Accelerating Fermionic Molecular Dynamics

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Abstract

We consider how to accelerate Fermionic Molecular Dynamics algorithms by introducing *n* pseudofermion fields coupled with the n^{th} root of the Fermionic kernel. The n^{th} roots may be computed efficiently using Чебышев rational approximations, and to this end we review the theory of optimal polynomial and rational Чебышев approximations.

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
  - $H = UDU^{-1}$
  - $f(H) = f(UDU^{-1}) = U f(D) U^{-1}$
- Rational functions do not require diagonalisation
  - $\alpha H^m + \beta H^n = U(\alpha D^m + \beta D^n) U^{-1}$
  - $H^{-1} = UD^{-1}U^{-1}$
- Rational functions have nice properties
  - Cheap (relatively)
  - Accurate

Polynomial approximation

- What is the best polynomial approximation $p(x)$ to a continuous function $f(x)$ for x in $[0,1]$?
  - Best with respect to the appropriate norm

$$\|p-f\|_n = \left(\int_0^1 dx \left| p(x) - f(x) \right|^n \right)^{1/n}$$

where $n \geq 1$

Weierstraß' theorem

- Taking $n \rightarrow \infty$ this is the "minimax" norm

$$\left\| p - f \right\|_\infty = \min_p \max_{0 \le x \le 1} \left| p(x) - f(x) \right|$$

- Weierstraß: Any continuous function can be arbitrarily well approximated by a polynomial

Бернштейне polynomials

- The explicit solution is provided by Бернштейне polynomials

$$p_n(x) \equiv \sum_{k=0}^{n} f\left(\frac{k}{n}\right) \binom{n}{k} x^n (1-x)^{n-k}$$

Чебышев's theorem

- Чебышев: There is always a unique polynomial of any degree d which minimises

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

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

Чебышев's theorem: Necessity

- Suppose p-f has less than $d+2$ extrema of equal magnitude
- Then at most $d+1$ maxima exceed some magnitude
- This defines a
- W… d which has the opposite sign to
  …olation)
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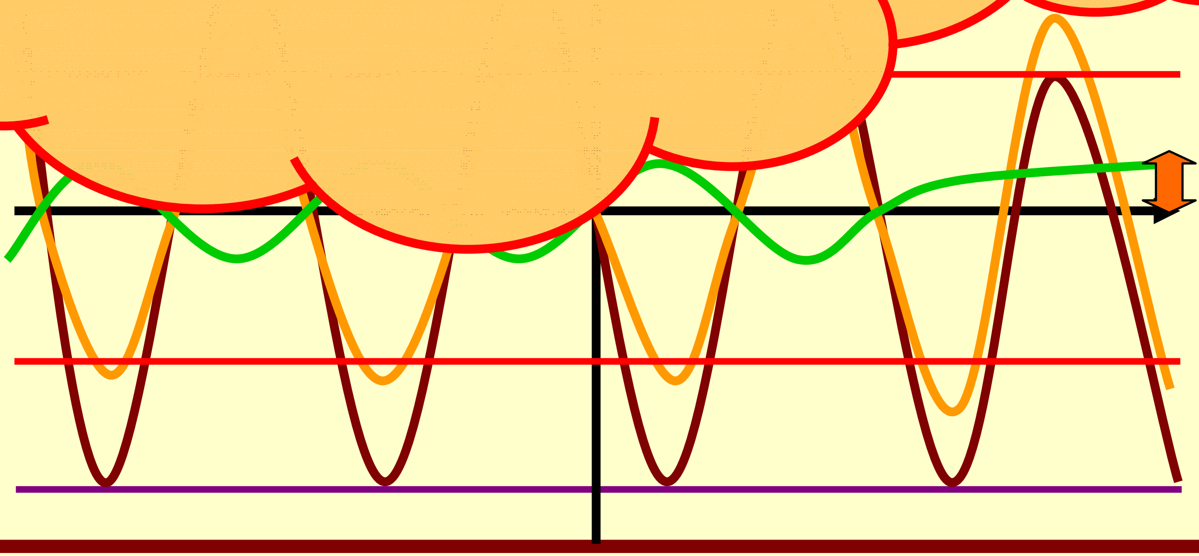
  …tion than p to f

