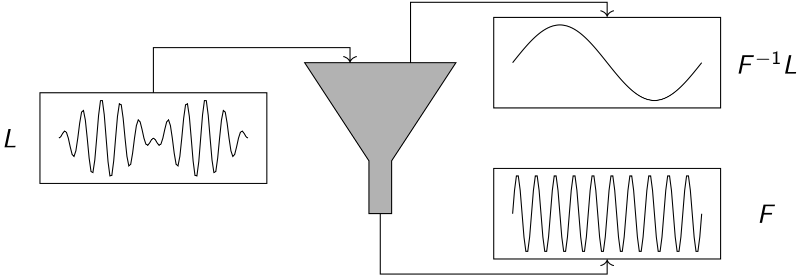
THE UNIVERSITY of ADELAIDE

Single flavour filtering for RHMC in BQCD

Waseem Kamleh

Collaborators

Taylor Haar, Yoshifumi Nakamura, James Zanotti



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- Single flavour fermion simulations pose additional computational challenges.

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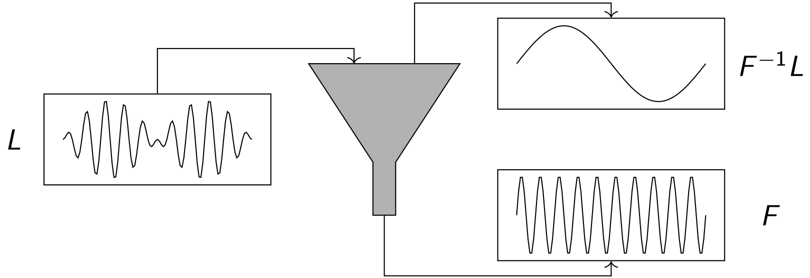
- $M^\dagger M$ is positive semi-definite, correct weight if $\det M > 0$.

Filtering methods

- One way to improve the performance of HMC is to split the action into multiple terms via a filter F on the fermion action kernel L

$$\phi^\dagger L\phi \to \phi_1^\dagger F\phi_1 + \phi_2^\dagger F^{-1}L\phi_2,$$

then integrate each term with a different step-size.



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  - e.g. Chebyshev approximations.

Single flavour filters: tRHMC

- The rational polynomial $R(K) \simeq K^{-1/2}$ in ordered product form is
$$R(K) = d_n \prod_{k=1}^{n} \frac{(K + a_k)}{(K + b_k)}$$
where $a_k, b_k, d_n > 0$ and $a_k > a_{k+1}, b_k > b_{k+1}$.

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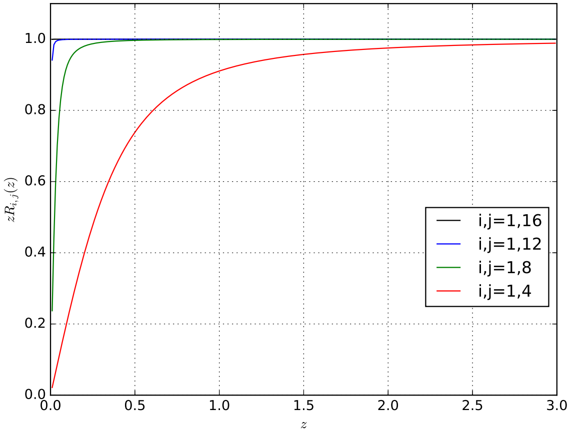
  - e.g. Luscher & Schaefer, *Comput.Phys.Commun. 184 (2013)*.

Single flavour filters: tRHMC

- The truncated product $R_{1,t}(K)$ also approximates $K^{-1/2}$.



