Rational Hybrid Monte Carlo

Modern Challenges for Lattice Field Theory

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- Motivation
- Current Algorithms
- Rational Hybrid Monte Carlo
- 2+1 ASQTAD Fermions
- 2+1 Domain Wall Fermions
- Conclusion

Introduction and Motivation

- Lattice QCD path integral

$$\langle\Omega\rangle = \frac{1}{Z}\int [dU] e^{-S(U)} [\det \mathcal{M}(U)]^{\alpha}\Omega(U)$$

  where $\alpha = \frac{N_f}{4}$ $(\frac{N_f}{2})$ for staggered (Wilson) fermions, $\mathcal{M} = M^\dagger M$.

  $\Rightarrow$ arbitrary N_f with non-integer α

- non-integer $\alpha \Rightarrow$ non-local action, conventional HMC fails
- Both ASQTAD and DWF programs want to do 2+1 physics
- Need non-local algorithms

The R Algorithm

Rewrite fermionic determinant:

$$\det \mathcal{M}^{\alpha} = \exp \alpha \operatorname{tr} \ln \mathcal{M}$$

- Approximate trace by noisy estimator $\equiv$ pseudo-fermions
- Use integrator $(O(\delta\tau^2))$
  - Non-reversible
  - Jacobian $\neq 1$

  $\Rightarrow$ Cannot include Monte Carlo acceptance test
- R: HMD algorithm which is inexact $\Rightarrow$ naïvely cheap, but extrapolation to zero stepsize (strictly) required

Polynomial Hybrid Monte Carlo

Write in pseudo-fermion notation

$$\begin{aligned} \det \mathcal{M}^{\alpha} &= \int \mathcal{D}\bar{\psi}\mathcal{D}\psi e^{-\bar{\psi}\mathcal{M}^{-\alpha}\psi} \\ &\approx \int \mathcal{D}\bar{\psi}\mathcal{D}\psi e^{-\bar{\psi}P(\mathcal{M})\psi}, \end{aligned}$$

where $P(\mathcal{M})$ is MiniMax polynomial approximation over spectral range.

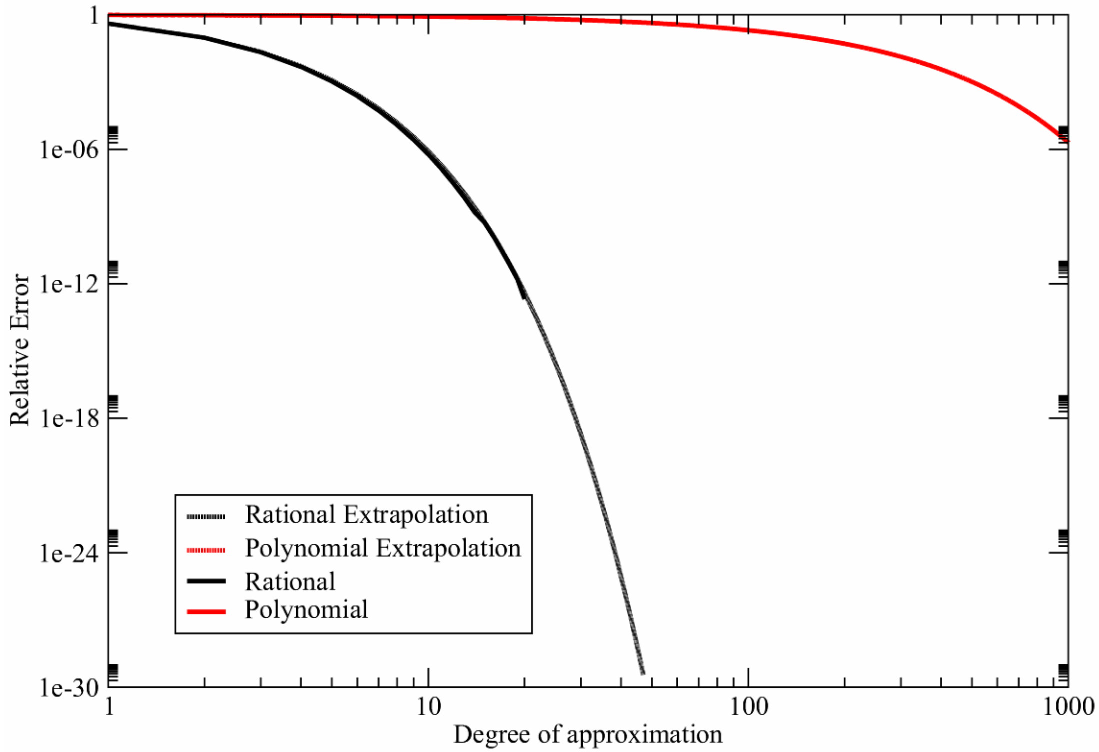
- Pseudo-fermion heatbath easily realised since $P(\mathcal{M}) = p^{\dagger}(\mathcal{M})p(\mathcal{M})$
- Use standard MD leapfrog $\Rightarrow$ exact

