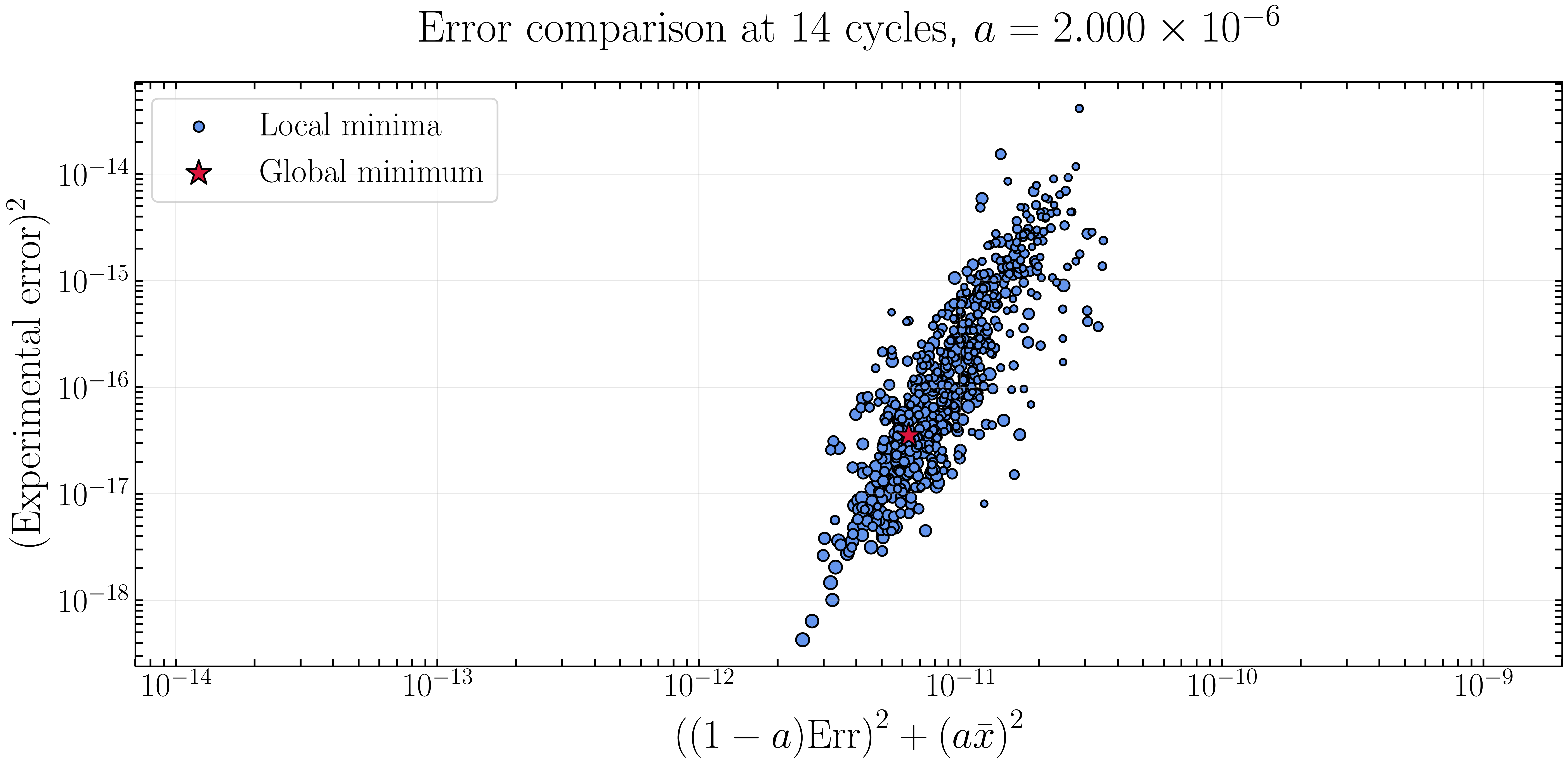
$$\bar{x} = \sum_i (a_i - x_{\text{opt.}}) + \sum_i (b_i - x_{\text{opt.}})$$

