High-degree polynomials for Hopping Parameter Expansion in LQCD

Comparing HPE and GMRES expansions with efficient coloring

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Goal: cheaper time-slice traces through polynomial expansions

Target: the pseudoscalar quark loop.

$$\tau_t = \sum_{\boldsymbol{x}} \mathrm{tr}_{\mathrm{sc}}\left[\gamma_5 D^{-1}(x,x)\right] = \mathrm{tr}(\Pi_t \Gamma_5 D^{-1}), \qquad x = (t, \boldsymbol{x}).$$

Π_t projects onto time slice t; $\mathrm{tr}_{\mathrm{sc}}$ traces spin–color; Γ_5 applies γ_5 site-wise.

- **Compare HPE and GMRES expansions** of the inverse Wilson–clover operator D^{-1}.
- **Split D^{-1} into a finite-range polynomial and a remainder**

HPE versus GMRES expansions

Let $D = C - K$ (on-site C, nearest-neighbor K) and $A = C^{-1}D$. For a degree-d polynomial q_d,

$$D^{-1} = \underbrace{q_d(A)C^{-1}}_{P_d \text{ (exact)}} + \underbrace{p_{d+1}(A)D^{-1}}_{R_d \text{ (stochastic)}},$$

where $p_{d+1}(A) = I - Aq_d(A)$.

- **HPE: truncated Neumann series**

$$q_d^{\mathrm{HPE}}(A) = \sum_{j=0}^{d} (C^{-1}K)^j, \qquad p_{d+1}^{\mathrm{HPE}}(A) = (C^{-1}K)^{d+1}.$$

- **GMRES: residual-minimizing polynomial**

$$q_d^{\mathrm{GMRES}}(A) = \sum_{j=0}^{d} \alpha_j A^j, \qquad p_{d+1}(A) = I - Aq_d^{\mathrm{GMRES}}(A).$$

The coefficients α_j are chosen by GMRES to minimize $\|p_{d+1}(A)b\|_2$.

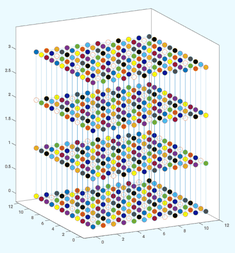
Exact traces with fewer colors

P_d reaches at most d hops, so coloring with same-colored sites separated by more than d hops makes the probing trace **exact**.

- Full spin–color dilution gives

$$N_{\mathrm{probes}} = 12\, N_c(d).$$

- **Multiplier-based coloring** uses fewer colors than hierarchical probing for the same distance.



$N_c(d)$: spatial colors. Illustration: distance-3 coloring of a 3D torus.

Cost: exact trace plus sampling

σ_d^2: measured variance per real remainder sample.

Exact trace: one-off cost

$$F_d = 12 N_c(d)\left[d\, t_K + (d+1) t_{C^{-1}}\right].$$

One remainder sample

$$c_d = t_{\mathrm{solve}} + (d+1)(t_K + t_{C^{-1}}).$$

Target standard error ϵ

$$N_d = \left\lceil \frac{\sigma_d^2}{\epsilon^2} \right\rceil, \qquad \boxed{T_d(\epsilon) = F_d + N_d c_d}.$$

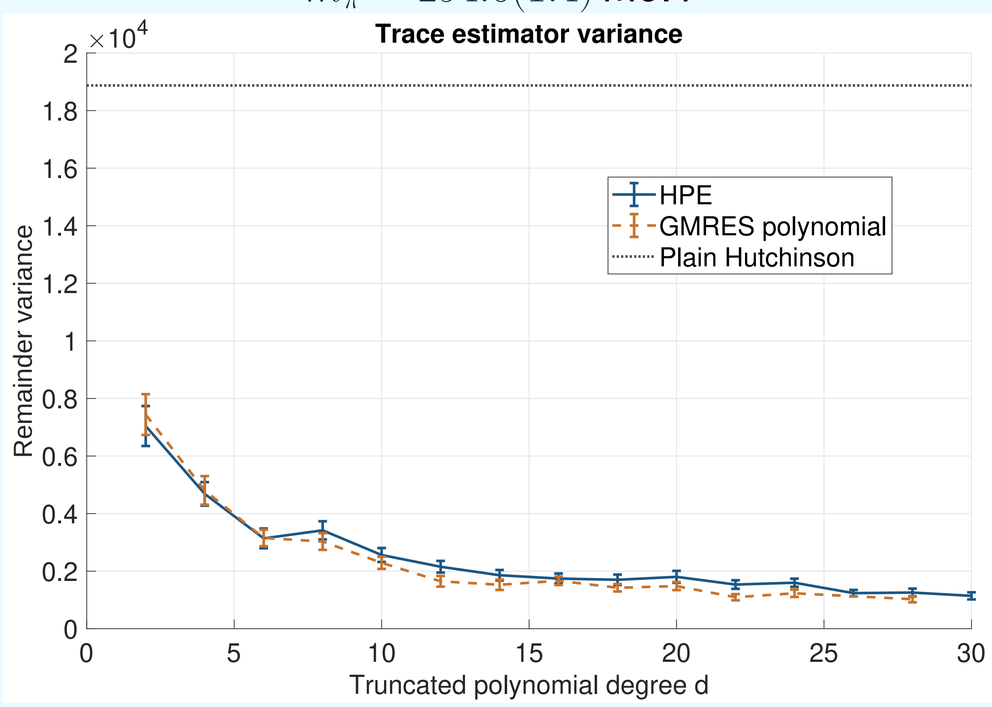
Plain Hutchinson: $F = 0$, $c = t_{\mathrm{solve}}$.