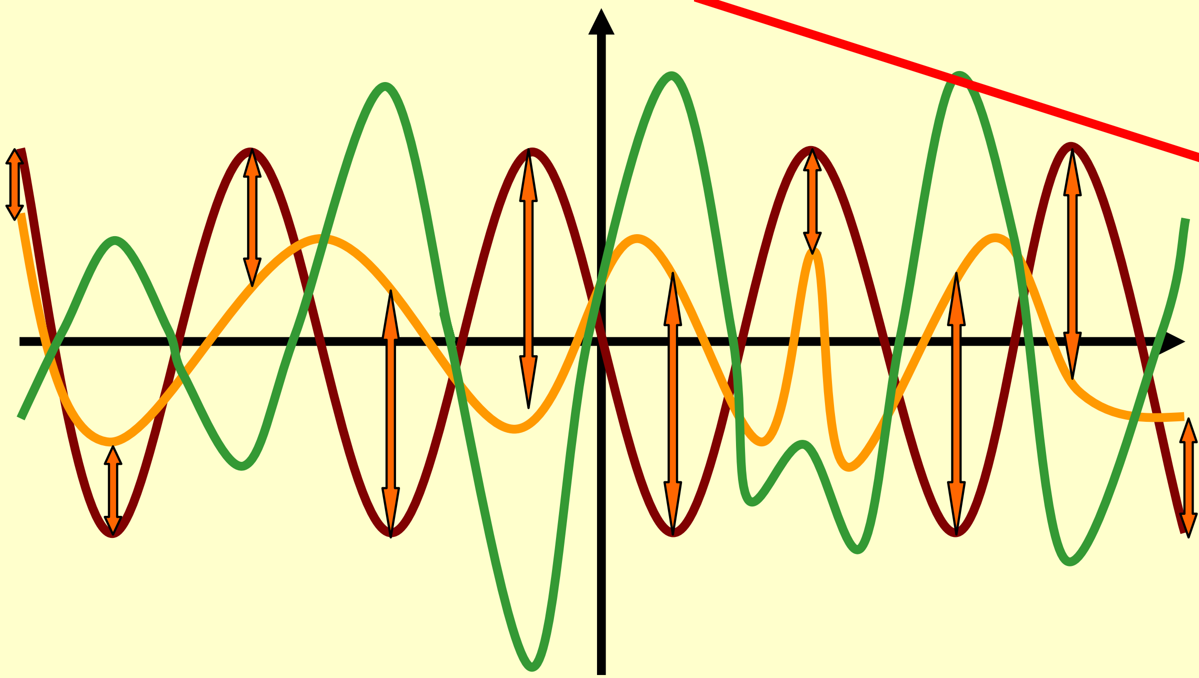
Lagrange was born in Turin!



Чебышев's theorem: Sufficiency

- Suppose there is a polynomial $\|p' - f\| < \|p - f\|$
- Then $|p'(x_i) - f(x_i)| \le |p(x_i) - f$
- Therefore $p' - p$ must have $d+1$ zero
- Thus $p' - p = 0$ as it is a polynomial of degree d

125th Anniversary of Чебышев's birth



Чебышев polynomials

- Convergence is often exponential in d
  - The best approximation of degree $d-1$ over $[-1,1]$ to x^d is $p_{d-1}(x) \equiv x^d - \left(\frac{1}{2}\right)^{d-1} T_d(x)$
    - Where the Чебышев polynomials are
      $$T_d(x) = \cos\left(d \cos^{-1}(x)\right)$$
    - The notation is an old transliteration of Чебышев !
    - In general, truncated Чебышев L^2 approximation is not L^∞ optimal even for polynomials
  - The error is $\left\| x^d - p_d(x) \right\|_\infty = \left(\frac{1}{2}\right)^{d-1} \left\| T_d(x) \right\|_\infty = 2e^{-d \ln 2}$

Чебышев rational functions

- Чебышев's theorem is easily extended to rational approximations
  - Rational functions with nearly equal degree numerator and denominator are usually best
  - Convergence is still often exponential
  - Rational functions usually give a much better approximation

  - A simple (but somewhat slow) numerical algorithm for finding the optimal Чебышев rational approximation was given by Ремез

Чебышев rationals: Example

- A realistic example of a rational approximation is

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

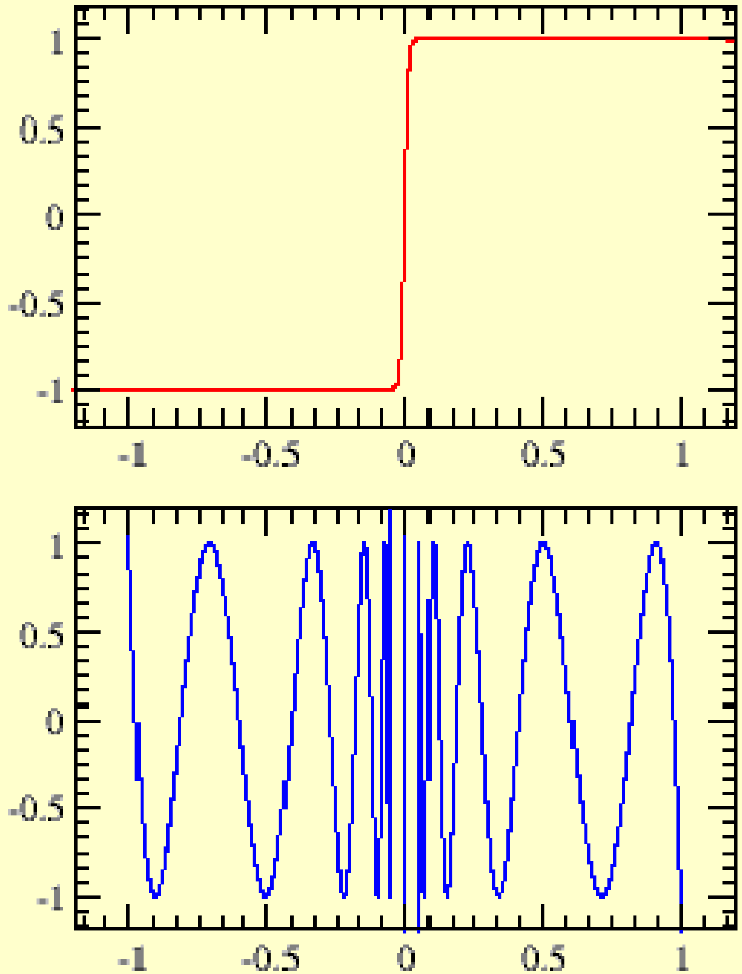
  - This is accurate to within almost 0.1% over the range $[0.003,1]$
- Using a partial fraction expansion of such rational functions allows us to use a multishift linear equation solver, thus reducing the cost significantly.
- The partial fraction expansion of the rational function above is

