



The RHMC Algorithm

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Outline

- Approximation theory
 - Polynomials versus Rationals
- Symplectic Integrators
 - Multiple timescale integrators
 - Instabilities
 - Higher-order integrators
- Multiple pseudofermions
 - Hasenbusch's trick
- RHMC
 - Comparison with R algorithm
 - Testimonials from satisfied customers
 - Domain Wall fermions
 - Wilson-like fermions
- Berlin Wall
- Conclusions

Чебышев's theorem

- Чебышев: There is always a unique rational function of any degree (n,d) which minimises

$$\|r - f\|_{\infty} = \max_{0 \leq x \leq 1} |r(x) - f(x)|$$

- The error $|r(x) - f(x)|$ reaches its maximum at exactly $n+d+2$ points on the unit interval



Чебышев rationals: Example

- A realistic example of a rational approximation is

$$\frac{1}{\sqrt{x}} \approx 0.3904603901 \frac{(x + 2.3475661045)(x + 0.1048344600)(x + 0.0073063814)}{(x + 0.4105999719)(x + 0.0286165446)(x + 0.0012779193)}$$

- This is accurate to within almost *0.1%* over the range $[0.003, 1]$
- Using a partial fraction expansion of such rational functions allows us to use a multishift linear equation solver, thus reducing the cost significantly.
- The partial fraction expansion of the rational function above is

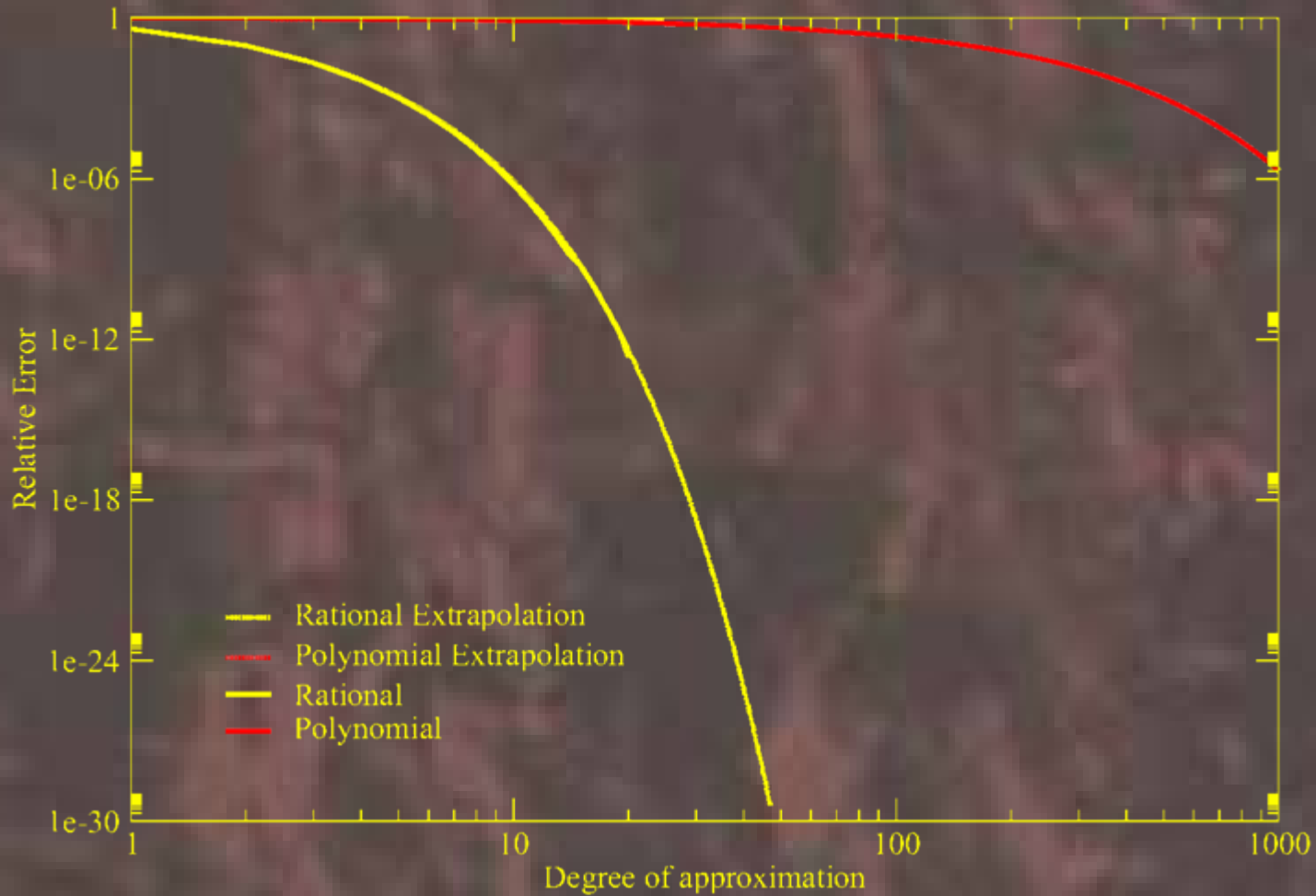
$$\frac{1}{\sqrt{x}} \approx 0.3904603901 + \frac{0.0511093775}{x + 0.0012779193} + \frac{0.1408286237}{x + 0.0286165446} + \frac{0.5964845033}{x + 0.4105999719}$$

- This appears to be numerically stable.

Polynomials v Rationals: Theory

- Золотарев's formula has L_∞ error $\Delta \leq e^{\frac{n}{\ln \varepsilon}}$
- Optimal L_2 approximation with weight $\frac{1}{\sqrt{1-x^2}}$ is
$$\sum_{j=0}^n \frac{(-1)^j 4}{(2j+1)\pi} T_{2j+1}(x)$$
- This has L_2 error of $O(1/n)$
- Optimal L_∞ approximation cannot be too much better (or it would lead to a better L_2 approximation)

Polynomials v Rationals: Data



Symplectic Integrators: I

● Baker-Campbell-Hausdorff (BCH) formula

- If A and B belong to any (non-commutative) algebra then $e^A e^B = e^{A+B+\delta}$, where δ constructed from commutators of A and B (i.e., is in the Free Lie Algebra generated by $\{A, B\}$)
- More precisely, $\ln(e^A e^B) = \sum_{n \geq 1} c_n$ where $c_1 = A + B$ and

$$c_{n+1} = \frac{1}{n+1} \left\{ -\frac{1}{2} [c_n, A+B] + \sum_{m=0}^{\lfloor n/2 \rfloor} \frac{B_{2m}}{(2m)!} \sum_{\substack{k_1, \dots, k_{2m} \geq 1 \\ k_1 + \dots + k_{2m} = n}} [c_{k_1}, [\dots, [c_{k_{2m}}, A+B] \dots]] \right\}$$