Polynomial Hybrid Monte Carlo

- Significant Error $|P(\mathcal{M}) - \mathcal{M}^{-\alpha}| >$ CG residual
  - Noisy acceptance test or appropriate reweighting (V^2)
- High degree polynomial
  - costly in memory (for non-analytic force)
  - rounding errors
  - ASQTAD force term very expensive
- Multi-boson algorithm has similar problems

Optimal rational approximations

- Very accurate
- Generated using Remez algorithm
- Real non-degenerate roots (poles are always +ve)



- Partial fractions - multimass solver

Rational Hybrid Monte Carlo

- Pseudo-fermionic action
  $S_{\mathrm{pf}} = \phi^\dagger r^2(\mathcal{M})\phi = \phi^\dagger \left(\alpha_0 + \sum_{i=1}^{n} \frac{\alpha_i}{\mathcal{M}+\beta_i}\right)^2 \phi$
  with
  $r(\mathcal{M}) = \mathcal{M}^{-\alpha/2}$
- Conventional Metropolis
- Proceed like HMC with $r^2(\mathcal{M})$ in place of $\mathcal{M}^{-\alpha}$

Rational Hybrid Monte Carlo

- Hybrid Molecular Dynamics Trajectory
  - Momentum refreshment heatbath ($P(\pi) \propto e^{-\pi^*\pi/2}$).
  - Pseudo-fermion heatbath ($\phi \propto r(\mathcal{M})^{-1}\xi$, where $P(\xi) \propto e^{-\xi^*\xi/2}$).
  - MD trajectory with $\tau/\delta\tau$ steps.
- Metropolis Acceptance Test $P_{\text{acc}} = \min(1, e^{-\delta H})$

Rational Hybrid Monte Carlo

- MD trajectory
  - Double inversion from $r^2(\mathcal{M})$
  - MC must be exact, MD governed by acceptance
  - Use low degree approx $\bar{r} \approx \mathcal{M}^{-\alpha} \approx r^2$
  - Pseudo-fermion force

$$S'_{\mathsf{pf}} = -\sum_{i=1}^{\bar{n}} \bar{\alpha}_i \phi^\dagger (\mathcal{M} + \bar{\beta}_i)^{-1} \mathcal{M}' (\mathcal{M} + \bar{\beta}_i)^{-1} \phi.$$

- CG cost per trajectory $\approx$ R alg, $(2 + \tau/\delta\tau) \approx (\tau/\delta\tau)$

2+1 ASQTAD Fermions

- Action has the form

$$S_f = \bar{\psi}\,(\mathcal{M}_{\bar{m}})^{-1/2}\,\psi + \bar{\chi}\,(\mathcal{M}_{m_s})^{-1/4}\,\chi,$$

  where $\bar{m} = (m_u + m_d)/2$
- Use rational approximation for each

$$S_f = \bar{\psi}\,r^2_{\bar{m}}(\mathcal{M})\psi + \bar{\chi}\,r^2_{m_s}(\mathcal{M})\chi$$

- $\mathcal{M}$ bounded explicitly by $m \Rightarrow$ approx easy
- Proceed as above with two fields?

2+1 ASQTAD Fermions

- ASQTAD force expensive

  $\Rightarrow$ Naïve RHMC has factor n more force computation than R
- Calculate force as matrix

$$\sum_{i=1}^{n} U...UX_iX_i^\dagger U...U = U...U \sum_{i=1}^{n} X_iX_i^\dagger U...U$$

  $\Rightarrow$ 3$\times$overhead, BUT
  - For 2+1 can perform force calculation simultaneously
  - No heatbath overhead
- 5% cost difference between R and RHMC

2+1 ASQTAD Fermions

- $V = 24^3 64$, $\beta = 6.76$, $\bar{m} = 0.0078$, $m_s = 0.039$.
- MILC $\delta\tau = \frac{2}{3}\bar{m} \approx 0.005$
- Use $\{\frac{1}{2}, \frac{1}{4}\}$
  - $\delta\tau = 0.005$, $\langle A \rangle = 70(6)\%$.
- Can we do better?

