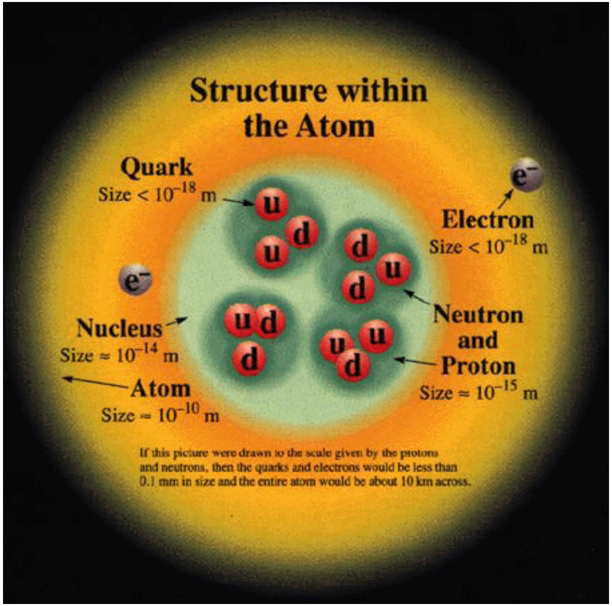
Computational Challenges in Lattice QCD

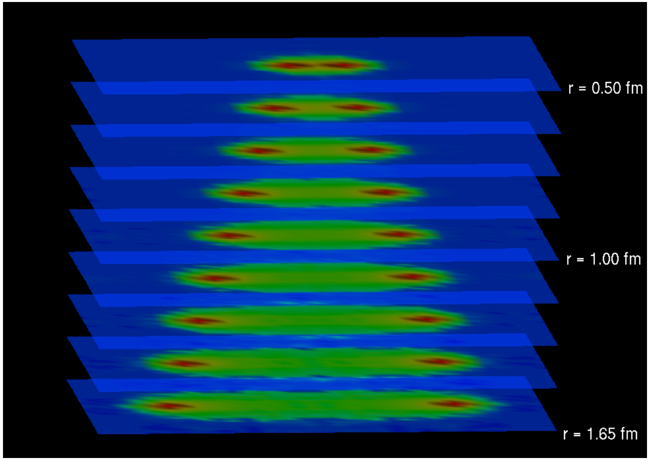
Andreas Frommer
Bergische Universität Wuppertal
Fachbereich Mathematik
frommer@math.uni-wuppertal.de
http://www.math.uni-wuppertal.de/SciComp

Outline

1. a page of physics . . .
2. a basic object: the Wilson fermion matrix
   - parameters
   - spectral and structural properties
3. stochastic simulation techniques
   - quenched
   - dynamical
4. (meanwhile) standard methods from linear algebra
   - multishift methods
5. overlap fermions
   - matrix sign function
   - nested iteration and inexact methods

A Page of Physics . . .

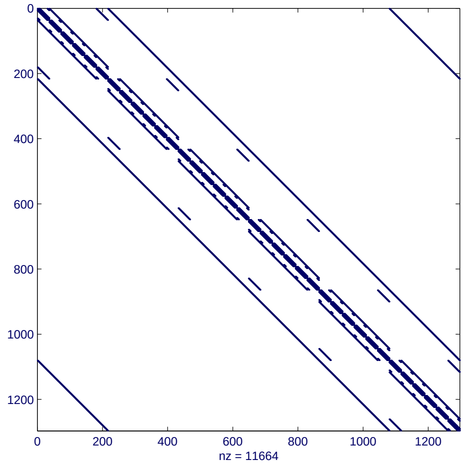




Back
Close

Basic Object: the Wilson Fermion Matrix

- $M = I - \kappa D$
- $M \in \mathbb{C}^{n \times n}$
- nearest neighbor coupling on 4-dimensional torus
- 12 variables per grid point
- $n = 12 \cdot n_1 \cdot n_2 \cdot n_3 \cdot n_4$
- $n_i = 16 \ldots 128$



$$(M\psi)_x = \psi_x - \kappa \left(\sum_{\mu=1}^{4} ((I - \gamma_\mu) \otimes U_\mu(x))\, \psi_{x+e_\mu} + \sum_{\mu=1}^{4} ((I + \gamma_\mu) \otimes U_\mu^H(x - e_\mu))\, \psi_{x-e_\mu} \right)$$