Symplectic Integrators: II

- Explicitly, the first few terms are

$$\ln(e^A e^B) = \{A+B\} + \frac{1}{2}[A,B] + \frac{1}{12}\{[A,[A,B]] - [B,[A,B]]\} - \frac{1}{24}[B,[A,[A,B]]] \\ + \frac{1}{720}\left\{ \begin{aligned} & -[A,[A,[A,[A,B]]]] - 4[B,[A,[A,[A,B]]]] \\ & -6[[A,B],[A,[A,B]]] + 4[B,[B,[A,[A,B]]]] \\ & -2[[A,B],[B,[A,B]]] + [B,[B,[B,[A,B]]]] \end{aligned} \right\} + \dots$$

- In order to construct reversible integrators we use symmetric symplectic integrators
- The following identity follows directly from the BCH formula

$$\ln(e^{A/2} e^B e^{A/2}) = \{A+B\} + \frac{1}{24}\{[A,[A,B]] - 2[B,[A,B]]\} \\ + \frac{1}{5760}\left\{ \begin{aligned} & 7[A,[A,[A,[A,B]]]] + 28[B,[A,[A,[A,B]]]] \\ & + 12[[A,B],[A,[A,B]]] + 32[B,[B,[A,[A,B]]]] \\ & - 16[[A,B],[B,[A,B]]] + 8[B,[B,[B,[A,B]]]] \end{aligned} \right\} + \dots$$

Symplectic Integrators: III

- We are interested in finding the classical trajectory in phase space of a system described by the Hamiltonian $H(q, p) = T(p) + S(q) = \frac{1}{2} p^2 + S(q)$

- The basic idea of such a symplectic integrator is to write the time evolution operator as

$$\begin{aligned}\exp\left(\tau \frac{d}{dt}\right) &\equiv \exp\left(\tau \left\{ \frac{dp}{dt} \frac{\partial}{\partial p} + \frac{dq}{dt} \frac{\partial}{\partial q} \right\}\right) \\ &= \exp\left(\tau \left\{ -\frac{\partial H}{\partial q} \frac{\partial}{\partial p} + \frac{\partial H}{\partial p} \frac{\partial}{\partial q} \right\}\right) \equiv e^{\tau \hat{H}} \\ &= \exp\left(\tau \left\{ -S'(q) \frac{\partial}{\partial p} + T'(p) \frac{\partial}{\partial q} \right\}\right)\end{aligned}$$

Symplectic Integrators: IV

- Define $Q \equiv T'(p) \frac{\partial}{\partial q}$ and $P \equiv -S'(q) \frac{\partial}{\partial p}$ so that $\hat{H} = P + Q$
- Since the kinetic energy T is a function only of p and the potential energy S is a function only of q , it follows that the action of $e^{\tau P}$ and $e^{\tau Q}$ may be evaluated trivially

$$e^{\tau Q} : f(q, p) \mapsto f(q + \tau T'(p), p)$$

$$e^{\tau P} : f(q, p) \mapsto f(q, p - \tau S'(q))$$

Symplectic Integrators: V

- From the BCH formula we find that the PQP symmetric symplectic integrator is given by

$$\begin{aligned}
 U_0(\delta\tau)^{\tau/\delta\tau} &= \left(e^{\frac{1}{2}\delta\tau P} e^{\delta\tau Q} e^{\frac{1}{2}\delta\tau P} \right)^{\tau/\delta\tau} \\
 &= \left(\exp \left[(P+Q)\delta\tau - \frac{1}{24} \left([P, [P, Q]] + 2[Q, [P, Q]] \right) \delta\tau^3 + O(\delta\tau^5) \right] \right)^{\tau/\delta\tau} \\
 &= \exp \left[\tau \left((P+Q) - \frac{1}{24} \left([P, [P, Q]] + 2[Q, [P, Q]] \right) \delta\tau^2 + O(\delta\tau^4) \right) \right] \\
 &= e^{\tau \hat{H}'} = e^{\tau(P+Q)} + O(\delta\tau^2)
 \end{aligned}$$

- In addition to conserving energy to $O(\delta\tau^2)$ such symmetric symplectic integrators are manifestly area preserving and reversible

Symplectic Integrators: VI

- For each symplectic integrator there exists a nearby Hamiltonian H' which is *exactly conserved*

- This is obtained by replacing commutators with Poisson brackets in the BCH formula

- For the PQP integrator we have

$$H' = P + Q - \frac{1}{24} \left(\{P, \{P, Q\}\} + 2 \{Q, \{P, Q\}\} \right) \delta\tau^2 + O(\delta\tau^4)$$

$$= H + \frac{1}{24} \left\{ 2p^2 S'' - S'^2 \right\} \delta\tau^2$$

$$+ \frac{1}{720} \left\{ -p^4 S^{(4)} + 6p^2 (S'S''' + 2S''^2) - 3S'^2 S'' \right\} \delta\tau^4 + O(\delta\tau^6)$$

- Note that H' cannot be written as the sum of a p -dependent kinetic term and a q -dependent potential term
- As H' is conserved, δH is of $O(\delta\tau^2)$ for arbitrary length trajectories

Symplectic Integrators: VII

Multiple timescales

- Split the Hamiltonian into pieces $H(q, p) = T(p) + S_1(q) + S_2(q)$
- Define $Q \equiv T'(p) \frac{\partial}{\partial q}$ and $P_i \equiv -S'_i(q) \frac{\partial}{\partial p}$ so that $\hat{H} = P_1 + P_2 + Q$
- Introduce a symmetric symplectic integrator of the form

$$U_{\text{SW}}(\delta\tau)^{\tau/\delta\tau} = \left(e^{\frac{1}{2}\delta\tau P_1} \left[e^{\frac{1}{2n}\delta\tau Q} e^{\frac{1}{n}\delta\tau P_2} e^{\frac{1}{2n}\delta\tau Q} \right]^{n_2} e^{\frac{1}{2}\delta\tau P_1} \right)^{\tau/\delta\tau}$$

- If $\frac{\|P_1\|_1}{2} \approx \frac{\|P_2\|_1}{n}$ then the instability in the integrator is tickled equally by each sub-step
- This helps if the most expensive force computation does not correspond to the largest force

Integrator Instability: Theory

- Consider a leapfrog integrator for free field theory
 - The evolution is given by

$$U(\tau) = \begin{pmatrix} \cos[\kappa(\delta\tau)\tau] & \frac{\sin[\kappa(\delta\tau)\tau]}{\rho(\delta\tau)} \\ -\rho(\delta\tau)\sin[\kappa(\delta\tau)\tau] & \cos[\kappa(\delta\tau)\tau] \end{pmatrix}$$