Multiple Pseudo-fermion fields

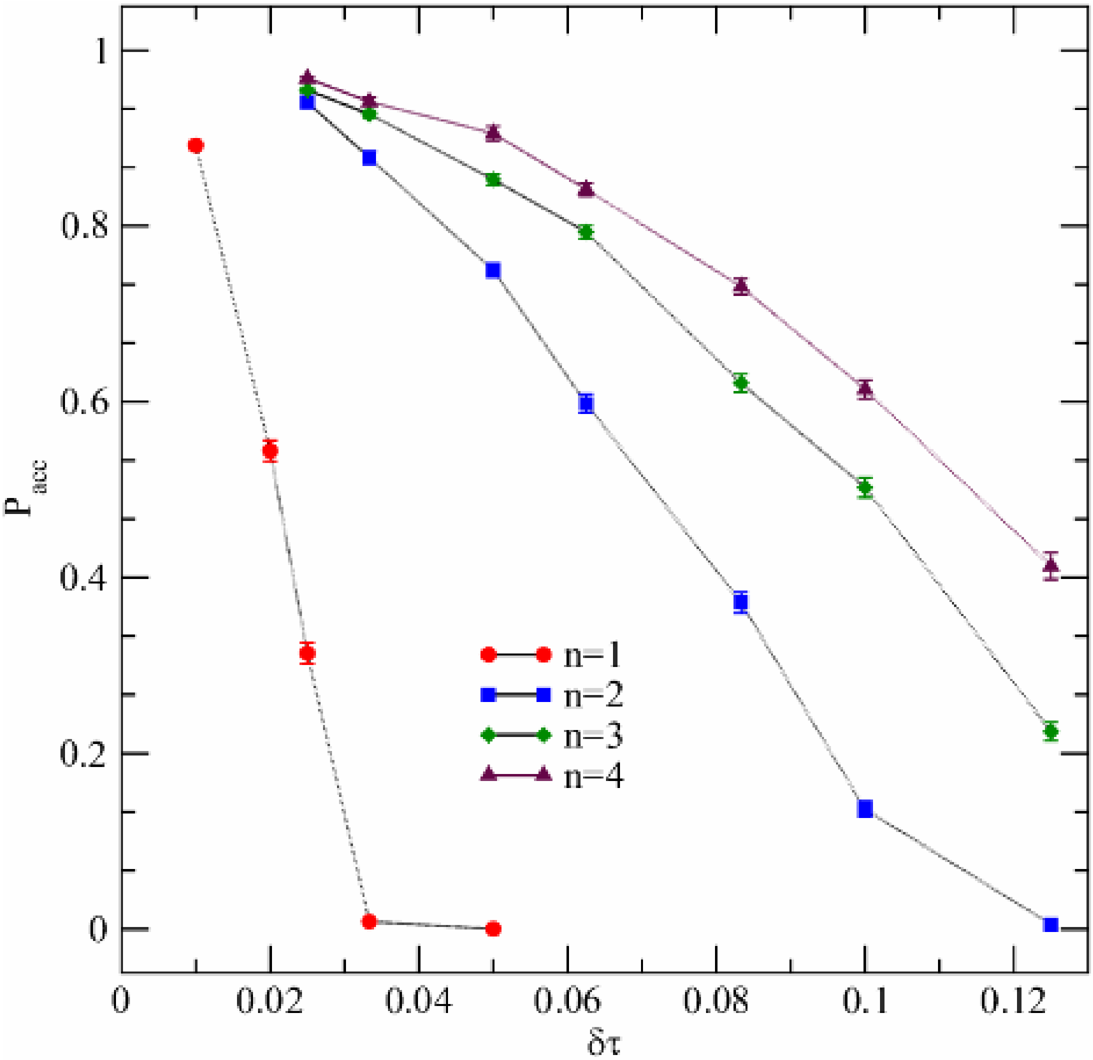
- Increased acceptance through multiple pseudo-fermions (Hasenbusch trick)

$$\begin{aligned}\det\mathcal{M} &= \det\mathcal{M}'\det(\mathcal{M}/\mathcal{M}')\\ &= \int\mathcal{D}\bar{\psi}\mathcal{D}\psi\mathcal{D}\bar{\psi}'\mathcal{D}\psi'\exp\left(-\bar{\psi}\mathcal{M}'\mathcal{M}^{-1}\psi - \bar{\psi}'\mathcal{M}'^{-1}\psi'\right)\end{aligned}$$

- Improves stochastic estimator of fermionic force
- Alternative multiple pseudo-fermions - Nroots

$$\begin{aligned}\det\mathcal{M}^{\alpha} &= (\det\mathcal{M}^{\alpha/n})^{n}\\ &= \prod_{k=1}^{n}\int\mathcal{D}\bar{\psi}_k\mathcal{D}\psi_k\exp(-\bar{\psi}_k\mathcal{M}^{-\alpha/n}\psi_k)\end{aligned}$$