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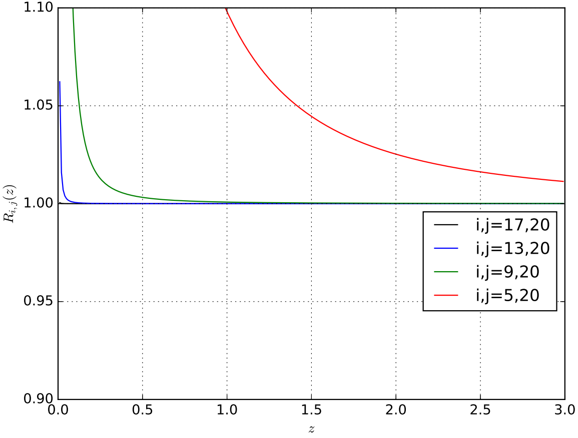
  - Reuse existing HMC code!
  - Distinct from partitioning the sum over poles.
- After truncating the ordered product, note that for small values of a_k and $b_k, (k > t)$ remainder term behaves like

$$R_{t+1,n}(K) = \prod_{k=t+1}^{n} \frac{(K + a_k)}{(K + b_k)} \simeq 1.$$

Single flavour filters: tRHMC

- The remainder term approximates unity.



BQCD lattice code

- All runs were performed using BQCD [see the poster (Stübern)].
- PF-RHMC and tRHMC filtering methods built into the latest release:
  www.rrz.uni-hamburg.de/services/hpc/bqcd
- Performance tests on $16^3 \times 32$ lattice.
  - Wilson gauge $\beta = 5.6$
  - Lattice spacing $a \sim 0.08$ fm.
  - $1 + 1$ (degenerate) single-flavour Wilson fermions.
  - $\kappa = 0.15825$ yields $m_\pi \sim 400$ MeV.

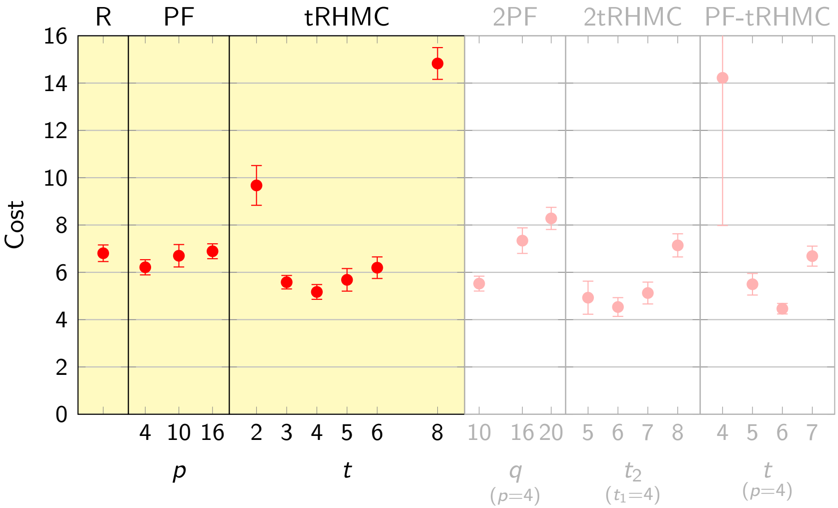
Step-size tuning (force-balanced)

- Step-sizes $h_i = \{h_G, h_1, h_2, \ldots, h_n\}$ for each action term can be tuned by force balancing.
- Given the forces F_i for each action term, the step-sizes follow

$$F_i h_i \approx \text{constant}$$

- F_i can be the average or maximum force.
- We then tune the only free step-size, the coarsest scale h_n, such that the acceptance rate $P_{acc} \sim 0.75$.

Filtering: Results (force-balanced)



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- For tRHMC, add another truncation point t_2:

$$S_{2tRHMC} = \phi_1^\dagger R_{1,t_1}(K)\phi_1 + \phi_2^\dagger R_{t_1+1,t_2}(K)\phi_2 + \phi_3^\dagger R_{t_2+1,n}(K)\phi_3.$$

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- Can also place a polynomial filter on top of tRHMC:

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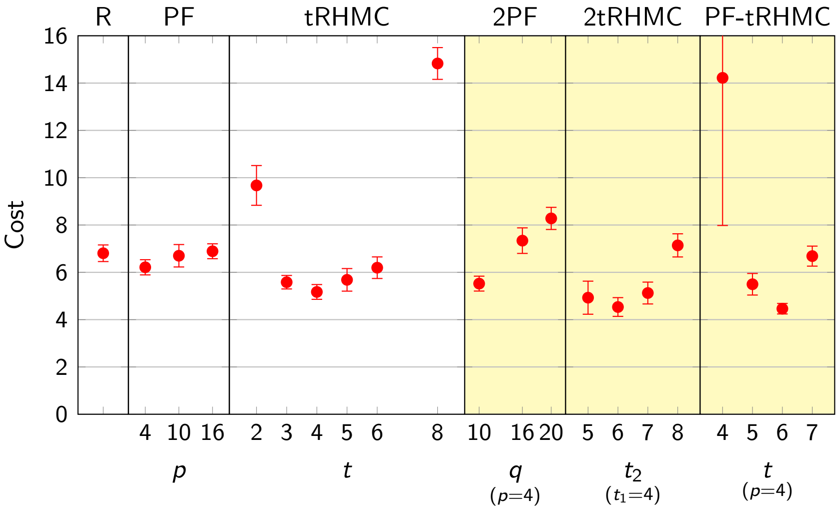

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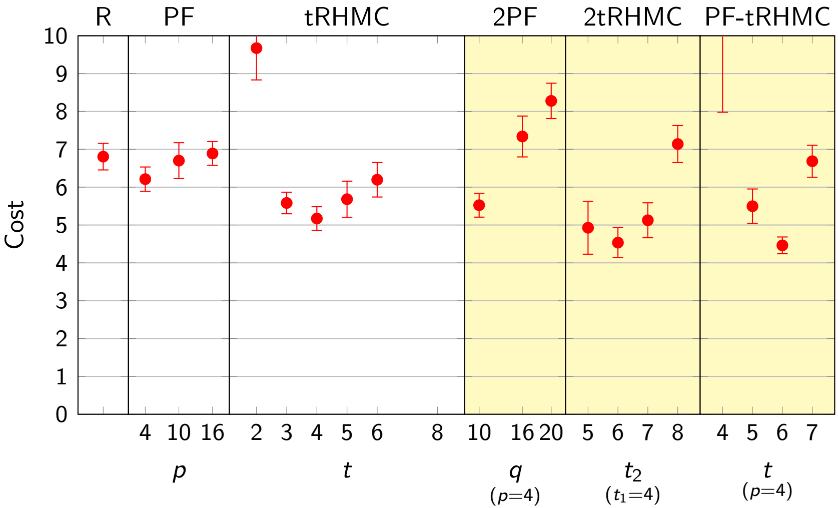
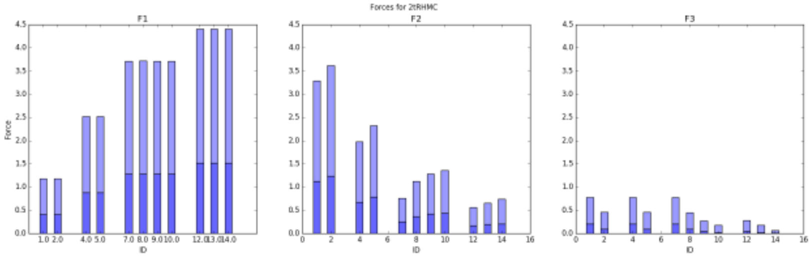


Step-size tuning (characteristic scale)



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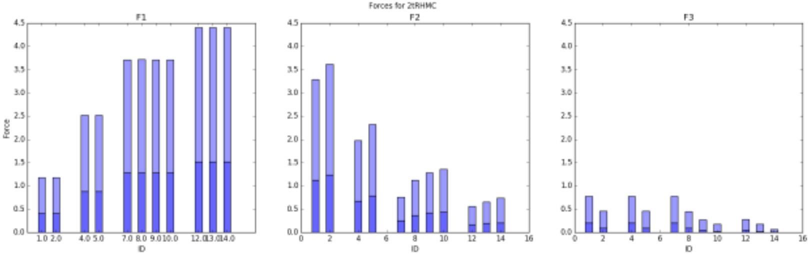