Numerical experiments





Numerical experiments



Outlook and future work

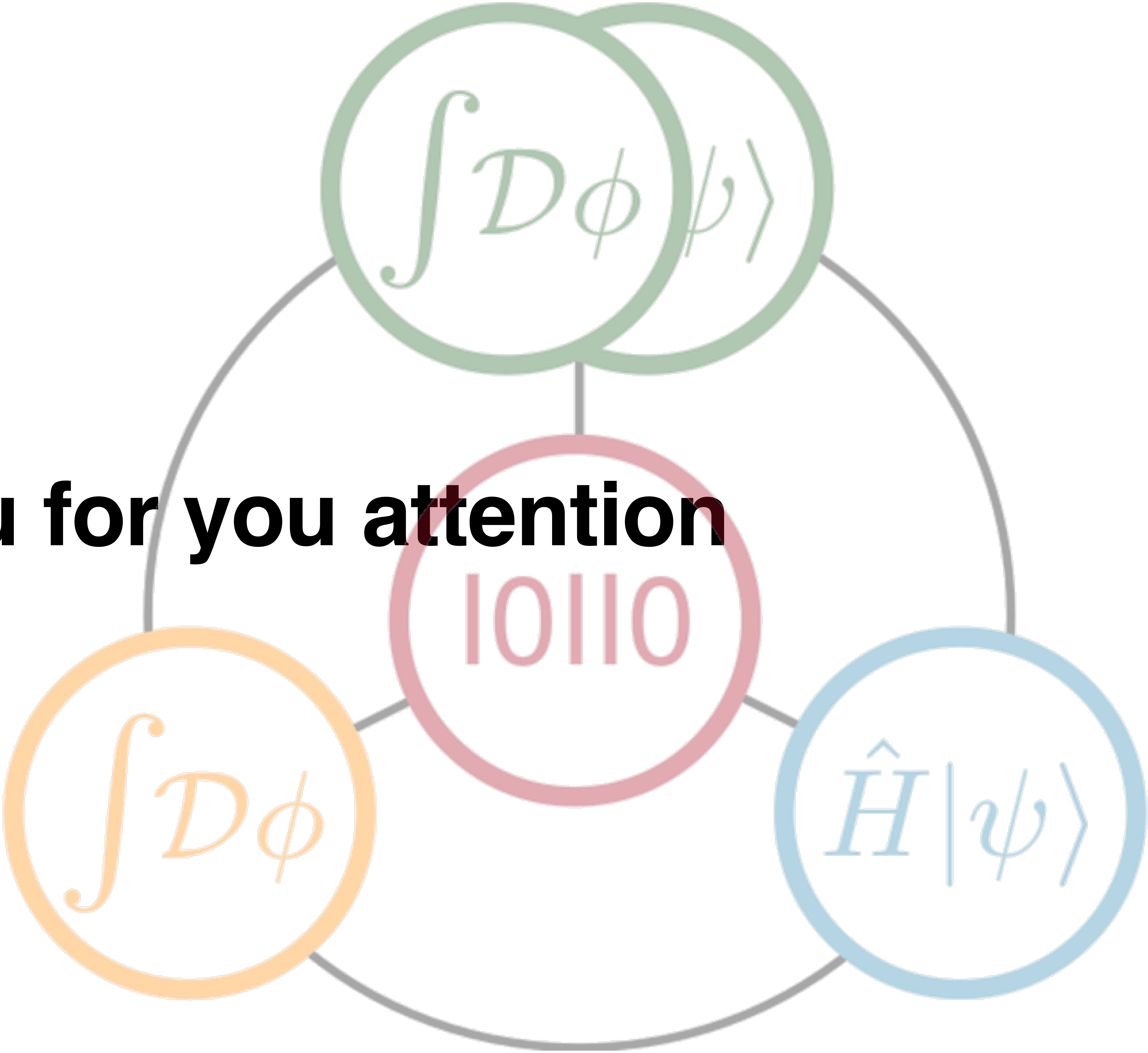
- We extended Omelyan's method to a general framework for optimizing Trotter-Suzuki decompositions and found novel schemes
- In progress: - Theoretical-Experimental error correspondence

  - Order 8 scheme optimization

  - Research of non-unitary schemes with complex parameters
- Future work: - Order 10 recursive formulae

  - Test optimized schemes on quantum hardware

Thank you for you attention

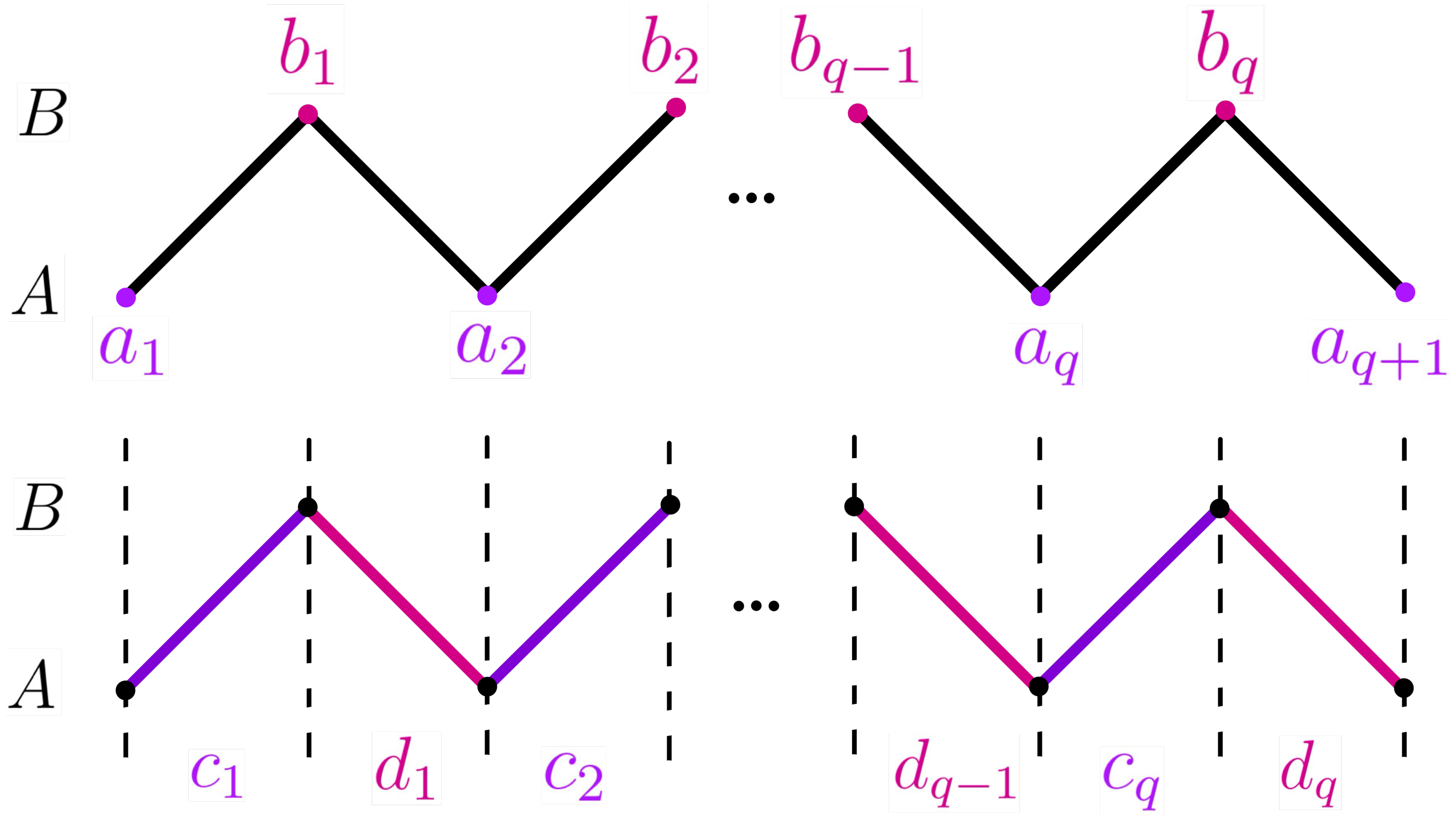


Additional slides

Arbitrary no. stages adaptation

- Every scheme with 2 stages is applicable to an arbitrary no. stages
- Transition from stage-based to a ramp based approach:

$$
\begin{aligned}
c_1 &= a_1\,, & d_1 &= b_1 - c_1\,,\\
&\ \vdots & &\ \vdots\\
c_i &= a_i - d_{i-1}\,, & d_i &= b_i - c_i
\end{aligned}
$$