- $U_\mu(x) \in SU(3)$
- $\gamma_\mu \in \mathbb{C}^{4\times 4}$
- $I \pm \gamma_\mu$ is projector on 2-dimensional subspace

Highly structured matrix and coefficients

- $m_{x,x\pm e_\mu}\psi_{x\pm e_\mu}$ computed as $U\cdot\psi^{3\times4}\cdot(I\pm\gamma_\mu)$
  $\longrightarrow$ saves factor 2
- storage for $m_{x,x\pm e_\mu}$ is 9 complex numbers instead of 144
  $\longrightarrow$ saves factor 16
- 'BLAS3' on the registers' level

Symmetries of the Wilson fermion matrix

γ_5-Symmetry:

$$\Gamma_5 M = M^H \Gamma_5,$$

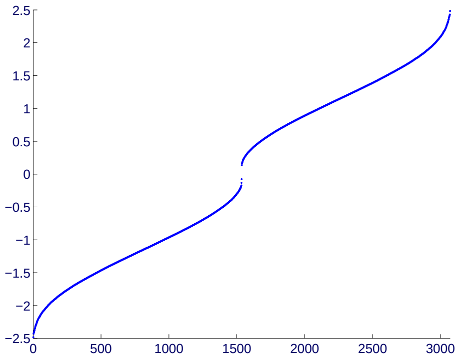
where Γ_5 simple permutation:

$$\Gamma_5 = I \otimes (\gamma_5 \otimes I_3),$$

$$\gamma_5 = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix} \text{ or } \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}.$$

Consequences:

- $\lambda \in \text{spec}(M) \Rightarrow \bar{\lambda} \in \text{spec}(M)$
- non-hermitian Lanczos process with Γ_5 instead of M^H
- $Q = \Gamma_5 M$ is hermitian (and maximally indefinite)

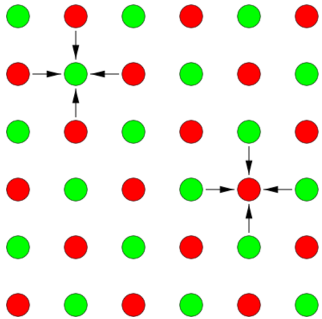


Odd-even Symmetry

- grid points x are even or odd (= red or green).
- odd-even-ordering yields

$$D = \begin{pmatrix} 0 & D_{oe} \\ D_{eo} & 0 \end{pmatrix}.$$

- Consequence:
  $\mu \in \text{spec}(D) \Rightarrow -\mu \in \text{spec}(D)$,
  $\lambda \in \text{spec}(M) \Rightarrow 2-\lambda \in \text{spec}(M)$

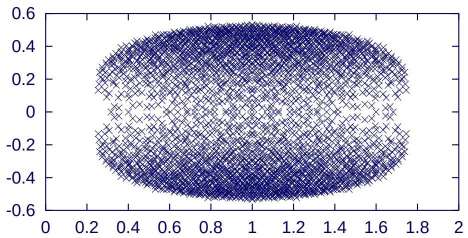


Spectrum of the Wilson fermion matrix

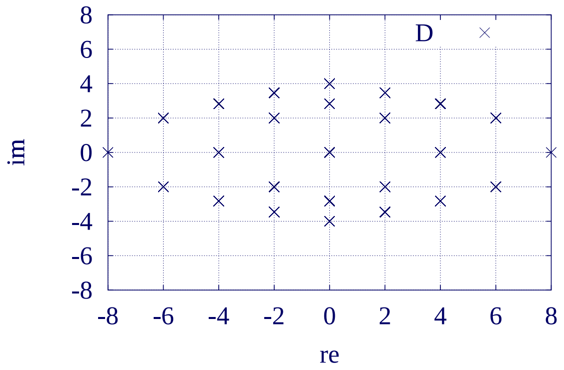
- M is positive real for $0 \leq \kappa < \kappa_c$.
- κ close to κ_c is interesting: relative quark mass