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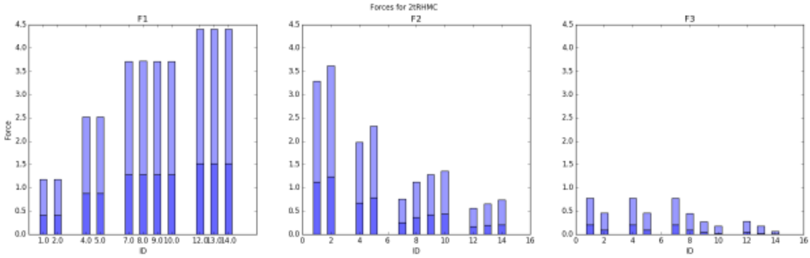

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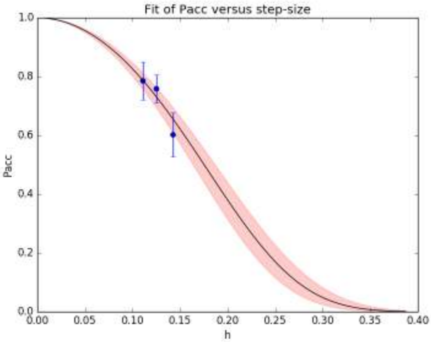
- Force-balanced approach to tuning becomes sub-optimal.
- Alternative approach: Note that for filtered actions the acceptance rate is primarily determined by the coarsest scale.

Step-size tuning (characteristic scale)

- Tune the coarsest scale by fitting the acceptance probability with the complementary error function,

$$P_{acc} \approx \mathrm{erfc}(h_n^2 c^2),$$

where the characteristic scale c is the only fit parameter.



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- This helps offset an unfavourable distribution of forces between action terms.

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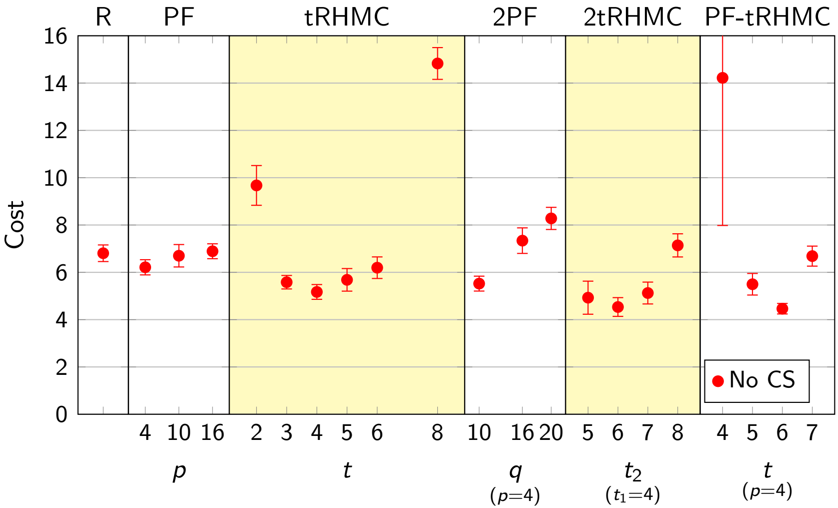

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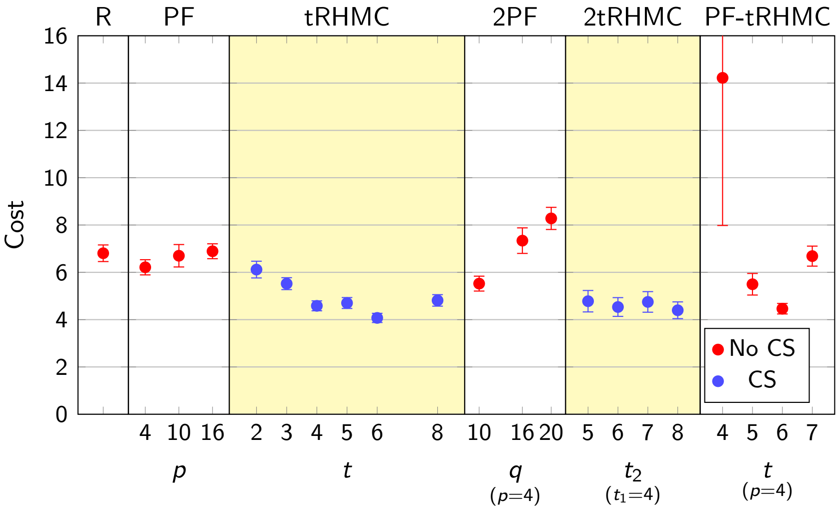