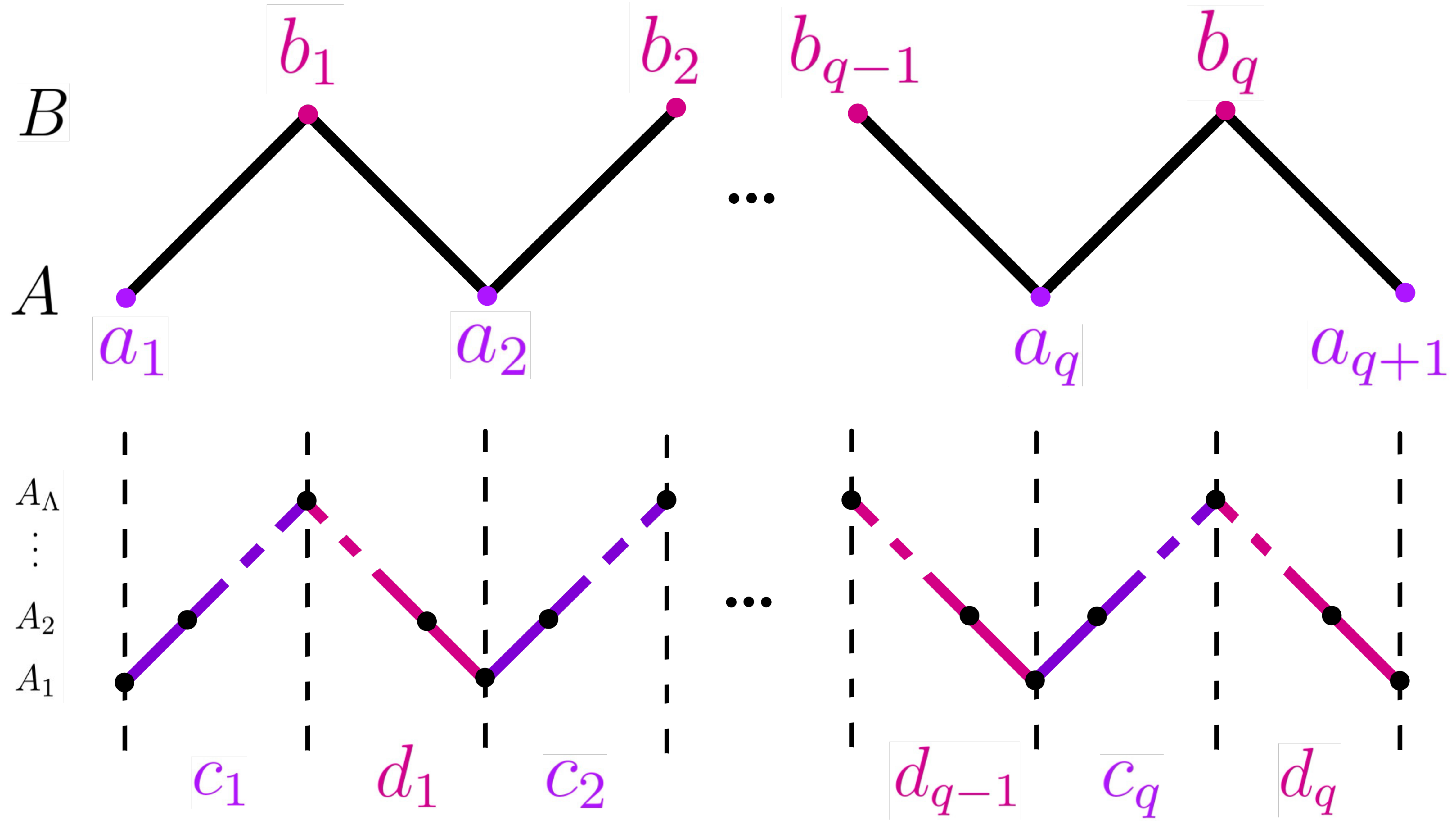


Additional slides

Arbitrary no. stages adaptation

- Every scheme with 2 stages is applicable to an arbitrary no. stages
- Transition from stage-based to a ramp based approach:

$$
\begin{aligned}
c_1 &= a_1\,, & d_1 &= b_1 - c_1\,,\\
&\vdots & &\vdots\\
c_i &= a_i - d_{i-1}\,, & d_i &= b_i - c_i
\end{aligned}
$$



$$
e^{h\sum_{k=1}^{\Lambda} A_k + \mathcal{O}(h^{n+1})} = \left(\prod_{k=1}^{\Lambda} e^{A_k c_1 h}\right)\left(\prod_{k=\Lambda}^{1} e^{A_k d_1 h}\right)\cdots\left(\prod_{k=1}^{\Lambda} e^{A_k c_q h}\right)\left(\prod_{k=\Lambda}^{1} e^{A_k d_q h}\right)
$$

Additional slides

Framework details

- Coefficients α , β and γ_j are polynomials of parameters a_i , b_i

$$e^{(A+B)h+O_1 h+O_3 h^3+O_5 h^5} = e^{\frac{a_2}{2}Ah} e^{\frac{b_1}{2}Bh} e^{a_1 Ah} e^{\frac{b_1}{2}Bh} e^{\frac{a_2}{2}Ah}$$

- Denote a scheme $\Phi^{(i_A, i_B)}$ at iteration (i_A, i_B)

$$e^{\frac{a_2}{2}Ah} e^{\frac{b_1}{2}Bh} e^{a_1 Ah} e^{\frac{b_1}{2}Bh} e^{\frac{a_2}{2}Ah} \to e^{\frac{a_2}{2}Ah} e^{\Phi^{(1,1)}} e^{\frac{a_2}{2}Ah} \to e^{\Phi^{(2,1)}}$$