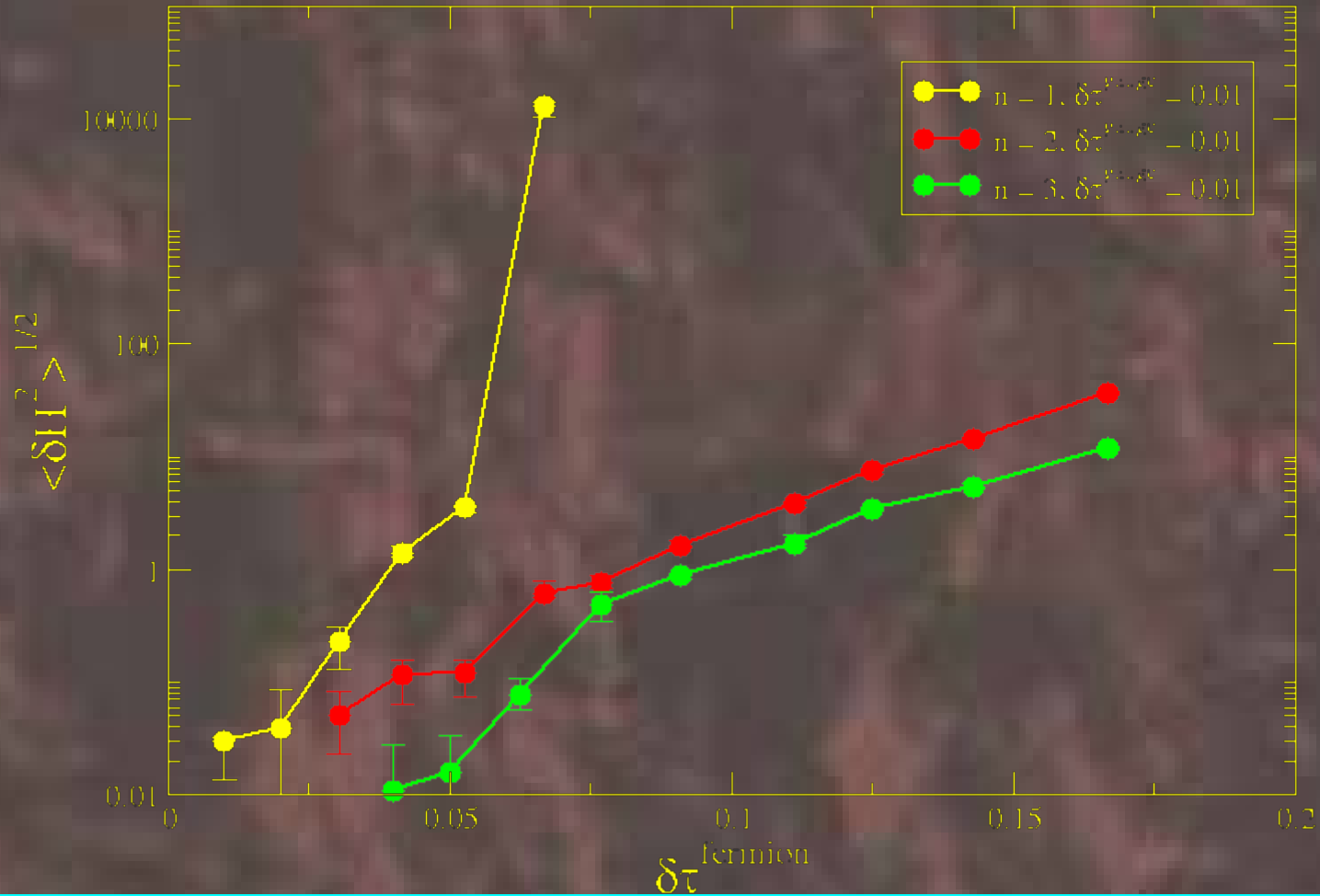
- where

$$\kappa(\delta\tau) = \frac{\cos^{-1}\left(1 - \frac{1}{2}\delta\tau^2\right)}{\delta\tau}, \rho(\delta\tau) = \sqrt{1 - \frac{1}{4}\delta\tau^2}$$

- This grows/oscillates with exponents

$$\nu = \pm \frac{1}{\delta\tau} \operatorname{Re} \ln \left[\frac{1}{2}\delta\tau^2 - 1 \pm \sqrt{\frac{1}{4}\delta\tau^2 - 1} \right]$$

Integrator Instability: Data



Higher-Order Integrators: I

- Campostrini and Rossi introduced an integrator with arbitrarily high-order errors
 - But the longest constituent step is longer than the overall step size, so integrator instabilities are worse
- Omelyan introduced an integrator to minimise the $\delta\tau$ error for a given number of sub-steps
 - I. P. Omelyan, I. M. Mryglod and R. Folk, *Comput. Phys. Commun.* 151 (2003) 272
 - Tetsuya Takaishi and Philippe de Forcrand, “Testing and tuning new symplectic integrators for Hybrid Monte Carlo algorithm in lattice QCD,” [hep-lat/0505020](https://arxiv.org/abs/hep-lat/0505020)

Higher-Order Integrators: II

- These techniques help if the force is extensive (i.e., a bulk effect)
 - Because the step size needs to be adjusted so that $V \delta\tau^n$ is constant for a fixed HMC acceptance rate
- They do not help if the force is due to one (or a small number) of light modes
 - Here the HMC acceptance goes to zero because the symplectic integrator becomes unstable for a single mode
 - Hasenbusch's trick reduces the maximum force if it is due to noise coming from the pseudofermion fields
 - But not if the intrinsic fermionic force contribution is large.
- The volume dependence of the spectral density of the Wilson Dirac operator needs to be investigated

Non-linearity of CG solver

- Suppose we want to solve $A^2x=b$ for Hermitian A by CG
 - It is better to solve $Ax=y$, $Ay=b$ successively
 - Condition number $\kappa(A^2) = \kappa(A)^2$
 - Cost is thus $2\kappa(A) < \kappa(A^2)$ in general
- Suppose we want to solve $Ax=b$
 - Why don't we solve $A^{1/2}x=y$, $A^{1/2}y=b$ successively?
- The square root of A is uniquely defined if $A>0$
 - This is the case for fermion kernels
- All this generalises trivially to n^{th} roots
 - No tuning needed to split condition number evenly
- How do we apply the square root of a matrix?

Rational matrix approximation

● Functions on matrices

- Defined for a Hermitian matrix by diagonalisation

- $H = U D U^{-1}$

- $f(H) = f(U D U^{-1}) = U f(D) U^{-1}$

● Rational functions do not require diagonalisation

- $\alpha H^m + \beta H^n = U (\alpha D^m + \beta D^n) U^{-1}$

- $H^{-1} = U D^{-1} U^{-1}$

No Free Lunch Theorem

- We must apply the rational approximation with each CG iteration
 - $M^{1/n} \approx r(M)$
 - The condition number for each term in the partial fraction expansion is approximately $\kappa(M)$
 - So the cost of applying $M^{1/n}$ is proportional to $\kappa(M)$
 - Even though the condition number $\kappa(M^{1/n}) = \kappa(M)^{1/n}$
 - And even though $\kappa(r(M)) = \kappa(M)^{1/n}$
- So we don't win this way...