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

  - This appears to be numerically stable.

Чебышев rationals: Example

- $\mathrm{sgn}(x) = x\,R(x^2) + O(\Delta)$
- $\varepsilon < |x| < 1$
- $\varepsilon = 0.01$
- R of degree $(10,10)$
- $\Delta = 0.00437985$
- Coefficients are known in closed form in terms of elliptic functions (Золотарев)

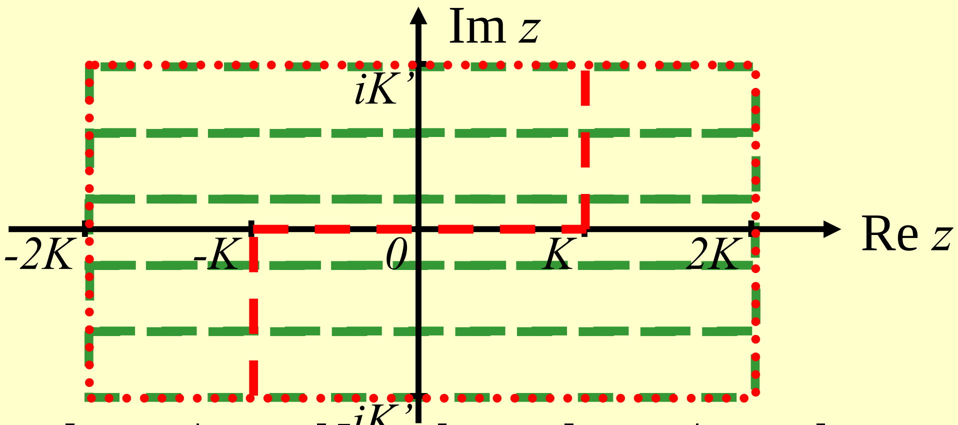


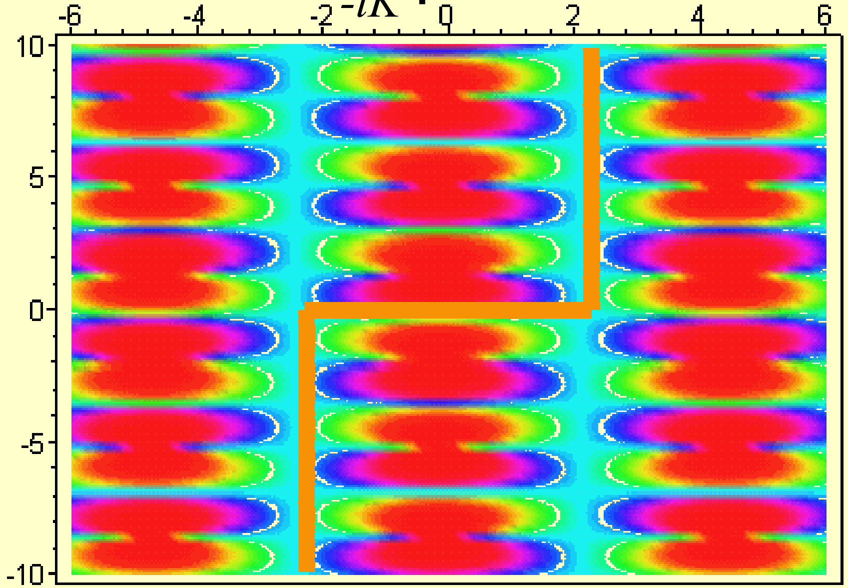
Золотарев's formula: I

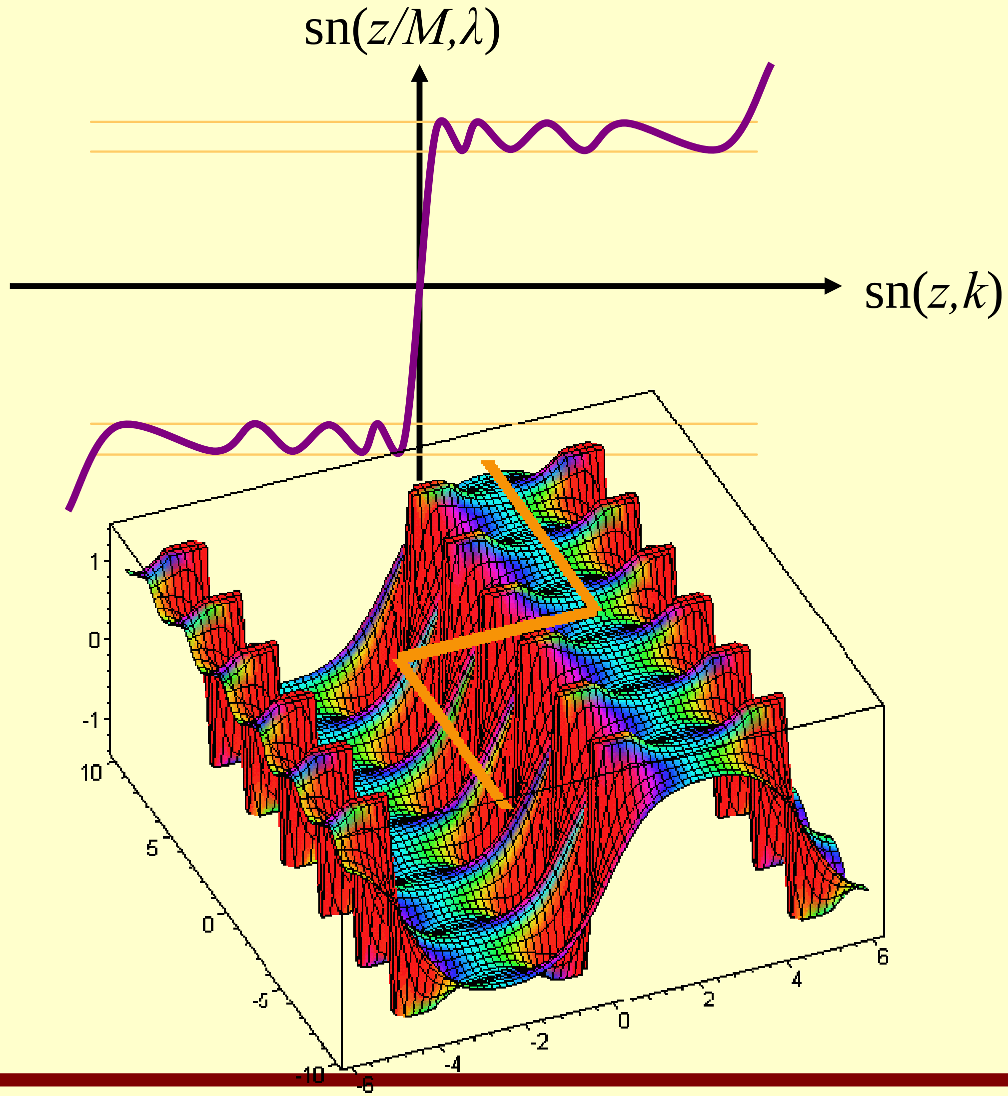
- Modular transformation of Jacobi elliptic functions of degree *n*

$$\frac{\operatorname{sn}(z/M;\lambda)}{\operatorname{sn}(z;k)} = \frac{1}{M}\prod_{m=1}^{\lfloor n/2 \rfloor} \frac{1-\dfrac{\operatorname{sn}(z;k)^2}{\operatorname{sn}(2iK'm/n;k)^2}}{1-\dfrac{\operatorname{sn}(z;k)^2}{\operatorname{sn}\left(2iK'\left(m-\frac{1}{2}\right)/n;k\right)^2}}$$

Золотарев's formula: II







Polynomials versus rationals

- Золотарев's formula has L_∞ error $\Delta \le e^{\frac{n}{\ln \varepsilon}}$
- Optimal L^2 approximation with weight $\dfrac{1}{\sqrt{1-x^2}}$ is