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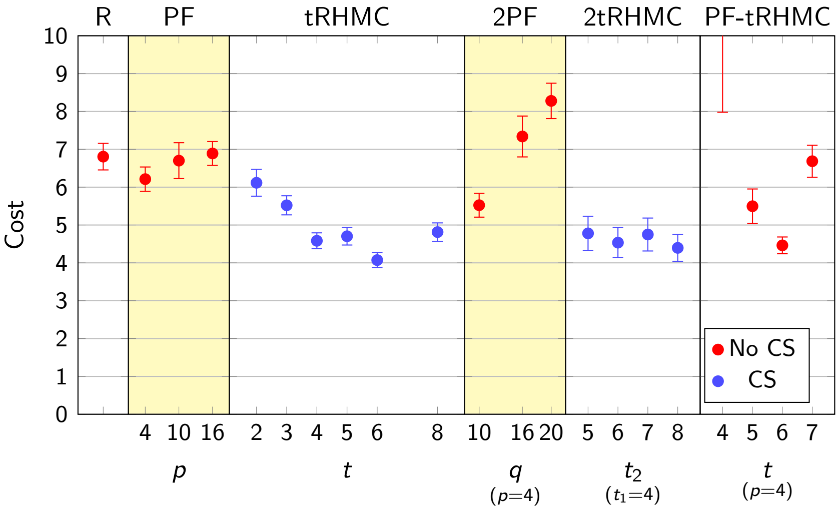

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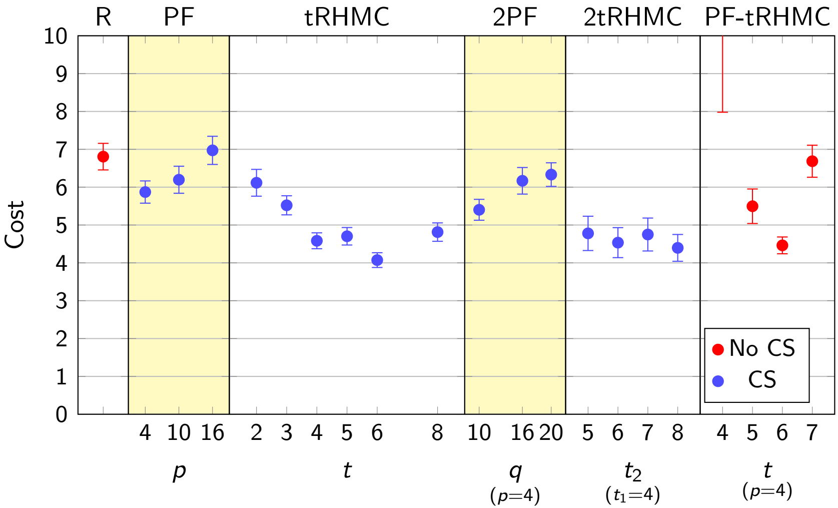

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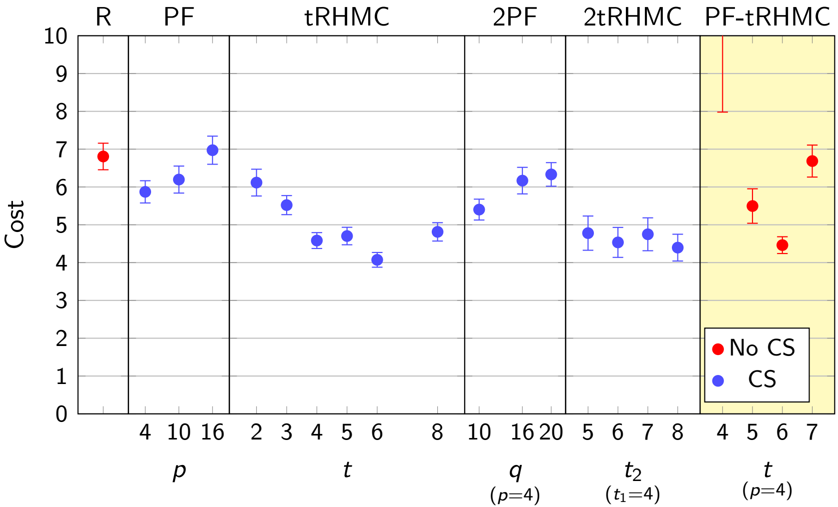