Pseudofermions

- We want to evaluate a functional integral including the fermionic determinant $\det M$
- We write this as a bosonic functional integral over a pseudofermion field with kernel M^{-1}

$$\det M \propto \int d\phi^* d\phi e^{-\phi^* M^{-1} \phi}$$

Multipseudofermions

- We are introducing extra noise into the system by using a single pseudofermion field to sample this functional integral
 - This noise manifests itself as fluctuations in the force exerted by the pseudofermions on the gauge fields
 - This increases the maximum fermion force
 - This triggers the integrator instability
 - This requires decreasing the integration step size

● A better estimate is $\det M = [\det M^{1/n}]^n$

$$\det M^{\frac{1}{n}} \propto \int d\phi^* d\phi e^{-\phi^* M^{\frac{1}{n}} \phi}$$

Hasenbusch's method

● Clever idea due to Hasenbusch

- Start with the Wilson fermion action $M=1 - \kappa H$
- Introduce the quantity $M'=1 - \kappa' H$
- Use the identity $M = M'(M'^{-1}M)$
- Write the fermion determinant as $\det M = \det M' \det (M'^{-1}M)$
- Introduce separate pseudofermions for each determinant
- Adjust κ' to minimise the cost

● Easily generalises

- More than two pseudofermions
- Wilson-clover action

Violation of NFL Theorem

- So let's try using our n^{th} root trick to implement multipseudofermions
 - Condition number $\kappa(r(M)) = \kappa(M)^{1/n}$
 - So maximum force is reduced by a factor of $n\kappa(M)^{(1/n)-1}$
 - This is a good approximation if the condition number is dominated by a few isolated tiny eigenvalues
 - This is so in the case of interest
- Cost reduced by a factor of $n\kappa(M)^{(1/n)-1}$
 - Optimal value $n_{\text{opt}} \approx \ln \kappa(M)$
 - So optimal cost reduction is $(e \ln \kappa) / \kappa$

Rational Hybrid Monte Carlo: I

- RHMC algorithm for fermionic kernel $(\mathcal{M}^\dagger \mathcal{M})^{\frac{1}{2n}}$

- Generate pseudofermion from Gaussian heatbath

$$P(\xi) \propto e^{-\frac{1}{2}\xi^\dagger \xi} \quad \chi = (\mathcal{M}^\dagger \mathcal{M})^{\frac{1}{4n}} \xi$$

$$P(\chi) \propto \int_{-\infty}^{\infty} d\xi e^{-\frac{1}{2}\xi^\dagger \xi} \delta\left(\chi - (\mathcal{M}^\dagger \mathcal{M})^{\frac{1}{4n}} \xi\right) \propto e^{-\frac{1}{2}\chi^\dagger (\mathcal{M}^\dagger \mathcal{M})^{-\frac{1}{2n}} \chi}$$

- Use accurate rational approximation $r(x) \approx \sqrt[4n]{x}$
- Use less accurate approximation for MD, $\tilde{r}(x) \approx \sqrt[2n]{x}$
 - $\tilde{r}(x) \neq r(x)^2$, so there are no double poles
- Use accurate approximation for Metropolis acceptance step

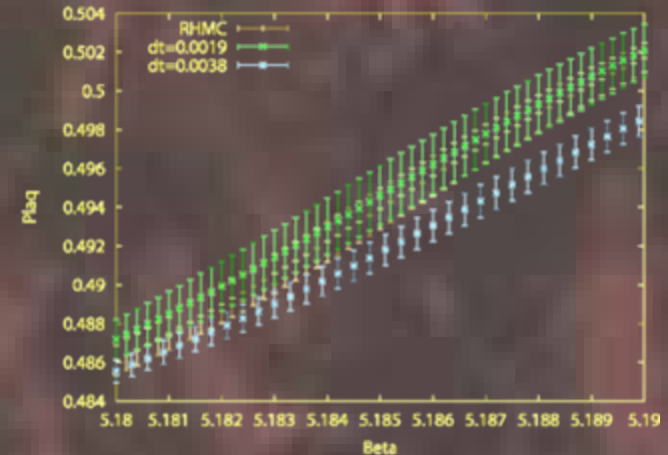
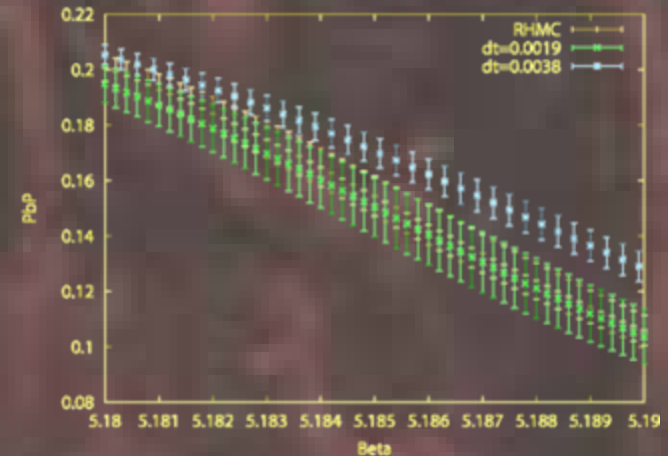
Rational Hybrid Monte Carlo: II

- Apply rational approximations using their partial fraction expansions
- Denominators are all just shifts of the original fermion kernel
 - All poles of optimal rational approximations are real and positive for cases of interest (Miracle #1)
 - Only simple poles appear (by construction!)
- Use multishift solver to invert all the partial fractions using a single Krylov space
 - Cost is dominated by Krylov space construction, at least for $O(20)$ shifts
- Result is numerically stable, even in 32-bit precision
 - All partial fractions have positive coefficients (Miracle #2)
- MD force term is of the usual form for each partial fraction
- Applicable to any kernel

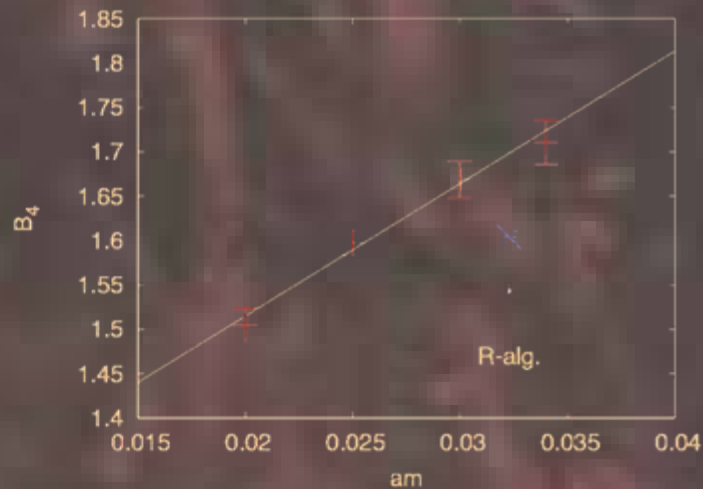
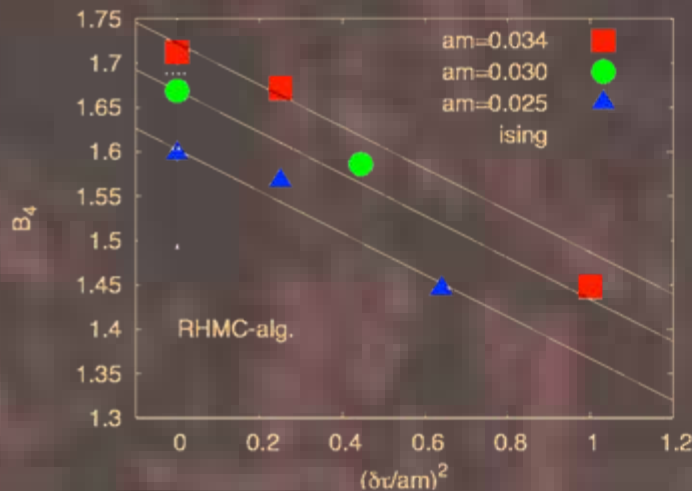
Comparison with R algorithm: I