- Test - 8^4 lattice $N_f = 4$ naive staggered quarks $\beta = 5.7$, $m = 0.01$.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0.8
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P_{acc}
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δτ
n=1
n=2
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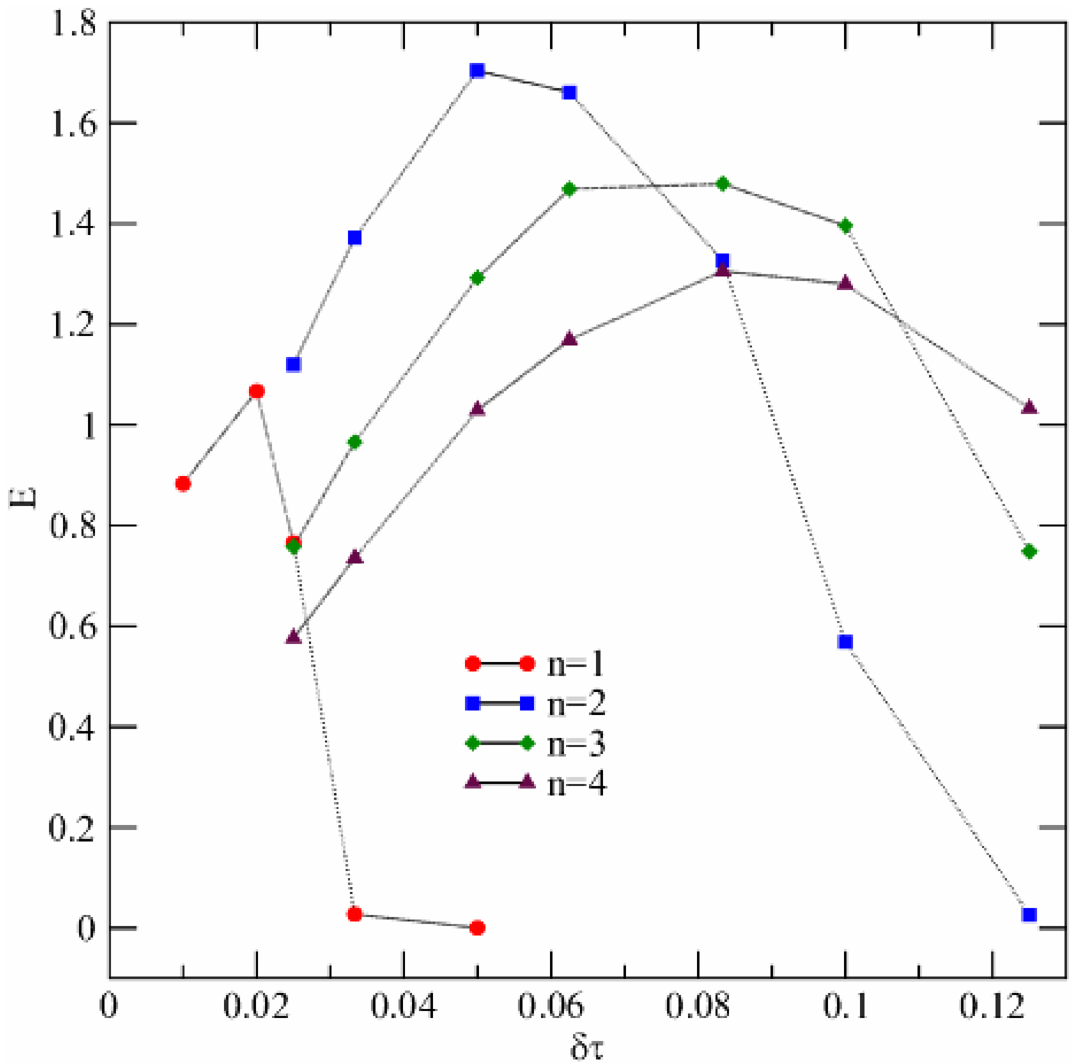
n=4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δτ
n=1
n=2
n=3
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2+1 ASQTAD Fermions

- $V = 24^3 64$, $\beta = 6.76$, $\bar{m} = 0.0078$, $m_s = 0.039$.
- MILC $\delta\tau = \frac{2}{3}\bar{m} \approx 0.005$
- Naive approach, use $\{\frac{1}{2}, \frac{1}{4}\}$
  - $\delta\tau = 0.005$, $\langle A \rangle = 70(6)\%$.
- Nroots acceleration, $\{\frac{1}{6}, \frac{1}{6}, \frac{1}{6}, \frac{1}{4}\}$,
  - $\delta\tau = 0.03$, $\langle A \rangle = 78(4)\%$.
  - $\delta\tau = 0.05$, $\langle A \rangle = 37(6)\%$.

2+1 Domain Wall Fermions

- Action now

$$S_f = \bar{\psi}\mathcal{M}_{\bar{m}}^{DW}\psi + \bar{\chi}(\mathcal{M}^{DW})^{1/2}\chi$$

with

$$\mathcal{M}_m^{DW} = M^{-1}(m)^{\dagger}M^{\dagger}(1)M(1)M^{-1}(m)$$

- BUT cannot write $r(\mathcal{M}^{DW})$ as shifted matrix
- Forced to write action as

$$S_f = \bar{\psi}\mathcal{M}_{\bar{m}}^{DW}\psi + \bar{\phi}\,(\mathcal{M}_1)^{1/2}\,\phi + \bar{\chi}\,(\mathcal{M}_{m_s})^{-1/2}\,\chi$$