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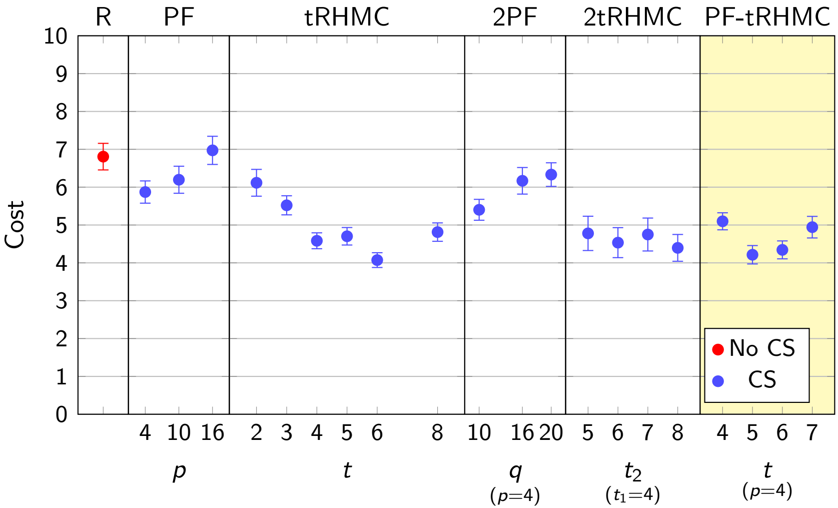


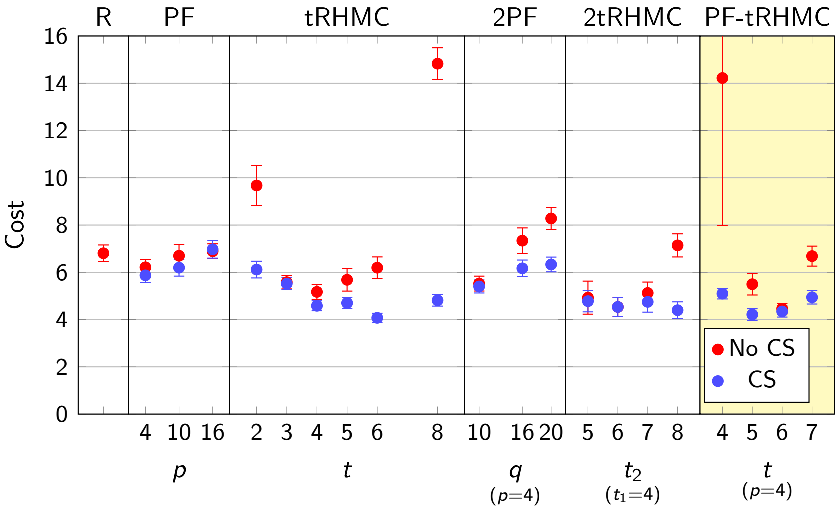
Summary

- Tested different filtering methods to improve the cost of generating single-flavour pseudofermions:
  - Polynomial-filtered RHMC.
  - Truncated-ordered-product filtering (tRHMC).
- tRHMC provides the best performance improvement, roughly factor of 2 speedup.
- Characteristic scale tuning works well for tRHMC across a wide range of truncation orders.
- tRHMC is provided by BQCD, but is also (almost) trivial to implement in existing RHMC codes.
- Multiple truncation filters can be used (should prove to be useful at light quark masses).

More lattice parameters

- The rational approximation used was the Zolotarev optimal rational approximation with order $n = 20$ and range $[5 \times 10^{-5}, 3]$.
- The polynomials used were Chebyshev approximations to $K^{-1/2}$ (or $P(K)^{-1}K^{-1/2}$ in the two filter case) with range $[5 \times 10^{-5}, 3]$.

Full cost plot



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