Measured kernel times

$t_K = 14.77$ ms, $t_{C^{-1}} = 3.00$ ms, $t_{\mathrm{solve}} = 8.67$ s.

Result: HPE versus GMRES

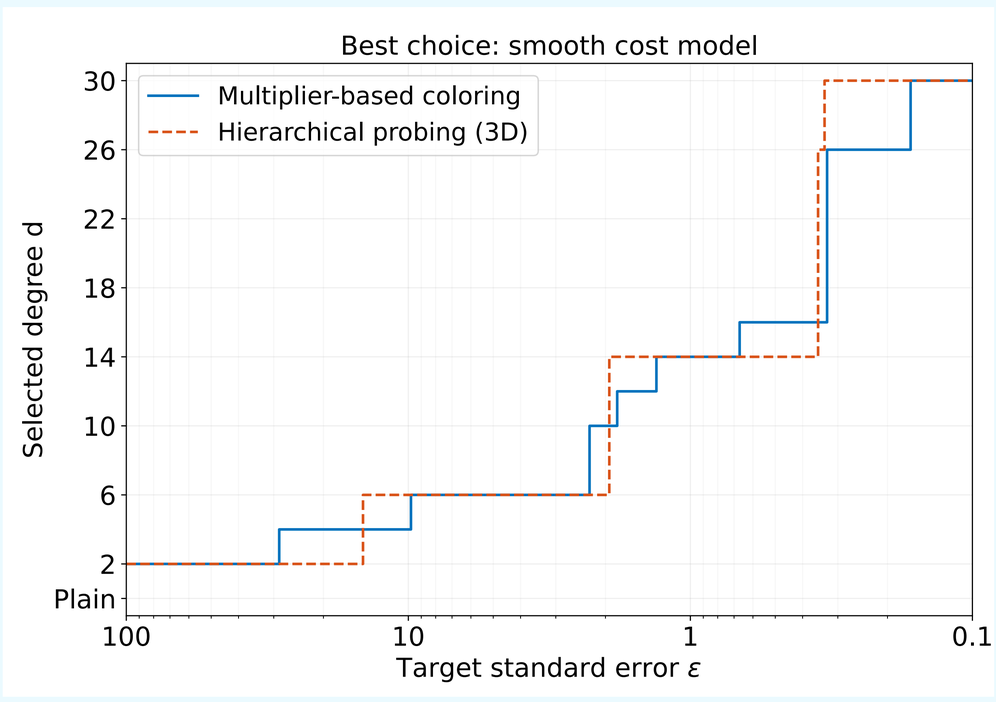
IV ensemble: 64×32^3, Wilson–clover, $N_f = 2$; $a = 0.071$ fm, $m_\pi = 294.6(1.4)$ MeV.



Unbiased time-slice trace estimator

$$\widehat{\tau}_{t,N} = \mathrm{tr}(\Pi_t \Gamma_5 P_d) + \frac{1}{N}\sum_{i=1}^{N} z_i^* \Pi_t \Gamma_5 R_d z_i.$$

Result: choosing the HPE degree



- At fixed degree, both colorings use the same polynomial and remainder; only the number of colors changes.
- **Up to 25% lower predicted total cost** with multiplier-based coloring versus hierarchical probing, at selected target accuracies in this model.

Outlook: when can higher degrees pay off?

Extend the study to less-local propagators.

- More ill-conditioned configurations generally have slower spatial decay, making high-degree polynomials promising.
- Efficient colorings may keep the exact trace affordable while higher degrees reduce remainder noise.

Useful references

[1] Giusti et al. *Frequency-splitting estimators of single-propagator traces.* Eur. Phys. J. C **79**, 586 (2019).

[2] Frommer, Schimmel and Schweitzer. *Analysis of probing techniques for sparse approximation and trace estimation of decaying matrix functions,* SIAM J. Matrix Anal. Appl. **42**(3), 1290–1318 (2021).

[3] Papace et al. *Probing and graph coloring techniques for trace estimation in Lattice QCD.* arXiv:2606.00394 (2026).