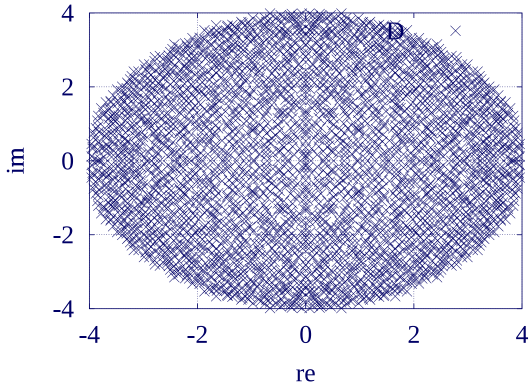
$$m_q = \frac{1}{2}\left(\frac{1}{\kappa} - \frac{1}{\kappa_c}\right),$$

becomes small.



spec(M) for 4^4 grid (realistic configuration)





spec(D) for cold ($U_\mu(x) = I$) and hot ($U_\mu(x)$ random) configuration

'Temperature' is controlled by parameter β.

Typical values: $5.0 - 6.0$; 'cold' $\Longleftrightarrow \beta = \infty$

Small eigenmodes are not smooth

- 'geometric' multigrid not available
- algebraic multigrid not (yet?) competitive [Medeke 99]

Stochastic Simulations

Statistical physics: compute values for physical observables Ω as

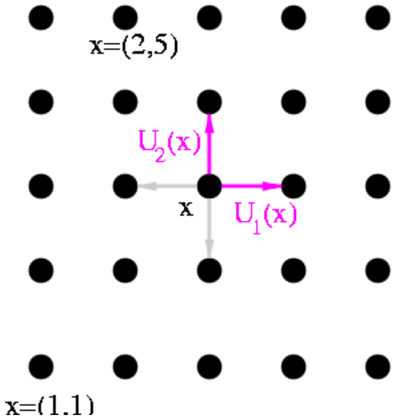
$$\langle\Omega\rangle = Z^{-1}\int \Omega(\Phi)e^{-S(\Phi)}d\Phi, \quad Z = \int e^{-S(\Phi)}d\Phi.$$

$\langle\Omega\rangle$: expected value, Φ: configuration, S: action

Challenge: Get good ensemble of configurations (small variance)

Lattice Gauge Theory

- QCD = standard theory of strong interaction between quarks
- lattice gauge theory = discretization of QCD



- approximation of gauge fields in Φ by configurations $\mathcal{U}$ of gauge links

$$\mathcal{U} = \{U_\mu(x) \mid x \in G, \mu = 1, \dots, 4\}.$$

Quenched vs Dynamical Simulations

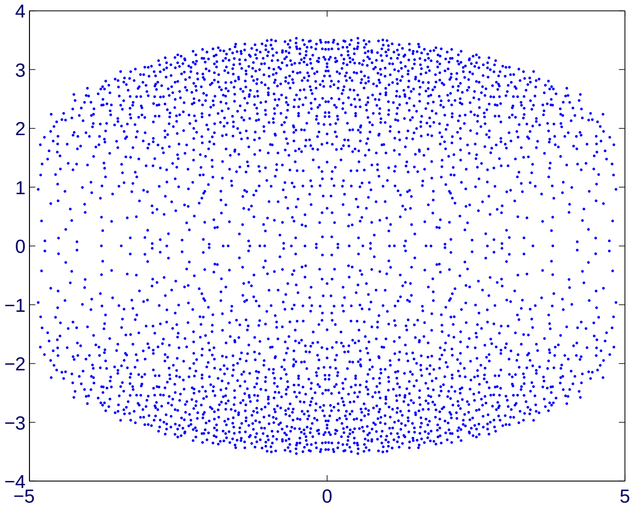
The Hybrid Monte-Carlo Method (HMC)

- generates a canonical ensemble of configurations (i.e. with distribution $Z^{-1}e^{-S(\mathcal{U})}$)
- includes
  - Metropolis acceptance test
  - leap frog integration scheme for ode's (exactly reversible in time)