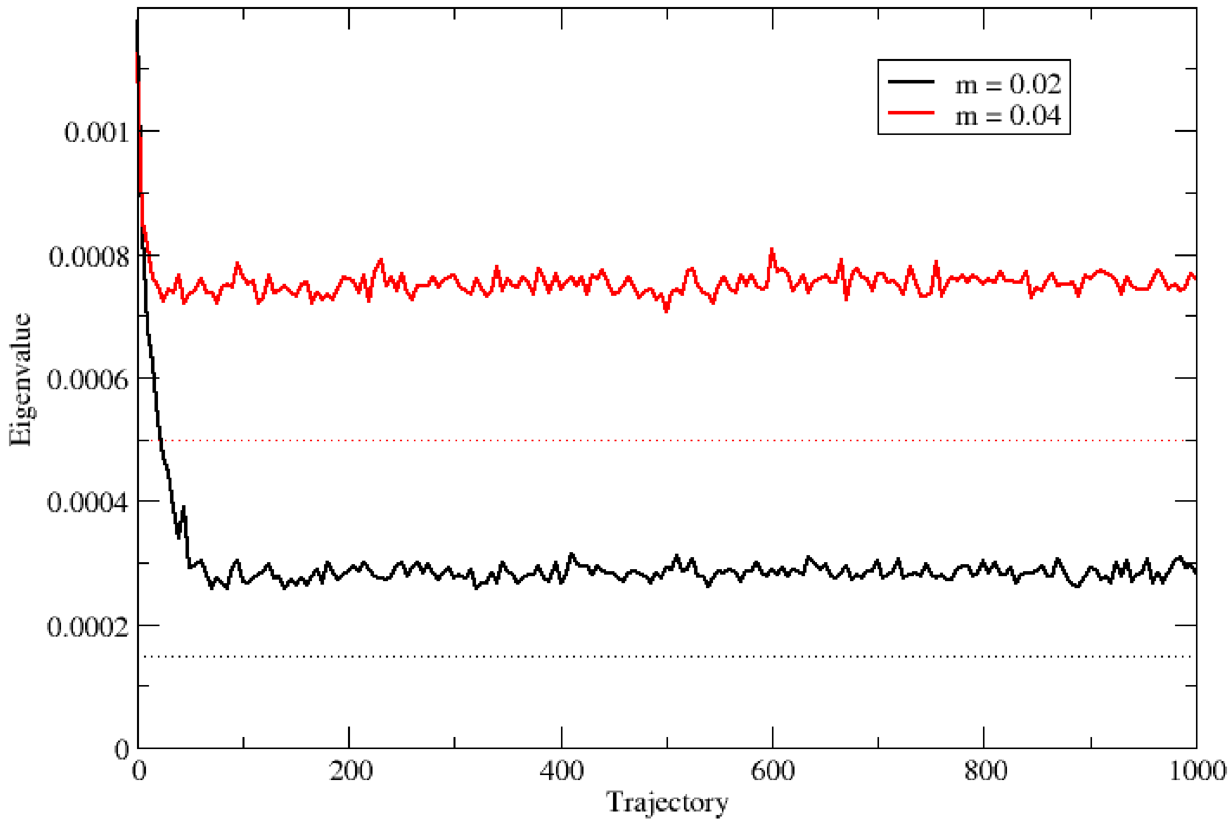
$\Rightarrow$ 2 fermion fields to simulate 1 flavour contribution