Binder cumulant of chiral condensate, B_4 , and RHMC acceptance rate A from a finite temperature study (2+1 flavour naive staggered fermions, Wilson gauge action, $V = 8^3 \times 4$, $m_{ud} = 0.0076$, $m_s = 0.25$, $\tau = 1.0$)

Algorithm	δt	A	B_4
R	0.0019		1.56(5)
R	0.0038		1.73(4)
RHMC	0.055	84%	1.57(2)



Comparison with R algorithm: II



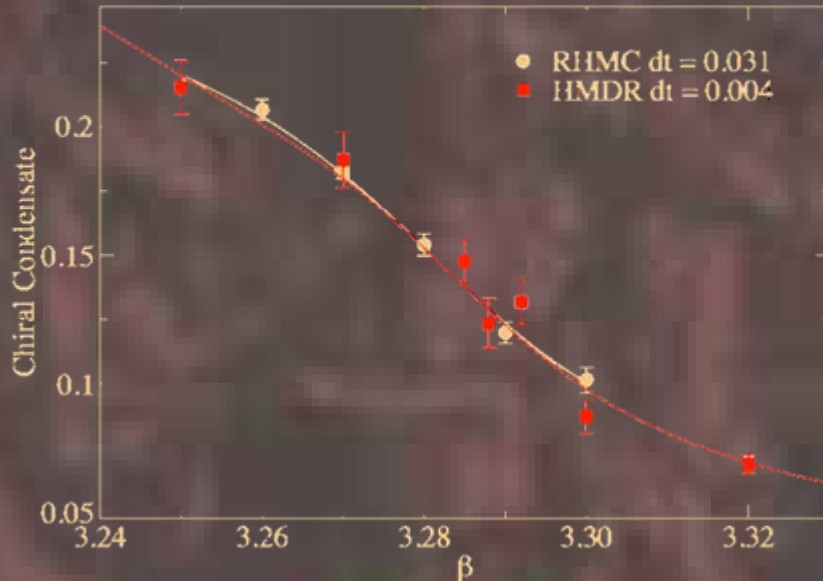
Naïve Staggered Fermions, $N_f = 3$, $V = 8^3 \times 4$

- Binder cumulant increases as step-size is reduced
- Step-size extrapolation is vital for R algorithm
- 25% reduction in critical quark mass at $\delta\tau = \frac{1}{2} m_c$
- 20% change in renormalized quark mass

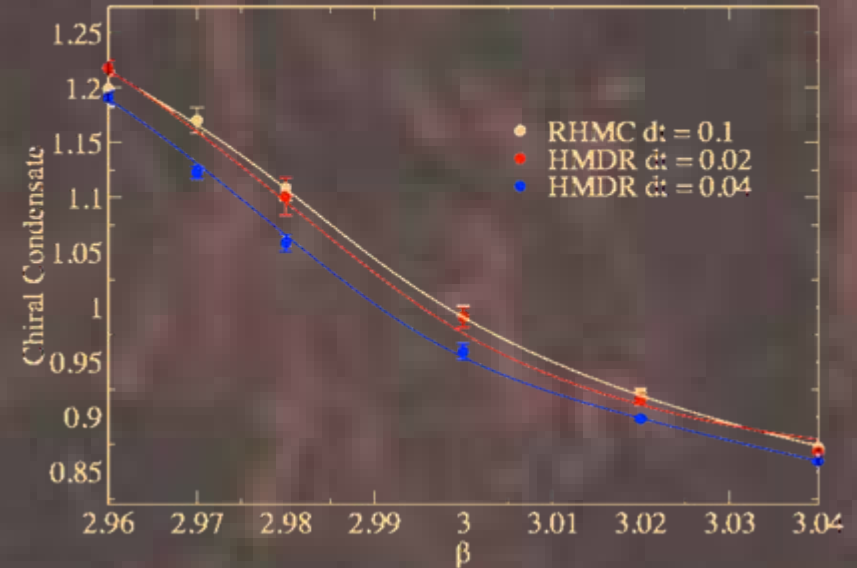
• “An exact algorithm is mandatory” (de Forcrand-Philipsen)

Comparison with R algorithm: III




RHMC vs. HMDR, p4fat3 $m_q=0.01, 8^3 \times 4$



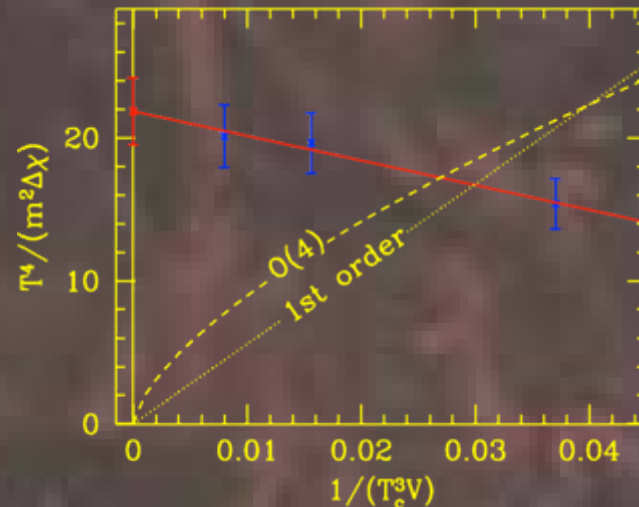
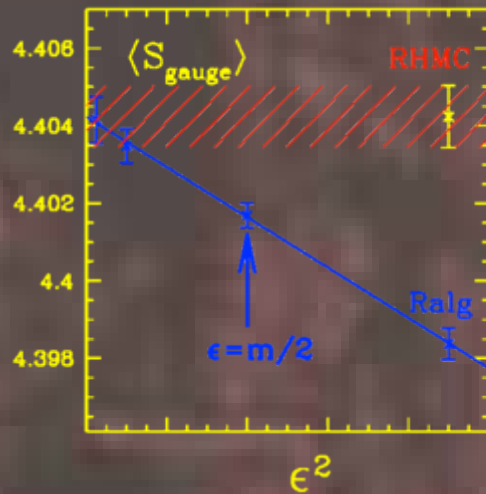
RHMC vs. HMDR, p4fat7, $m_q=0.1, 8^3 \times 4$



RBC-Bielefeld

-  P4 staggered fermions
-  RHMC allows an $O(10)$ increase in step-size
-  Speedup greater as $m_\ell \rightarrow 0$