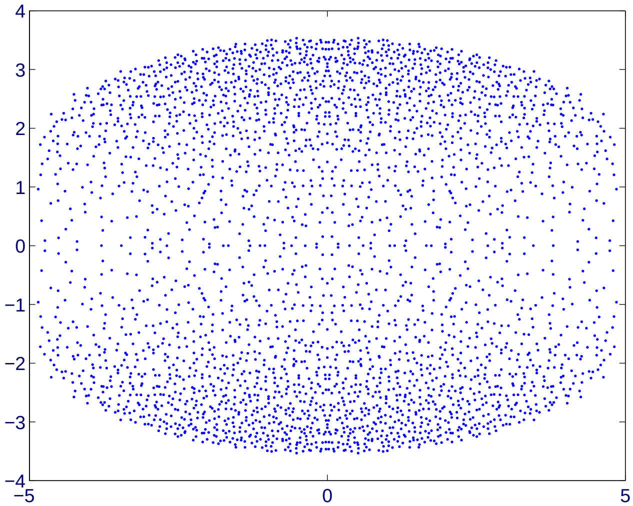
HMC comes in two flavours

- quenched: approximate fermionic part of S by a constant
  $\longrightarrow$ no linear system solves needed for generation of ensemble.
- dynamical: takes fermionic part of S into account
  $\longrightarrow$ each step in integrator requires solving systems with matrix $M = M(\mathcal{U})$.

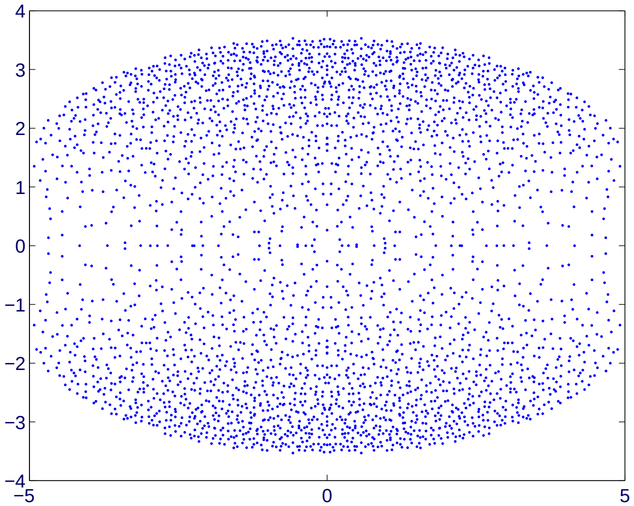
watch HMC on spec(M): Configuration 0



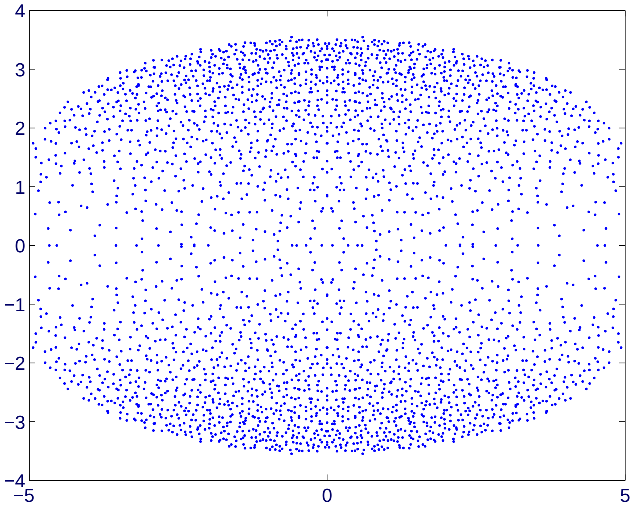
watch HMC on spec(M): Configuration 1000