- Additional cost small

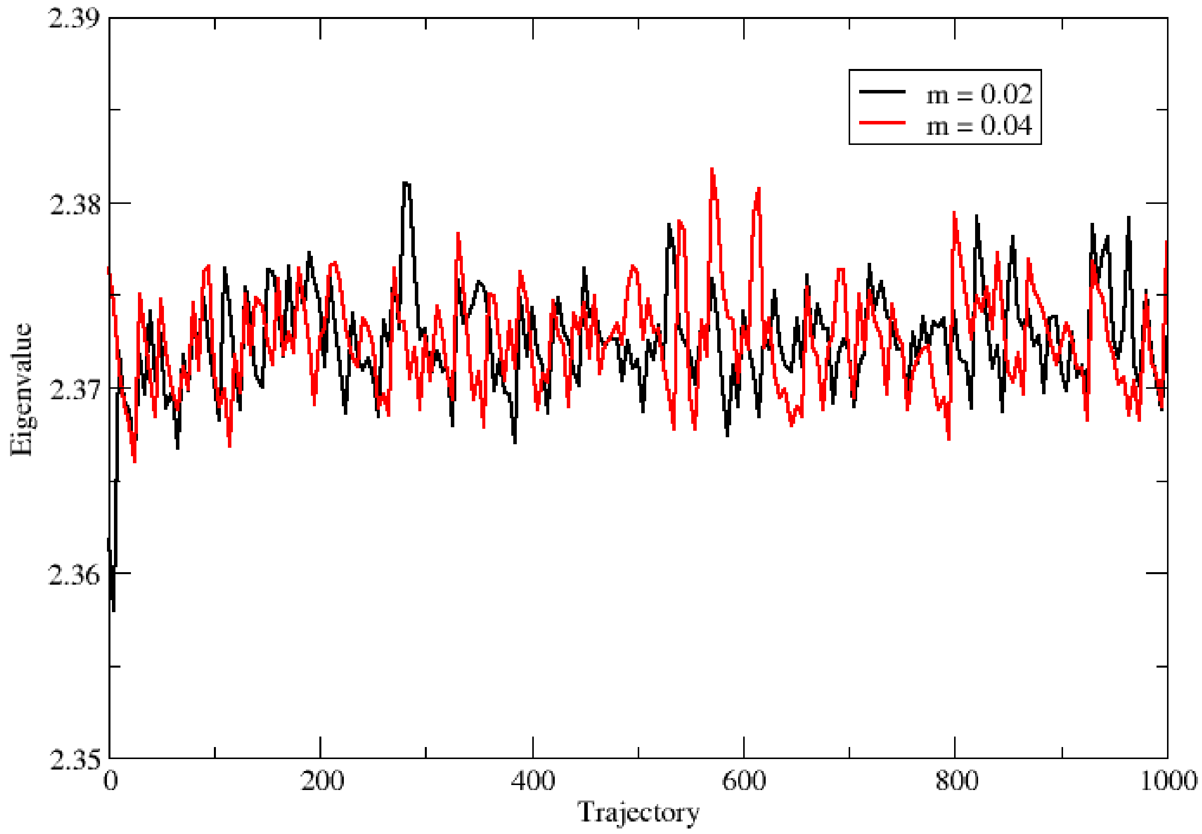
2+1 Domain Wall Fermions

- Lower bound of matrix?
- Use speculative lower bound
- $V = 16^3 32 \times 8$, $\beta = 0.72$, DBW2, $m_s = 0.04$, $\bar{m} = 0.02, 0.04$
- R algorithm $\delta\tau = 0.01$
- RHMC $\delta\tau = 0.02$, Nroots $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$
- $\langle A_{2+1} \rangle = 68\%$, $\langle A_3 \rangle = 72\%$.