$$\sum_{j=0}^{n} \frac{(-)^j 4}{(2j+1)\pi} T_{2j+1}(x)$$

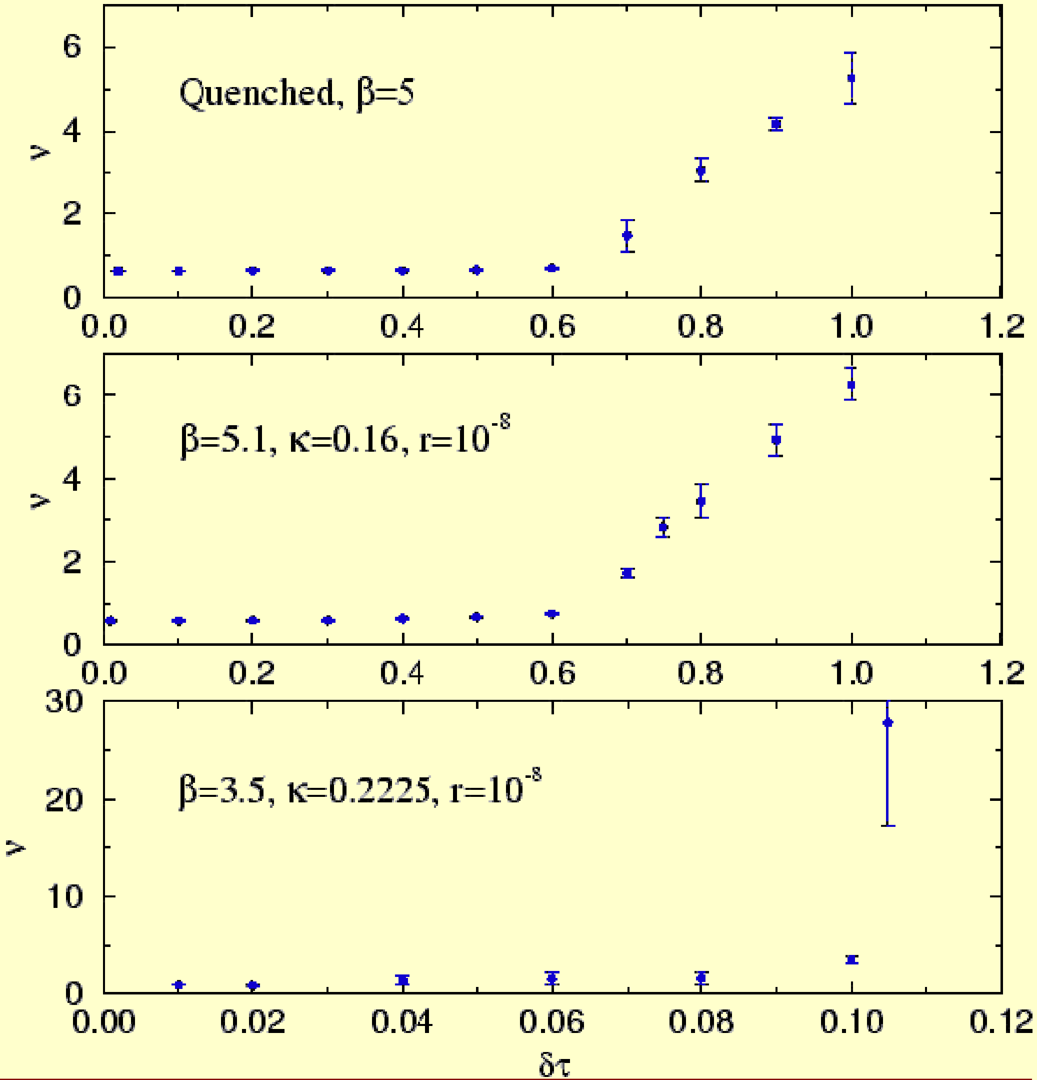
  - This has L^2 error of $O(1/n)$
- Optimal L^∞ approximation cannot be too much better (or it would lead to a better L^2 approximation)

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…

Instability of symplectic integrator

- Symmetry symplectic integrator
  - Leapfrog
    - Exactly reversible…
    - …up to rounding errors
- Ляпунов exponent ν
  - $\nu > 0 \ \forall \delta\tau$
    - Chaotic equations of motion (Liu & Jansen)
  - $\nu \propto \delta\tau$ when $\delta\tau$ exceeds critical value $\delta\tau_c$
    - Instability of integrator
  - $\delta\tau_c$ depends on quark mass