- General form:

$$\Phi^{(i_A, i_B)} = \left(\nu^{(i_A)} A + \sigma^{(i_B)} B\right) h + \left(\alpha^{(i_A, i_B)} C_1 + \beta^{(i_A, i_B)} C_2\right) h^3 + h^5 \sum_k \gamma_k^{(i_A, i_B)} D_k + \cdots$$

where: $\nu^{(i_A)} = \sum_{i=1}^{i_A} a_i, \quad \sigma^{(i_B)} = \sum_{i=1}^{i_B} b_i$

Additional slides

Framework details

- Use the BCH formula to derive the recursive formulae for the coefficients

$$e^{\Phi^{(i,i-1)}} = e^{\frac{a_i}{2}Ah} e^{\Phi^{(i-1,i-1)}} e^{\frac{a_i}{2}Ah}$$

- Order 2 coefficients recursive formulae:

$$\alpha^{(i,i-1)} = \alpha^{(i-1,i-1)} + \alpha a_i^2 \sigma^{(i-1)} - \beta a_i \nu^{(i-1)} \sigma^{(i-1)},$$

$$\beta^{(i,i-1)} = \beta^{(i-1,i-1)} + \beta a_i \left(\sigma^{(i-1)}\right)^2$$

- Higher order derivations become much more involved

Additional slides

Framework details

- The error function defines a high-dimensional manifold in parameters a_i and b_i
- Dimension: $n_p = q + 1$, $n_c \in (2, 4, 10, \ldots)$
- Goal: minimize this manifold to identify global and local minima

$$\mathrm{Err}_2(a_i, b_i) = \sqrt{|\alpha|^2 + |\beta|^2}$$

$$\mathrm{Err}_4(a_i, b_i) = \sqrt{\sum_{k=1}^{6} |\gamma_k|^2}$$

Additional slides

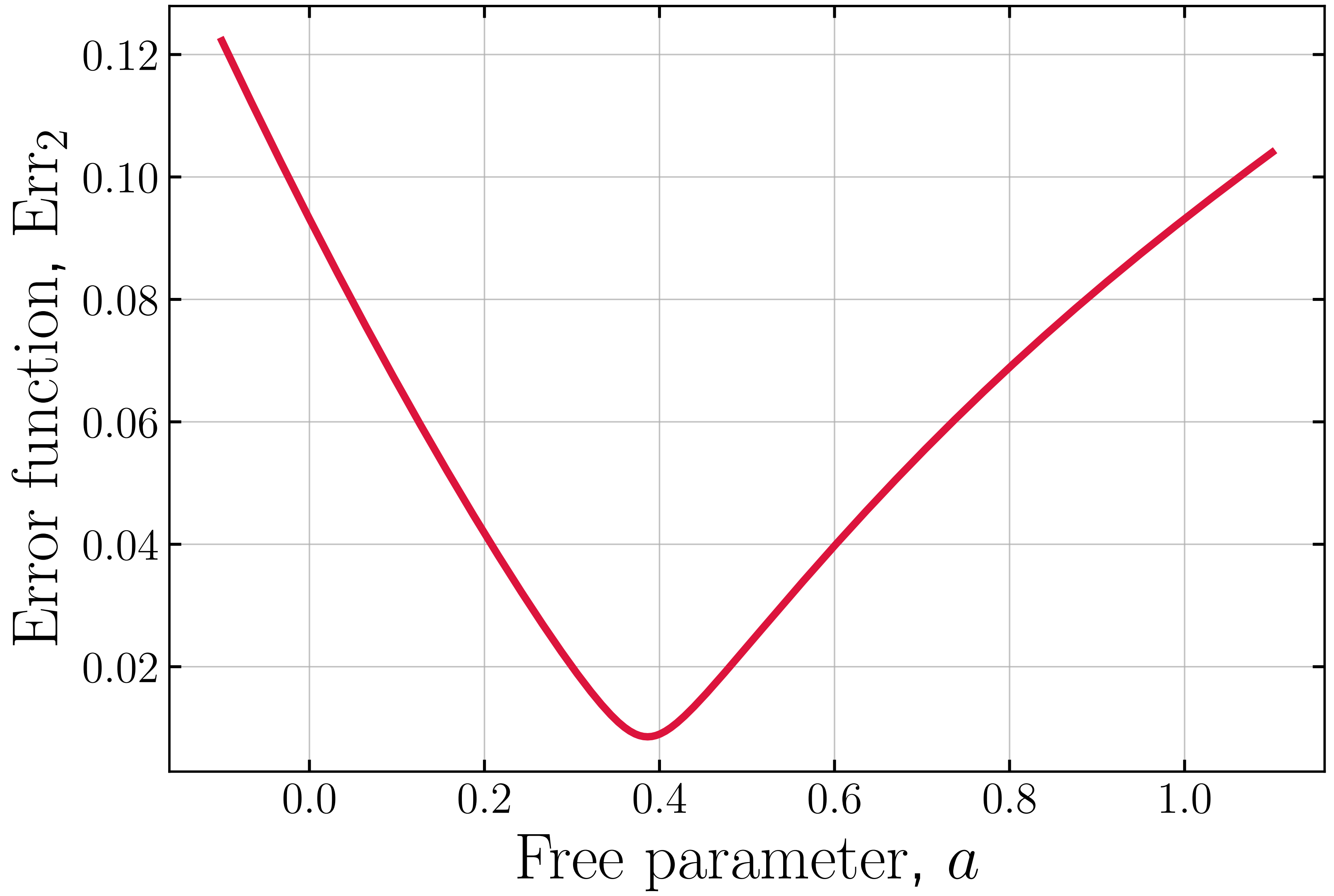
Framework details

- The error function defines a high-dimensional manifold in parameters a_i and b_i
- Dimension: $n_p = q + 1$, $n_c \in (2, 4, 10, \ldots)$
- Goal: minimize this manifold to identify global and local minima
- Example: q=2, 1 free parameter

$$\alpha(q=2) = \frac{a^2}{8} - \frac{a}{4} + \frac{1}{12}, \quad \beta(q=2) = -\frac{a}{8} + \frac{1}{24}$$