Comparison with R algorithm: IV



Wuppertal—Budapest

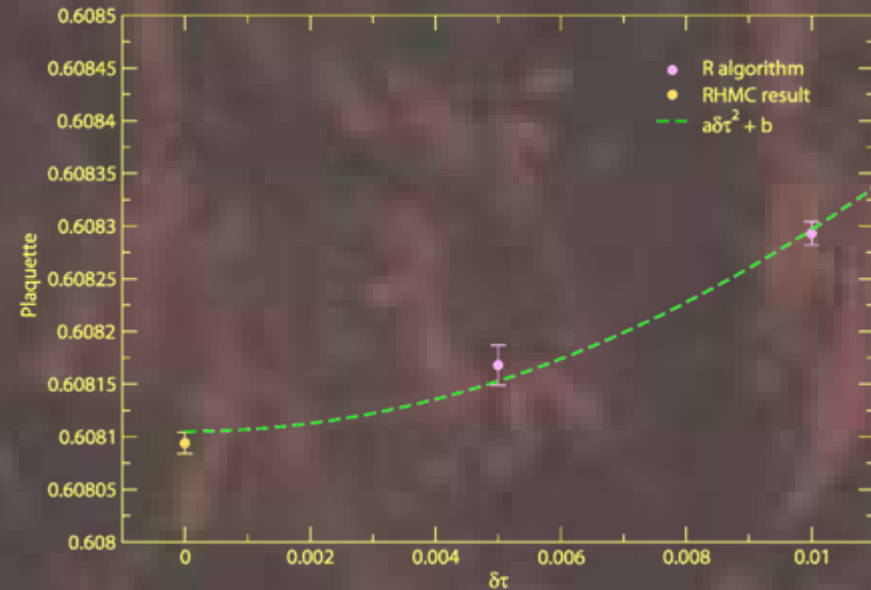
- Stout smeared staggered, $V = 16^4$, $m_\pi = 320$ MeV

- Subtraction required for equation of state and order of the transition
- At $\delta\tau \simeq \frac{2}{3} m_l$ finite step-size error \sim magnitude of subtraction
- RHMC is order of magnitude faster than the R algorithm
- Order of transition in continuum limit at physical quark masses for the first time

Comparison with R algorithm: V

The different masses at which domain wall results were gathered, together with the step-sizes δt , acceptance rates A , and plaquettes P ($V = 16^3 \times 32 \times 8$, DBW2 gauge action, $\beta = 0.72$)

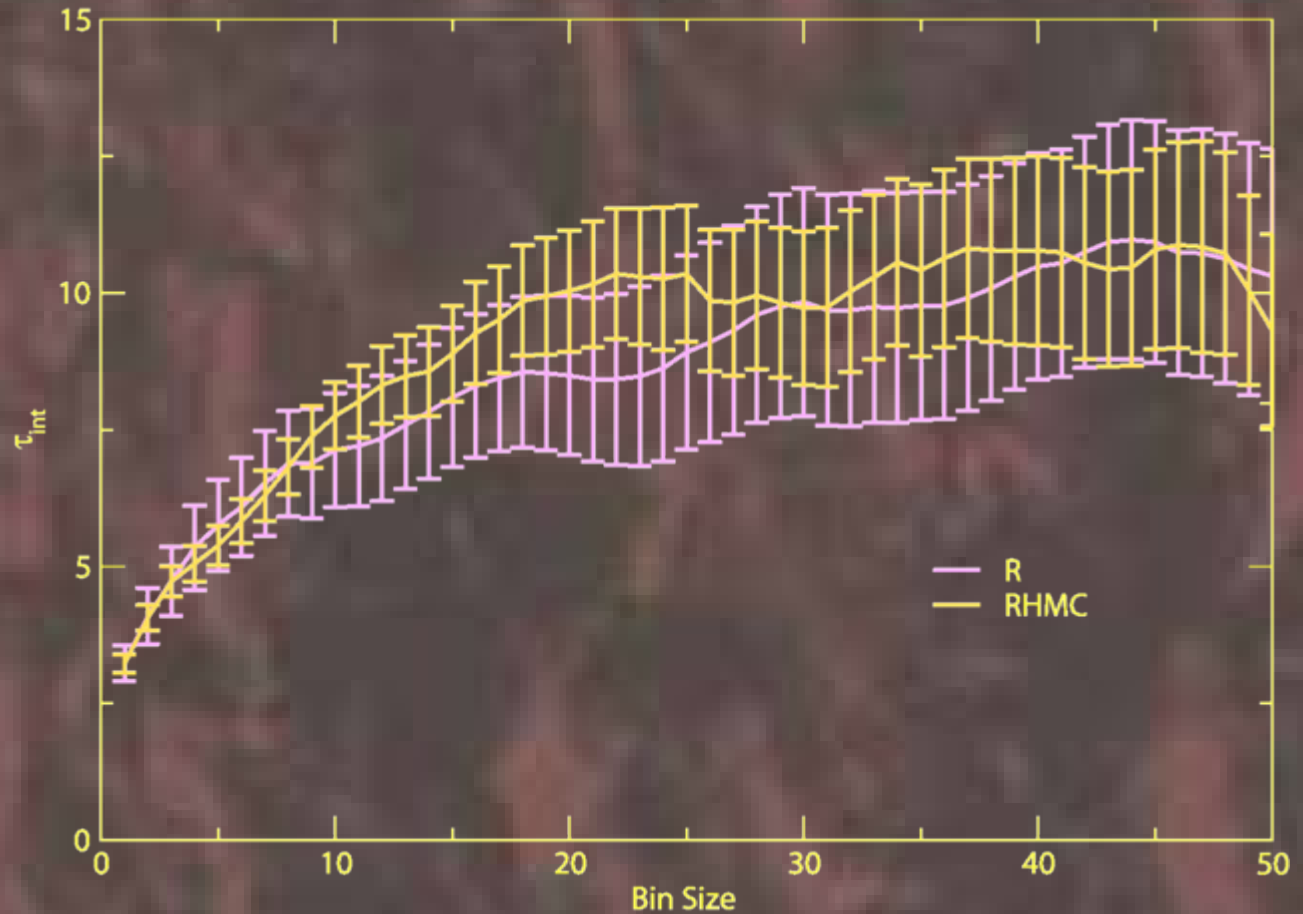
Algorithm	m_{ud}	m_s	δt	A	P
R	0.04	0.04	0.01		0.60812(2)
R	0.02	0.04	0.01		0.60829(1)
R	0.02	0.04	0.005		0.60817
RHMC	0.04	0.04	0.02	65.5%	0.60779(1)
RHMC	0.02	0.04	0.0185	69.3%	0.60809(1)