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

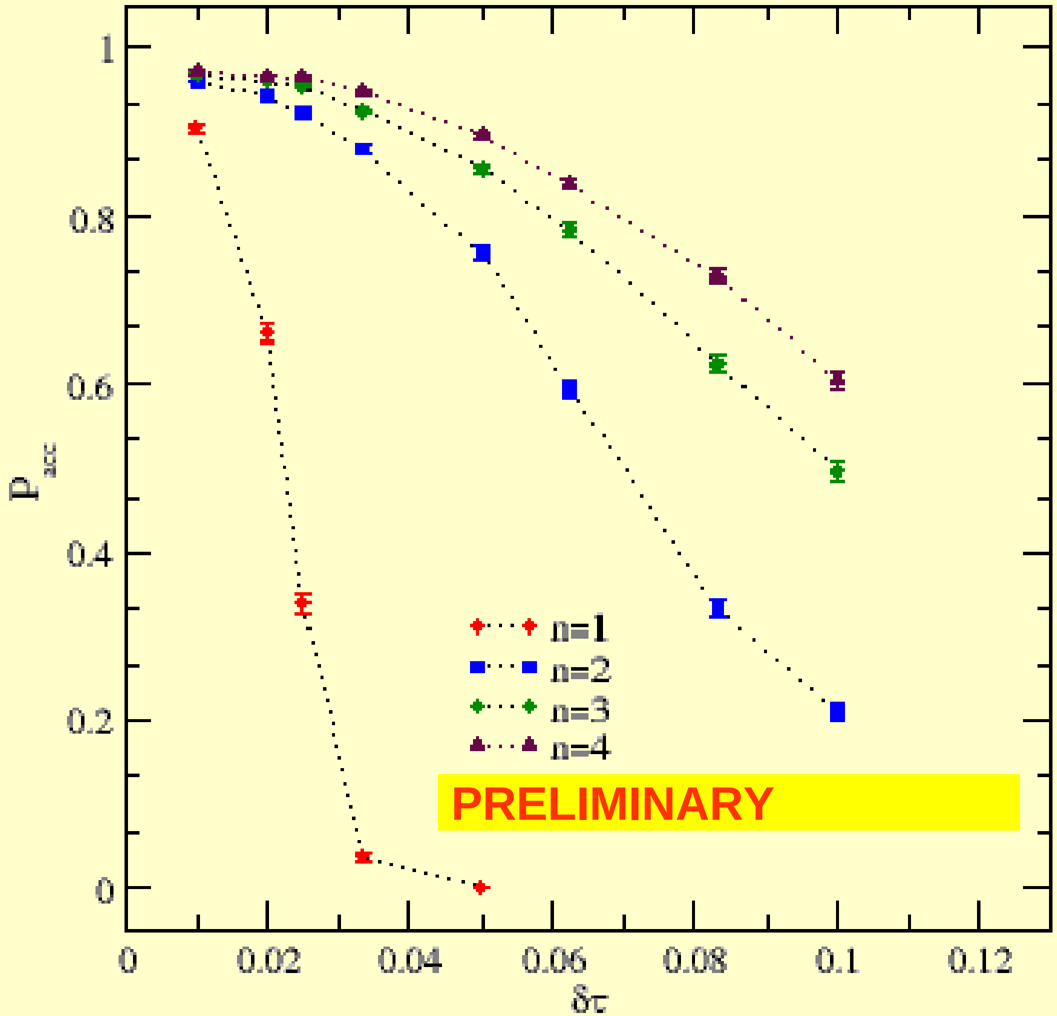
- Clever idea due to Hasenbusch
  - Start with the Wilson fermion action $M=1-\kappa H$
  - Introduce the quantity $M'=1-\kappa' H$
  - Use the identity $M = M'(M'^{-1}M)$
  - Write the fermion determinant as $\det M = \det M' \det (M'^{-1}M)$
  - Introduce separate pseudofermions for each determinant
  - 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
- Cost reduced by a factor of $n\kappa(M)^{(1/n)-1}$
  - Optimal value $n_{\mathrm{opt}} \approx \ln \kappa(M)$
  - So optimal cost reduction is $(e \ln\kappa)/\kappa$
- This works!
- Numerical results due to Mike Clark