$$\mathrm{Err}_2(a_i, b_i) = \sqrt{|\alpha|^2 + |\beta|^2}$$

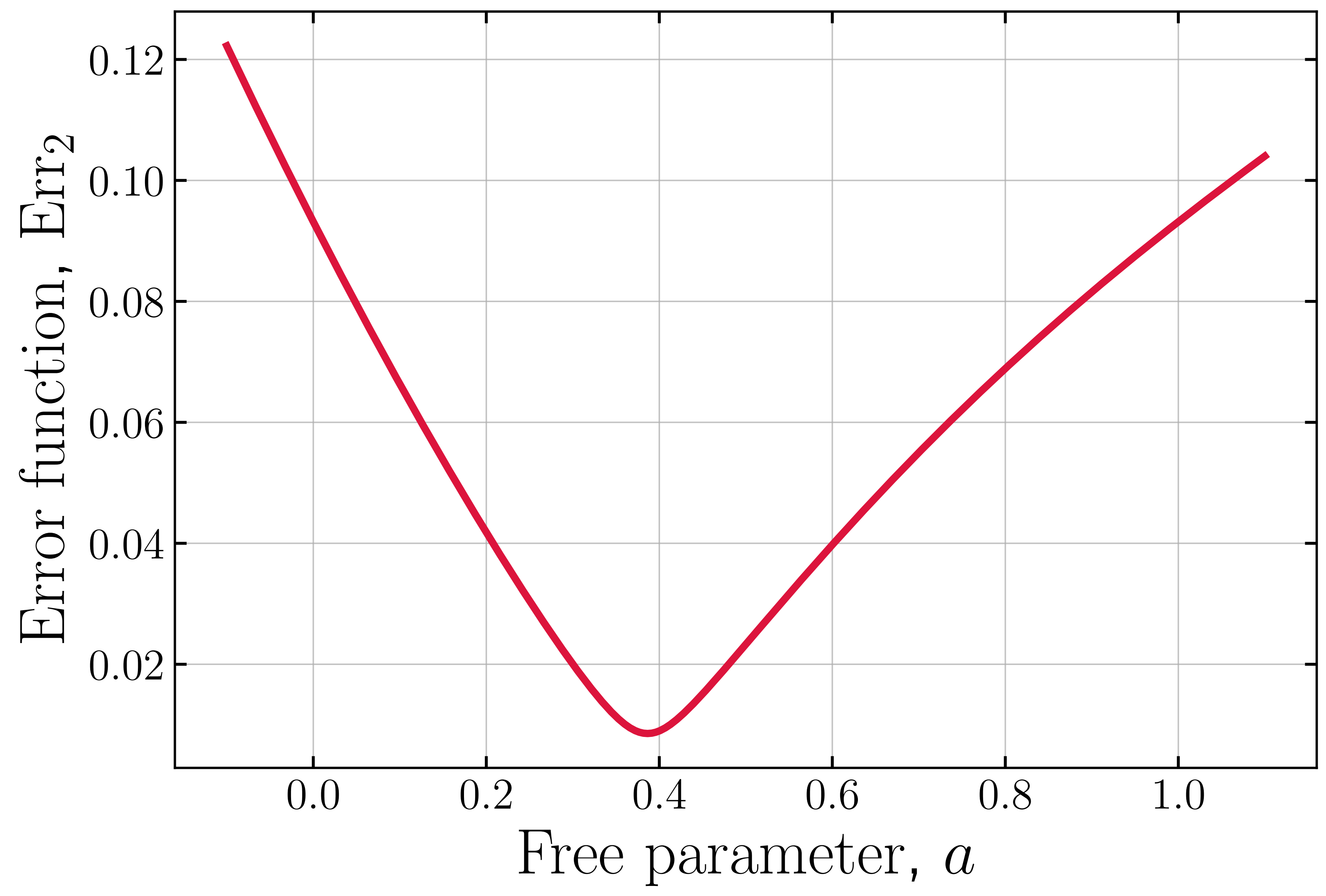
$$\mathrm{Err}_4(a_i, b_i) = \sqrt{\sum_{k=1}^{6} |\gamma_k|^2}$$