The step-size variation of the plaquette with $m_{ud} = 0.02$

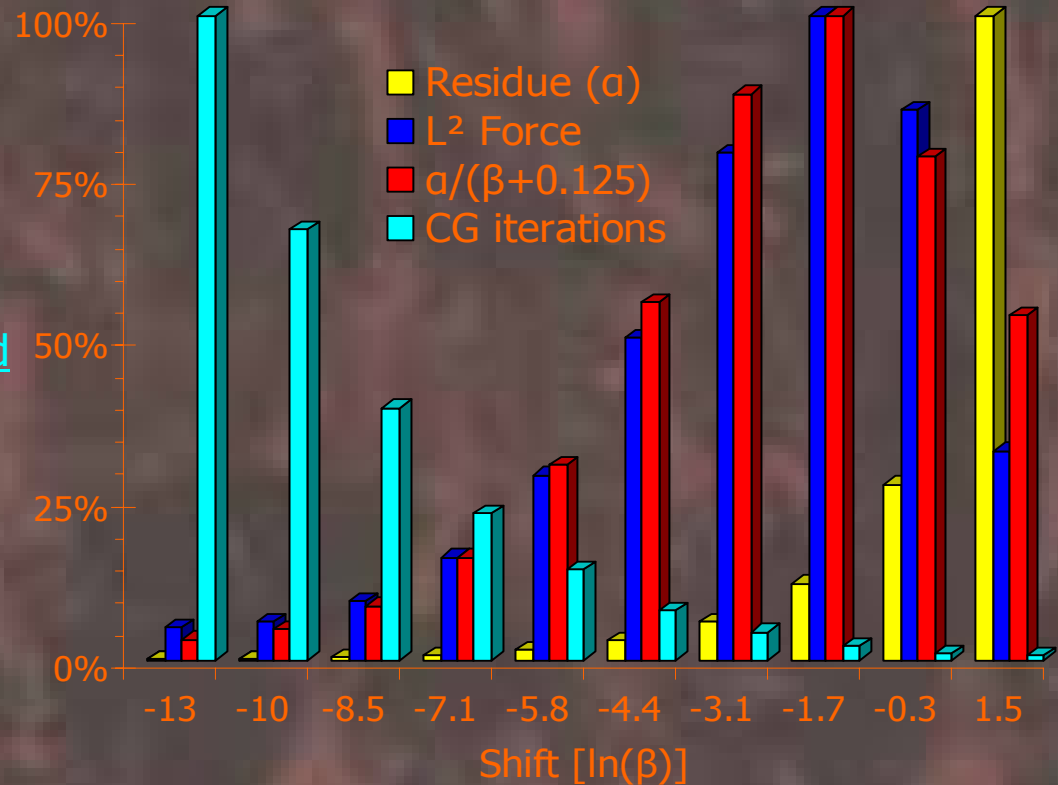
Comparison with R algorithm: VI

The integrated autocorrelation time of the 13th time-slice of the pion propagator from the domain wall test, with $m_{ud} = 0.04$



Multipseudofermions with multiple timescales

- Semiempirical observation: The largest force from a single pseudofermion does not come from the smallest shift
 - For example, look at the numerators in the [partial fraction expansion we exhibited earlier](#)
- Use a coarser timescale for expensive smaller shifts
- Invert small shifts less accurately
 - Cannot use chronological inverter with multishift solver anyhow



$$\frac{1}{\sqrt{x}} \approx 0.3904603901 + \frac{0.0511093775}{x + 0.0012779193} + \frac{0.1408286237}{x + 0.0286165446} + \frac{0.5964845033}{x + 0.4105999719}$$

Performance Comparison

$V = 24^3 \times 32$, $\beta = 5.6$, $N_f = 2$, Wilson fermions

Cost in units of $A_{plaq} \times N_{MV} \times 10^4$

κ	RHMC	Urbach <i>et al.</i>	Orth <i>et al.</i>
0.15750	9.6	9.0	19.1
0.15800	29.9	17.4	128
0.15825	52.5	56.5	—

DWF (RBRC—UKQCD)

- 2+1 Flavour determinant

$$\left(\frac{\det \mathcal{M}_\ell^\dagger \mathcal{M}_\ell}{\det \mathcal{M}_{PV}^\dagger \mathcal{M}_{PV}} \right) \left(\frac{\det \mathcal{M}_s^\dagger \mathcal{M}_s}{\det \mathcal{M}_{PV}^\dagger \mathcal{M}_{PV}} \right)^{\frac{1}{2}} = \left(\frac{\det \mathcal{M}_\ell^\dagger \mathcal{M}_\ell}{\det \mathcal{M}_s^\dagger \mathcal{M}_s} \right) \left(\frac{\det \mathcal{M}_s^\dagger \mathcal{M}_s}{\det \mathcal{M}_{PV}^\dagger \mathcal{M}_{PV}} \right)^{\frac{3}{2}}$$

- Mass (Hasenbusch) preconditioning using s quark
- Use multiple timescale integrator
 - Gauge, triple strange, light
- CG count reduced by factor of 10
- CPU time reduced by factor of 6
- Light quarks cost about 10% of total
- Cost has weak mass dependence

2+1 ASQTAD Staggered Fermions

- Mass preconditioning using s quark

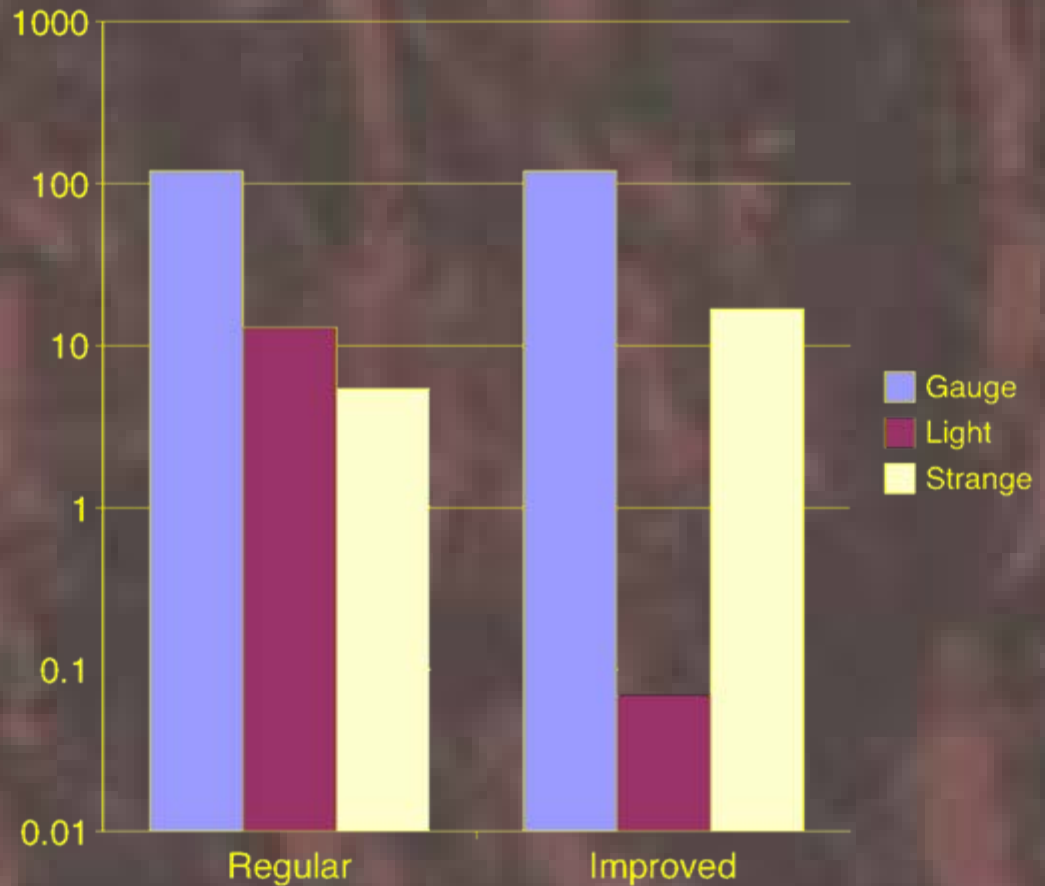
$$\det \mathcal{M}_\ell^{\frac{1}{2}} \mathcal{M}_s^{\frac{1}{4}} = \left(\frac{\det \mathcal{M}_\ell}{\det \mathcal{M}_s} \right)^{\frac{1}{2}} \det \mathcal{M}_s^{\frac{3}{4}}$$