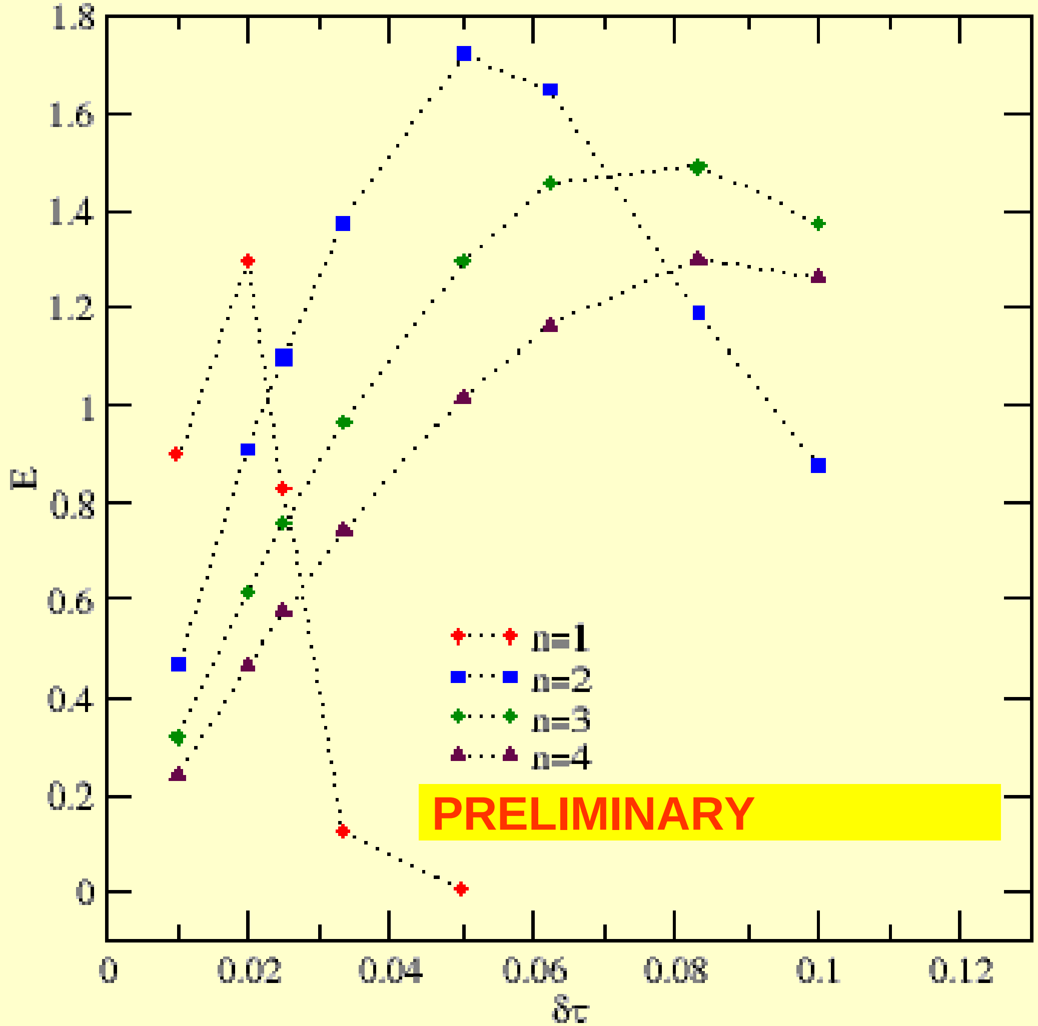
Acceptance rate at m=0.025

- 8^4 lattice
- $m=0.025$
- $\beta=5.26$
- $\tau=1.0$
- *4* flavours
- naïve staggered



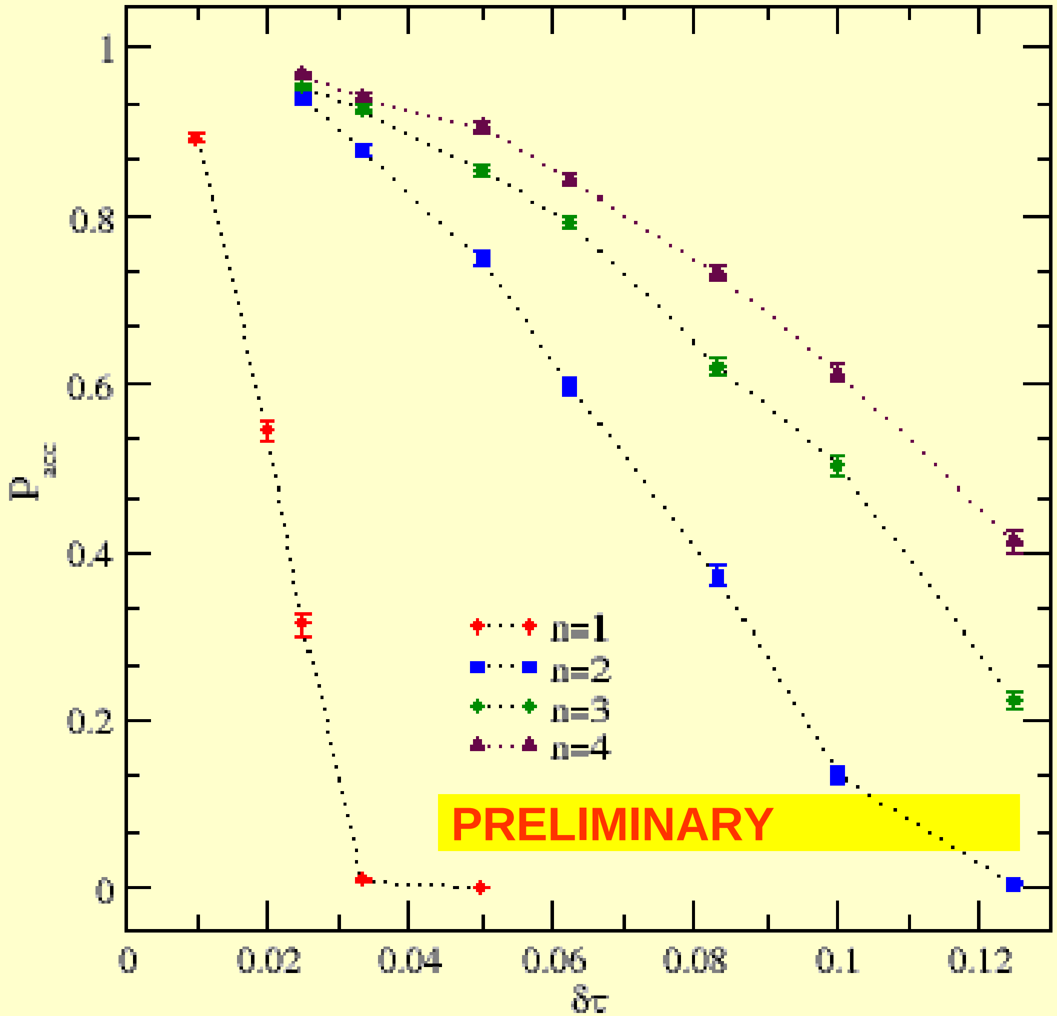
Efficiency at m=0.025

- 8^4 lattice
- $m=0.025$
- $\beta=5.26$
- $\tau=1.0$
- *4* flavours
- naïve staggered
- $n_{opt}=2$
- *33%* gain