Additional slides

Framework details

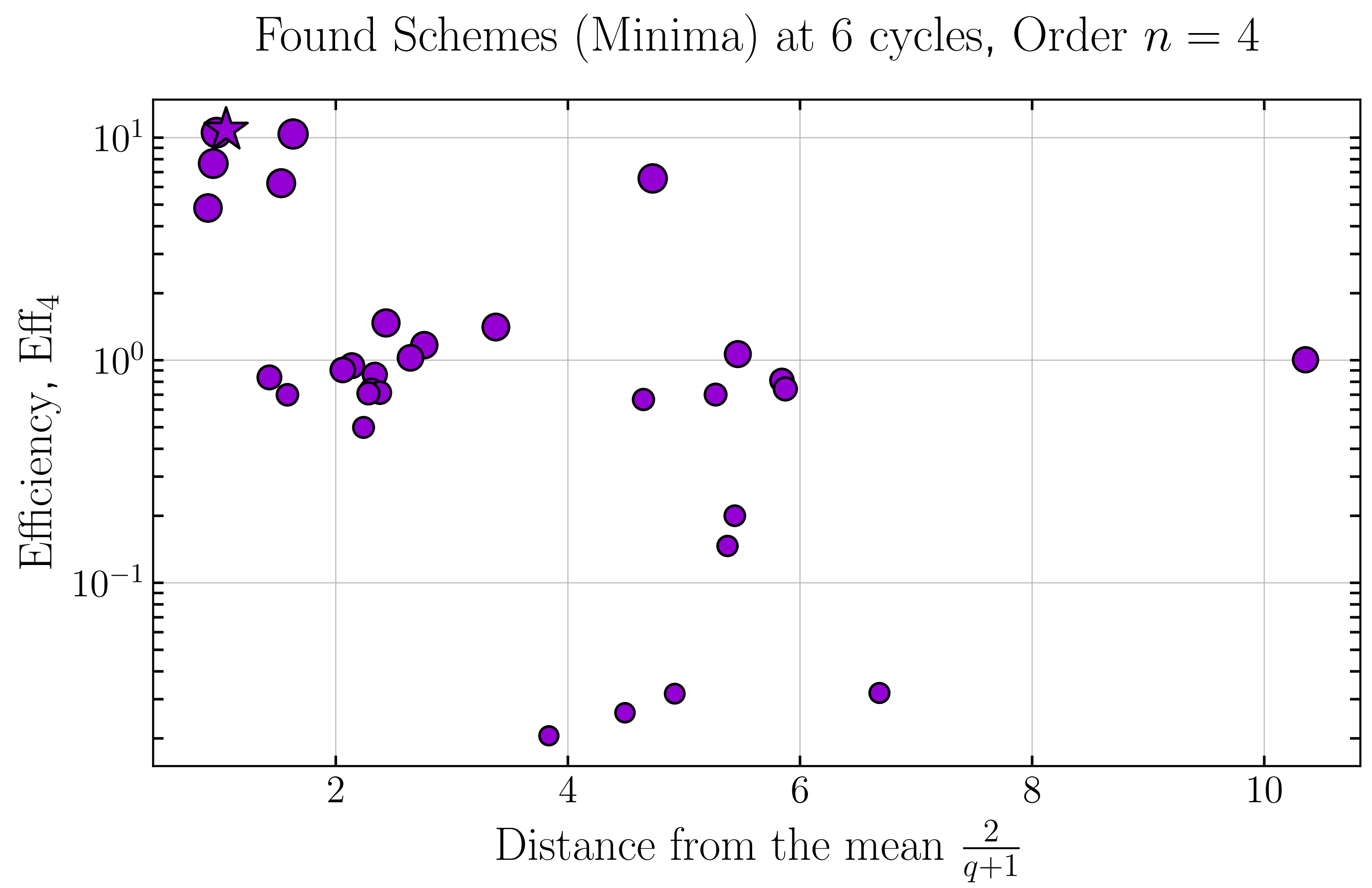
- Optimization method: The Levenberg-Marquard algorithm
- Combination of the Gradient descent and the Gauss-Newton method
- Gradient descent: quickly accelerates toward the minimum region
- Gauss-Newton: Assumes the minimum region and accurately pinpoints the minimum
- Fast convergence, but susceptible to local minima ⟶ Many random initial parameters

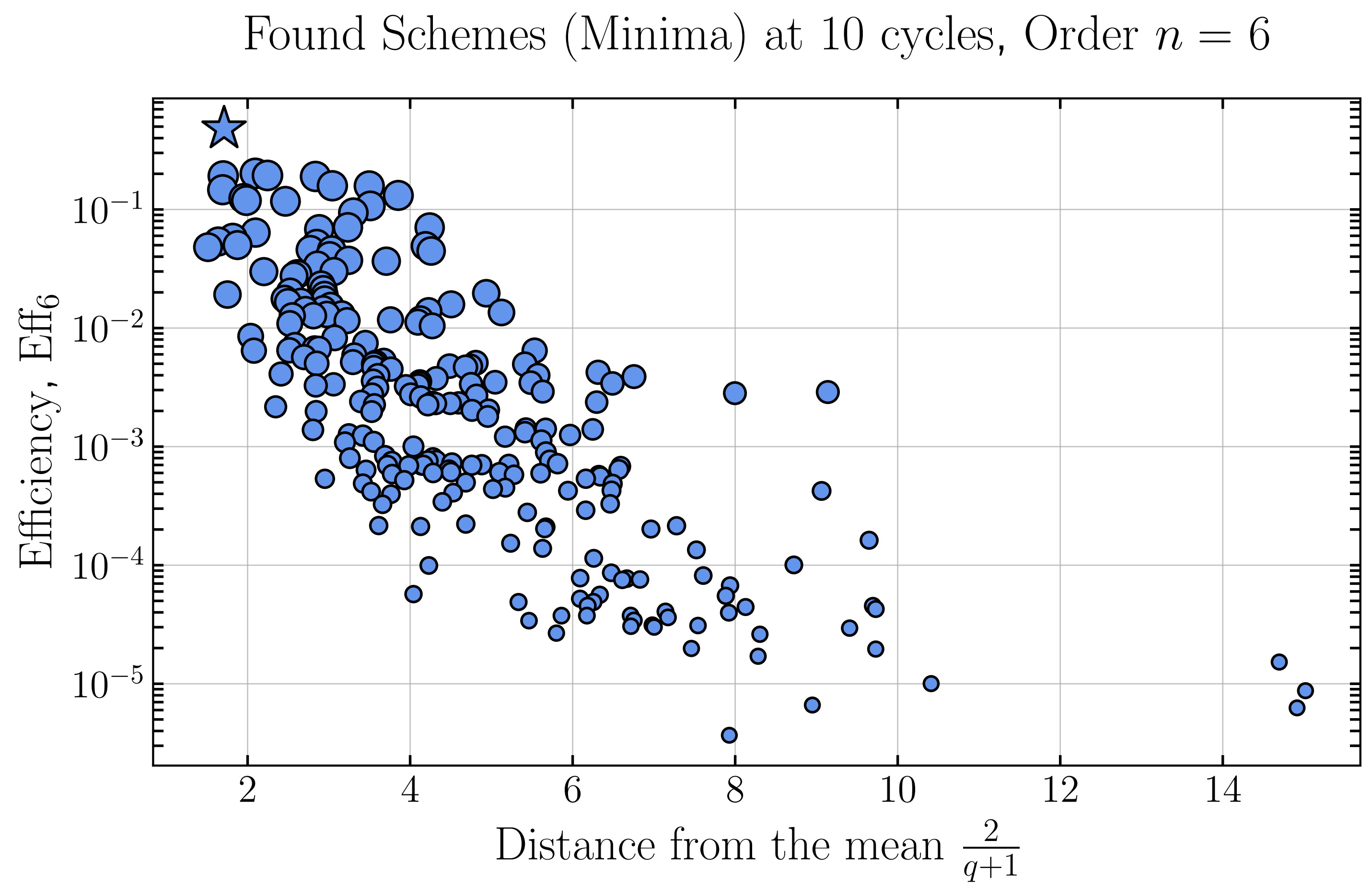


Additional slides

Local minima

- Global minimum is usually close to the average parameter value $\frac{2}{q+1}$
- Efficiency drops drastically far from this mean
- It is good to study less efficient schemes, which are closer to the mean