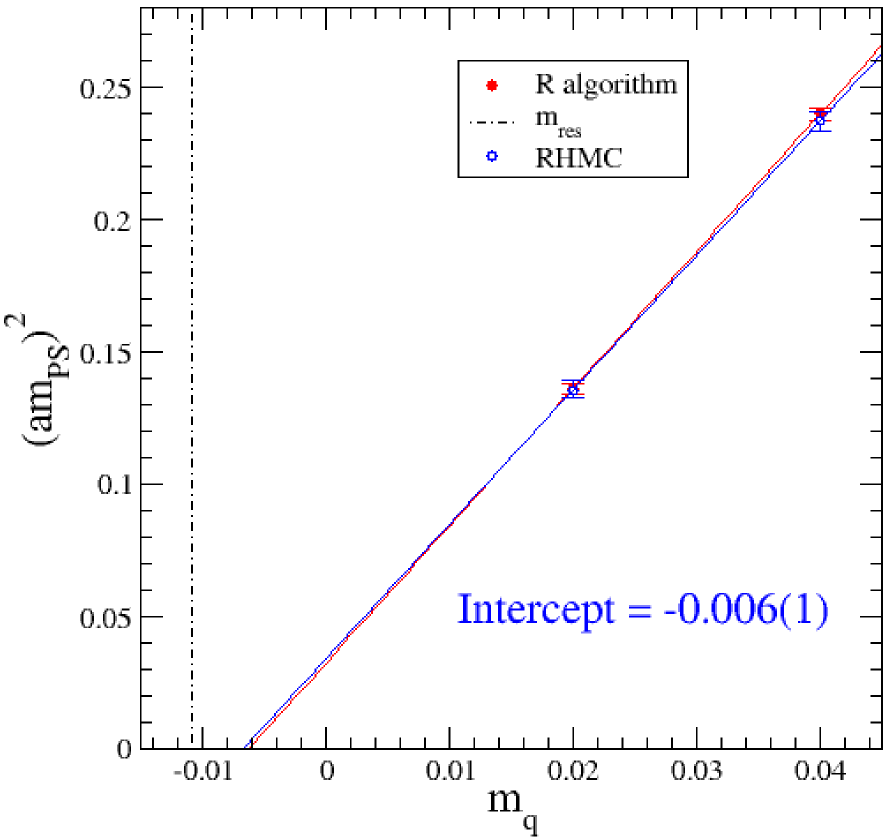
Lowest Eigen-value Behaviour



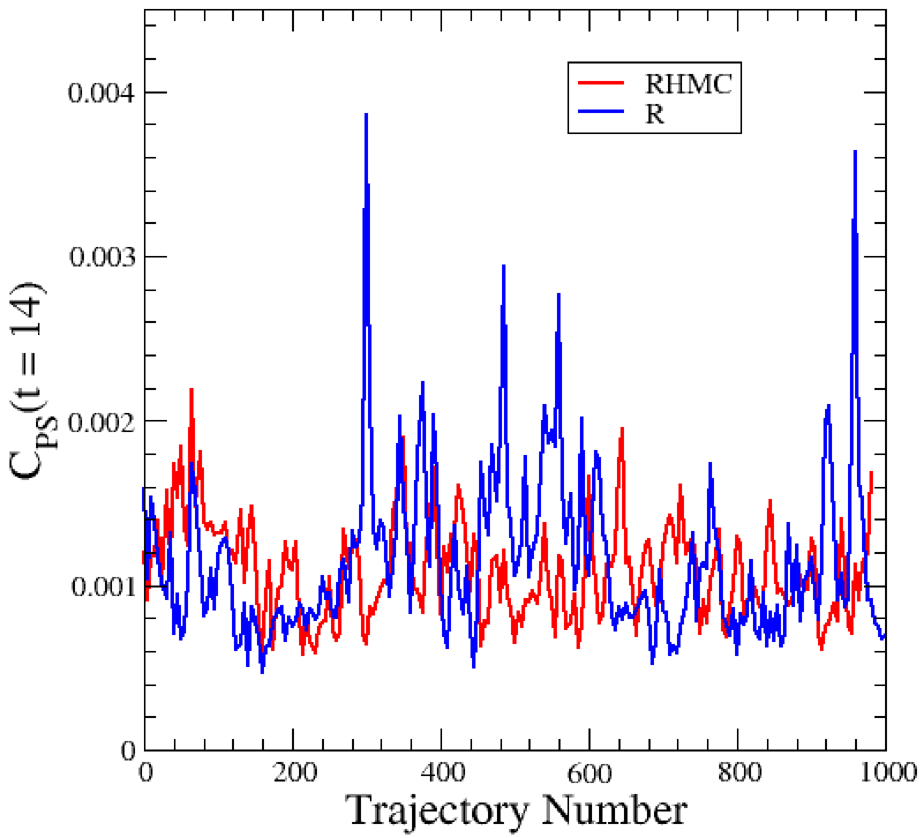
Highest Eigen-value Behaviour



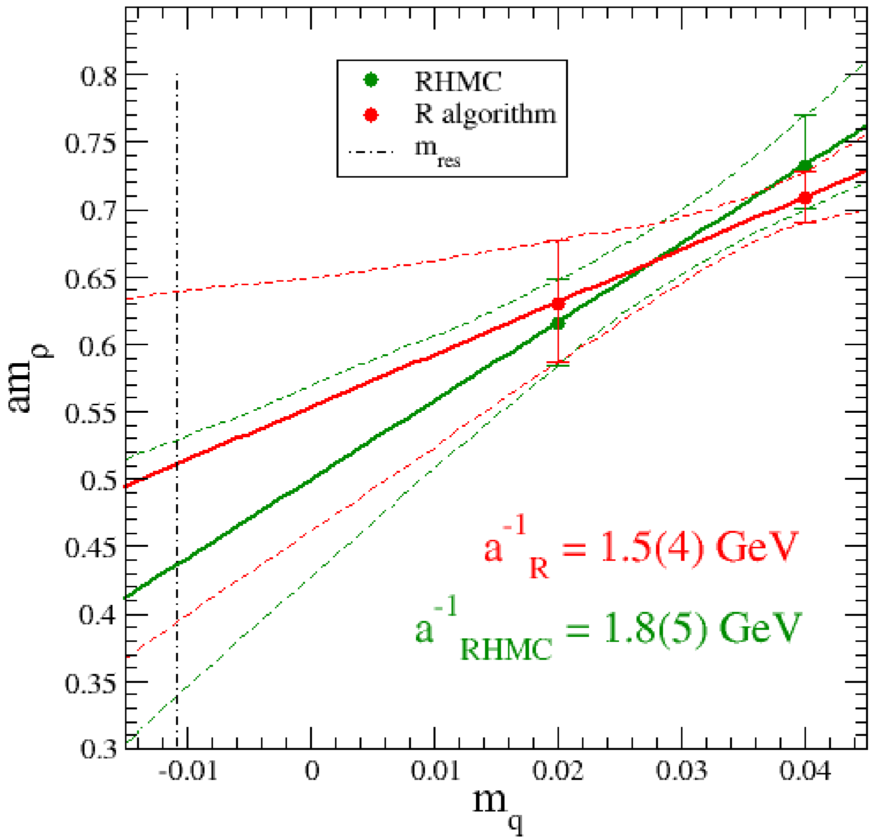
Pseudo-Scalar^2 vs dynamical, $m_s = 0.04$