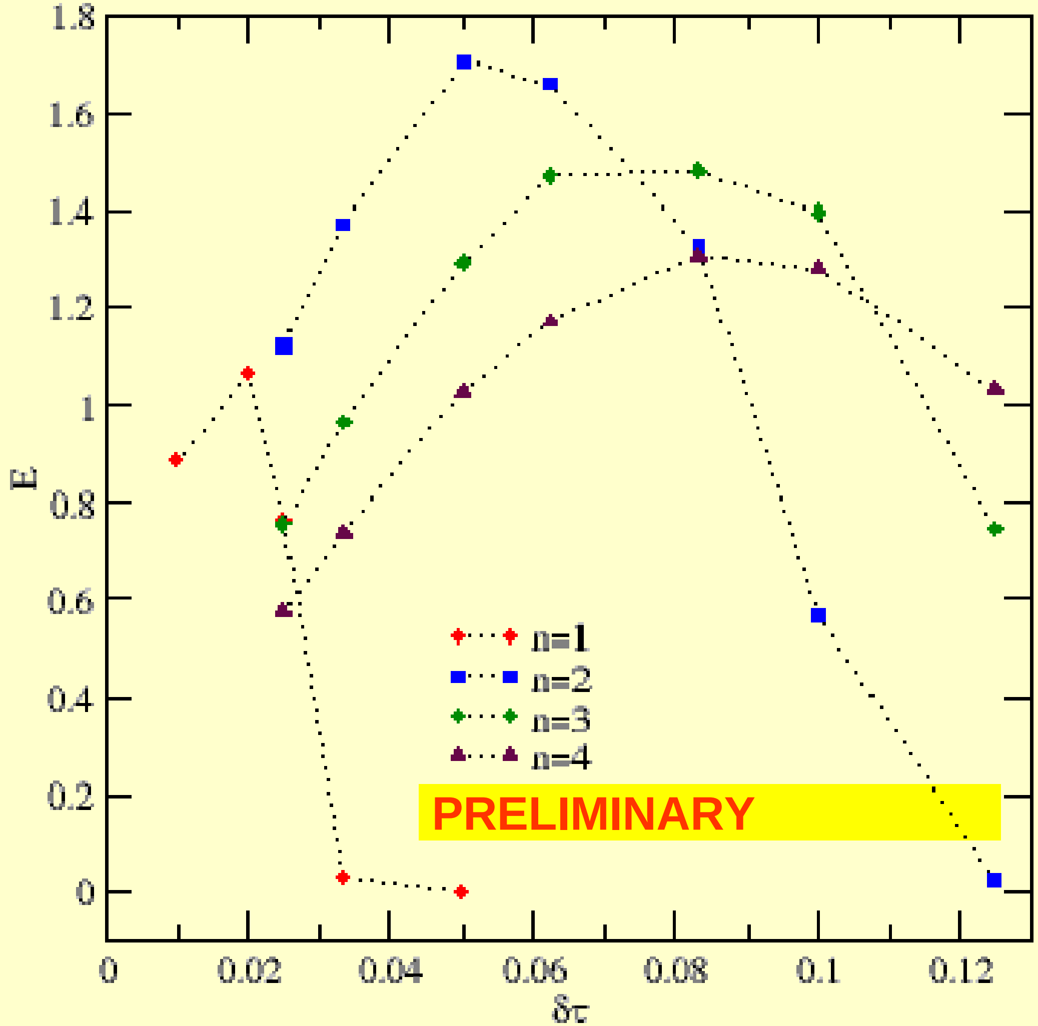
Acceptance rate at m=0.01

- *8⁴* lattice
- *m=0.01*
- *β=5.26*
- *τ=1.0*
- *4* flavours
- naïve staggered



Efficiency at m=0.01

- 8^4 lattice
- $m=0.01$
- $\beta=5.26$
- $\tau=1.0$
- 4 flavours
- naïve staggered
- $n_{opt}=2$
- 60% gain



RHMC technicalities

- In order to keep the algorithm exact to machine precision (as a Markov process)
  - Use a good (machine precision) rational approximation for the pseudofermion heatbath
  - Use a good rational approximation for the HMC acceptance test at the end of each trajectory
  - Use as poor a rational approximation as we can get away with to compute the MD force