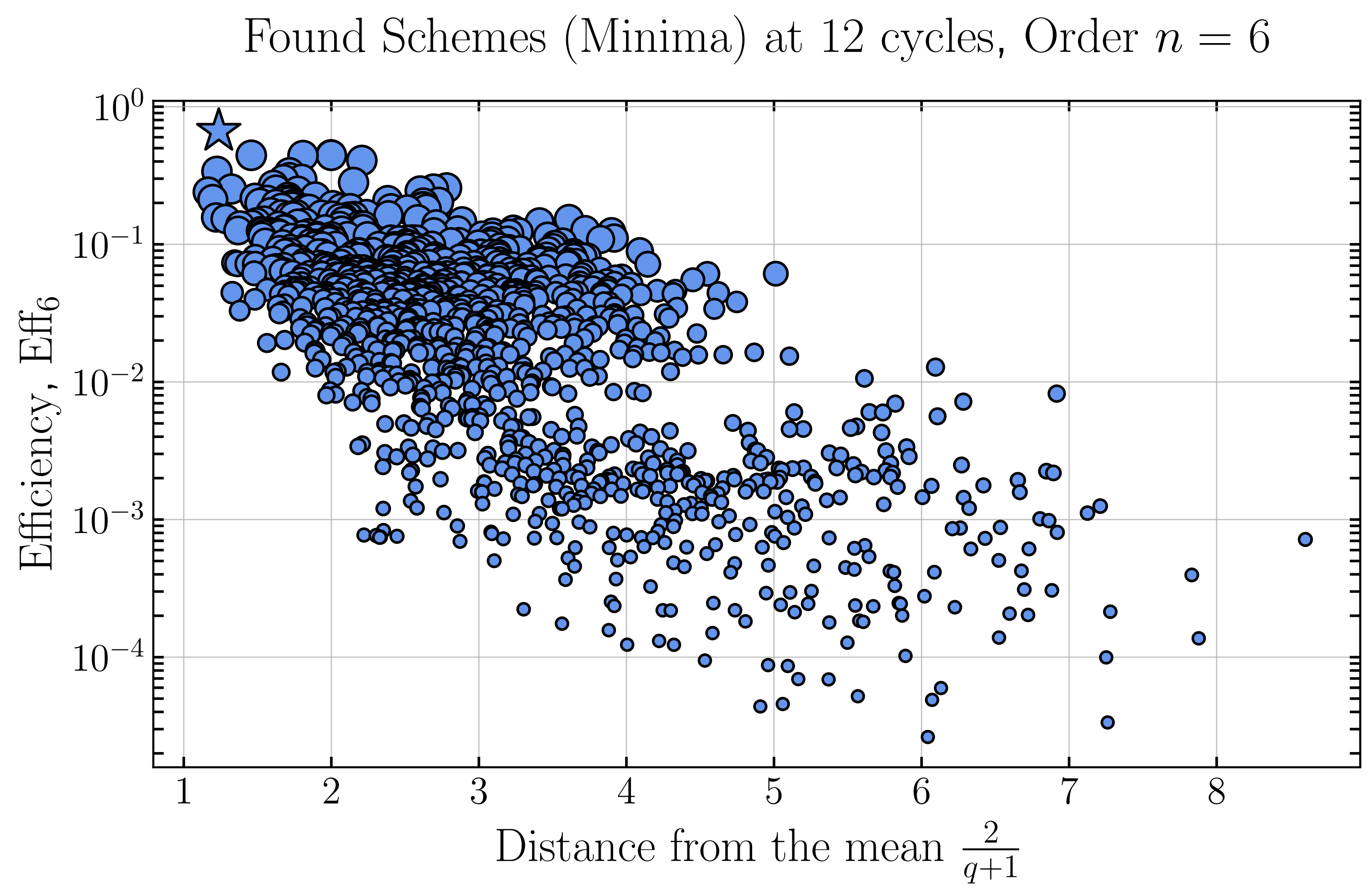


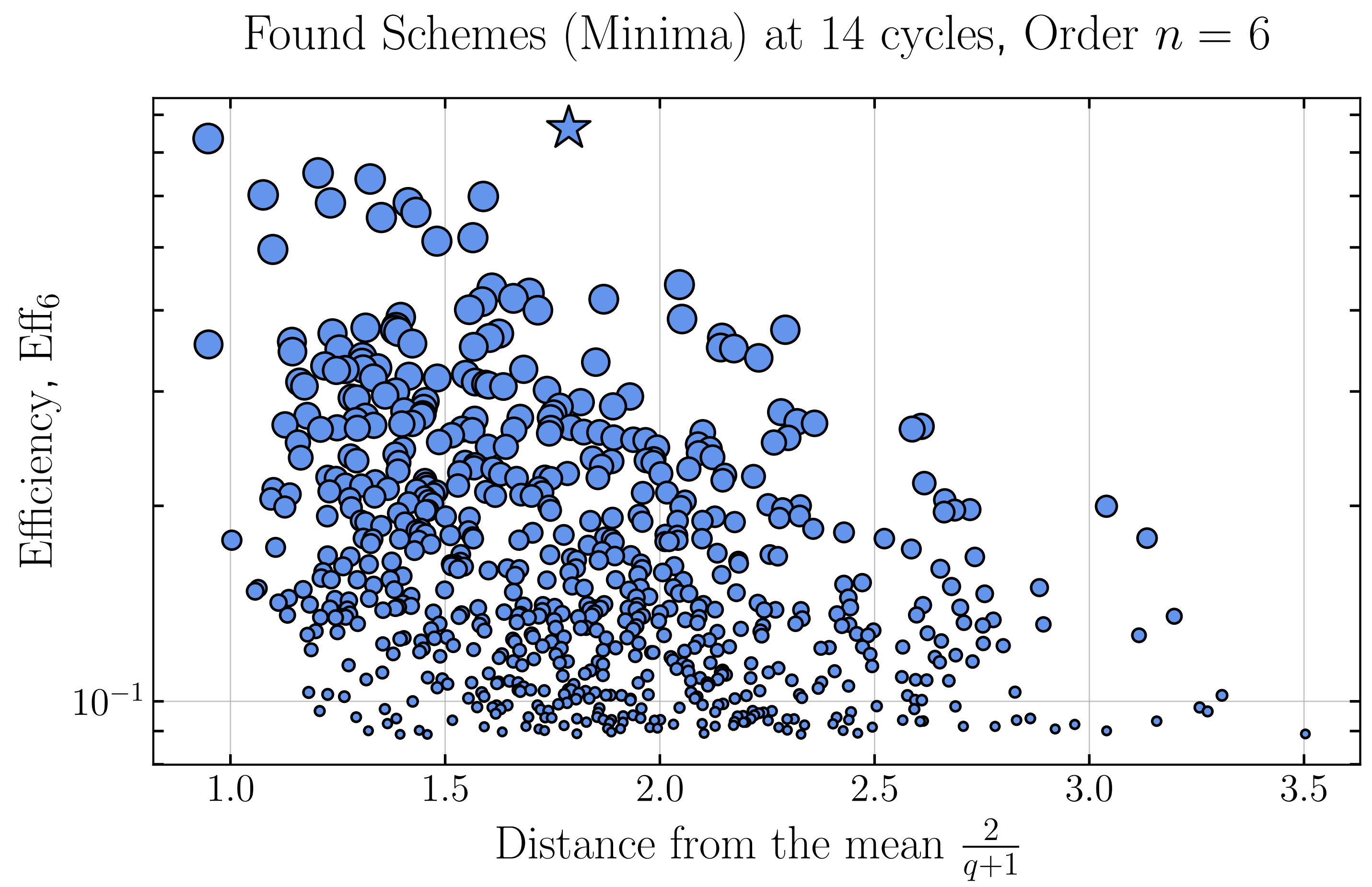


Additional slides

Local minima

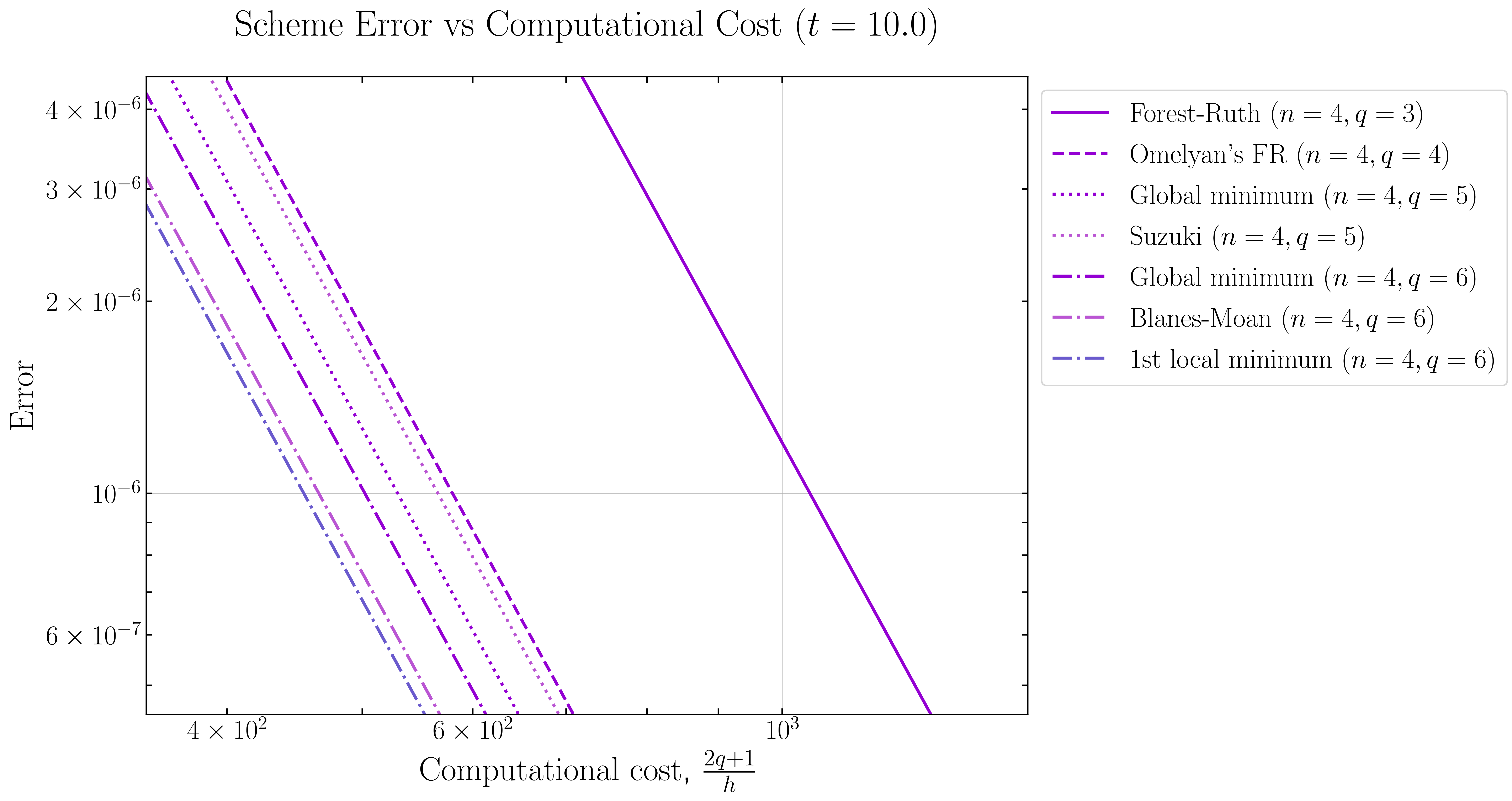
- Global minimum is usually close to the average parameter value $\frac{2}{q+1}$
- Efficiency drops drastically far from this mean
- It is good to study less efficient schemes, which are closer to the mean





Additional slides

Numerical experiments



Additional slides

Numerical experiments