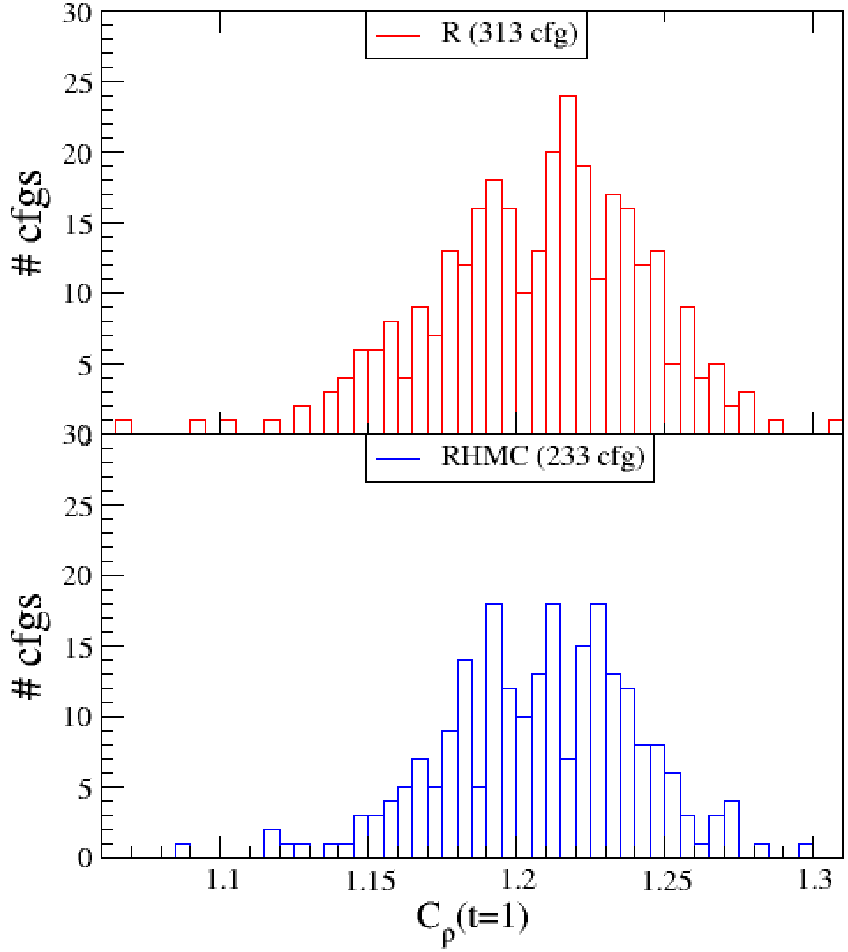
Pseudo-Scalar Correlator (t=14), $\bar{m} = 0.04$, $m_s = 0.04$



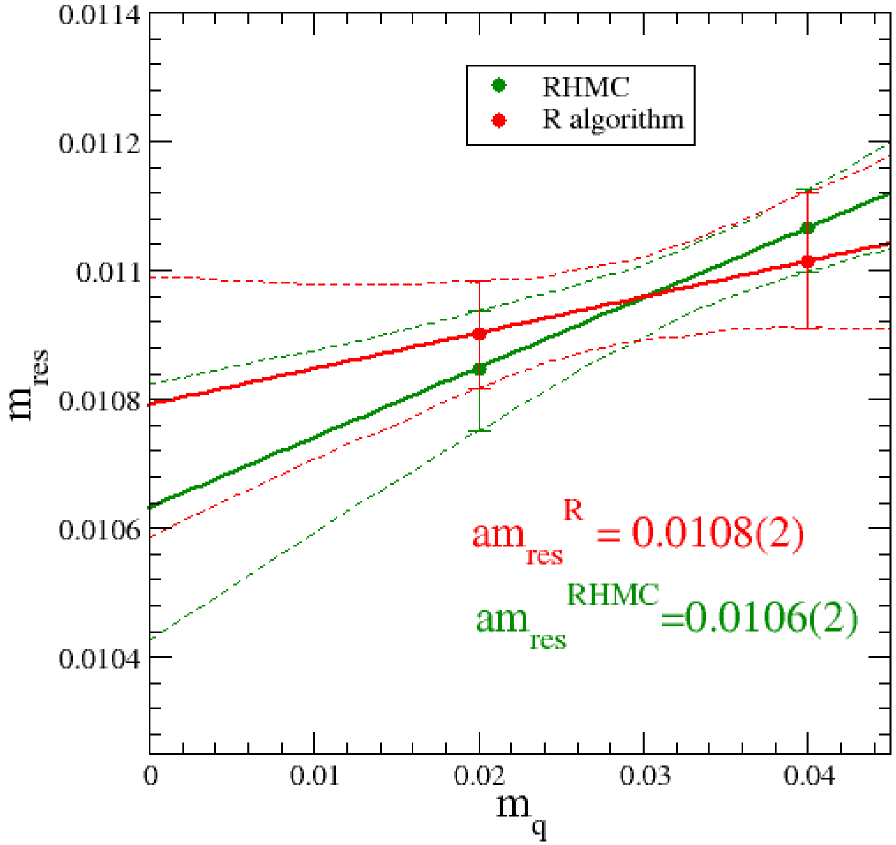
M_ρ vs dynamical, $m_s = 0.04$



Histogram of ρ correlator, $(t = 1)$, $\bar{m} = 0.04, m_s = 0.04$



m_{res} vs dynamical, $m_s = 0.04$



Conclusions and outlook

- Fast exact algorithm for non-local quantum field theories
- 2+1 ASQTAD
  - Naive cost R $\approx$ cost RHMC
  - At least factor of 2 gain over R algorithm
  - Further tuning required
  - Awaiting stability.......
- 2+1 DWF
  - RHMC verified for DWF
  - Naive cost R $\approx$ cost RHMC
  - Investigate noise in R
- Future work shall use RHMC exclusively