- Mass is just a shift for staggered fermions

$$\begin{aligned} S_F &= \phi_\ell^\dagger \left(\frac{\mathcal{M}_s}{\mathcal{M}_\ell} \right)^{\frac{1}{2}} \phi_\ell + \phi_s^\dagger \mathcal{M}_s^{-\frac{3}{4}} \phi_s = \phi_\ell^\dagger \left(\frac{\mathcal{M}_\ell + \delta m^2}{\mathcal{M}_\ell} \right)^{\frac{1}{2}} \phi_\ell + \phi_s^\dagger \mathcal{M}_s^{-\frac{3}{4}} \phi_s \\ &= \phi_\ell^\dagger r_1(\mathcal{M}_\ell) \phi_\ell + \phi_s^\dagger r_2(\mathcal{M}_s) \phi_s \end{aligned}$$

2+1 ASQTAD Staggered Fermions

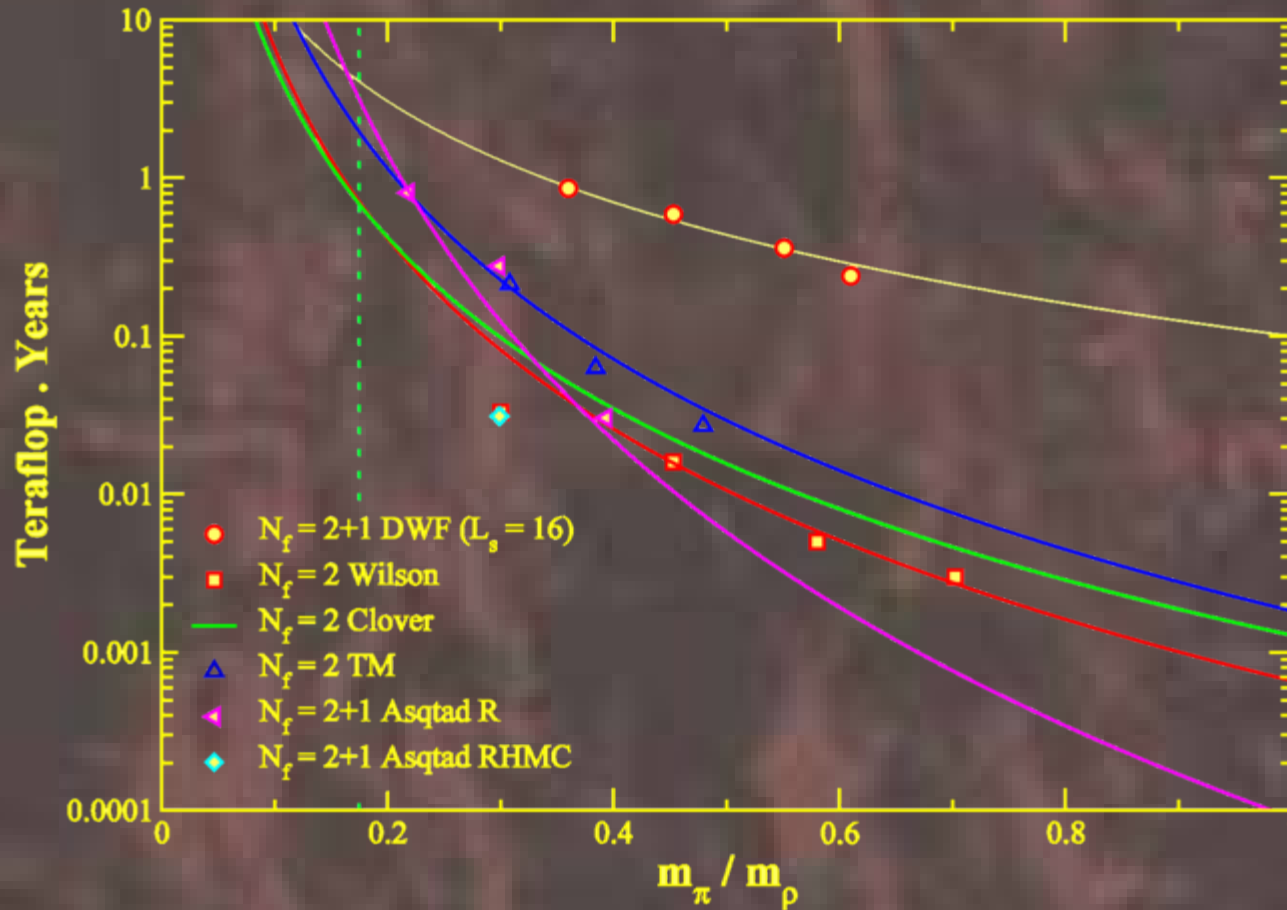
- Use multiple timescales
 - Gauge, triple strange, light
- Dominant cost from triple strange
 - Operator derivative cost \gg CG cost
 - Further mass preconditioning detrimental
- Use n^{th} root trick on triple strange
 - Optimum solution uses mass preconditioning and n^{th} root trick
 - Test at current run parameters
 - $V = 24^3 \times 64$, $\beta = 6.76$,
 $m_l = 0.005$, $m_s = 0.05$
 - Speed up factor 8 over R algorithm **and exact**



Berlin Wall

- Comparison of cost of fermion algorithms
 - $N_f = 2+1$ DWF RHMC (RBC-UKQCD)
 - $N_f = 2$ mass preconditioned Wilson (Urbach *et al.*)
 - $N_f = 2$ mass preconditioned Clover (QCDSF)
 - $N_f = 2+1$ mass preconditioned Clover + RHMC (Wuppertal-Jülich)
 - $N_f = 2$ mass preconditioned Twisted Mass (ETM)
 - $N_f = 2+1$ ASQTAD R (MILC)
 - $N_f = 2+1$ ASQTAD RHMC (Clark-Kennedy)
- All data scaled to $V = 24^3 \times 40$, $a = 0.08$
- Cost for generating 10^3 independent configurations
 - Independent plaquette measurements

Berlin Wall



Conclusions (RHMC)

Advantages of RHMC

- Exact
 - No step-size errors; no step-size extrapolations
- Significantly cheaper than the R algorithm
- Allows easy implementation of Hasenbusch (multipseudofermion) acceleration
 - Combination of both can be helpful
- Further improvements possible
 - Such as multiple timescales for different terms in the partial fraction expansion

Disadvantages of RHMC

- ???