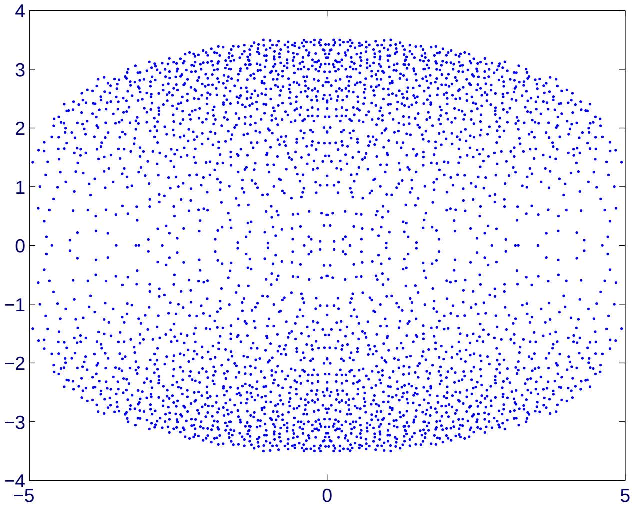
watch HMC on spec(M): Configuration 1400



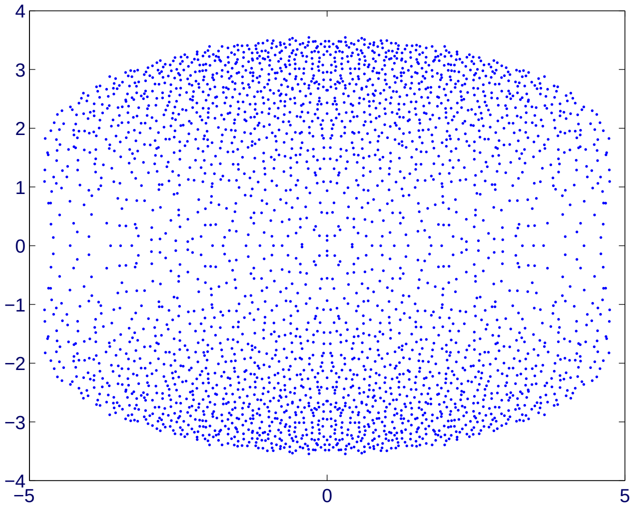
watch HMC on spec(M): Configuration 1800



watch HMC on spec(M): Configuration 2200



watch HMC on spec(M): Configuration 2600



Computational Effort

In Hybrid Monte Carlo one repeatedly solves very large linear systems.

```
for i = 1, ..., 100 000 do
    solve M(U_i)ψ_i = φ
    compute U_{i+1} from ψ_i
    store every 1000th conf. U_i
end for
```

Lattice QCD continues to be an HPC challenge.

- Earth Simulator (Japan)
- APE (Europe)
- QCDOC (USA-UK)
- cluster computers

Methods from Linear Algebra

Systems and Solvers

M positive real $\leftrightarrow$ $Q = \Gamma_5 M$ hermitian and indefinite

- Solve $Mx = b$ using non-hermitian solver
- Solve $Qx = \Gamma_5 b$ using hermitian indefinite solver
- Solve $M^H M y = M^H b$ using CGNR

A Recurring Theme: Shifted Systems

$$M = M(\kappa) = I - \kappa D.$$

Solve

$$\left(\frac{1}{\kappa} I - D\right) \psi = \varphi$$

for several values of κ.

Observation: Krylov subspaces independent of κ.

Potential: Solve

- for several κ at the same time

with

- just one matrix vector multiplication per step for all systems.

Multishift methods:

'one Lanczos for all' approach:

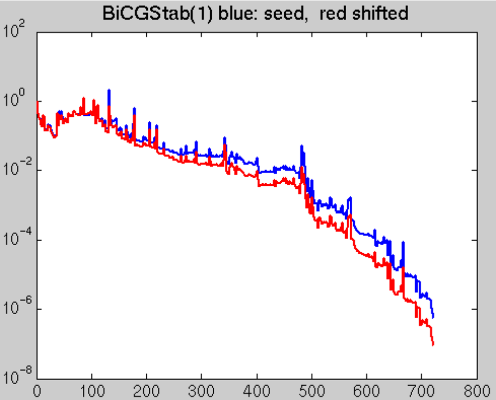
- shifted CG
- shifted QMR (Freund)
- shifted Chebyshev
- shifted BiCG
- shifted restarted FOM (Simoncini)

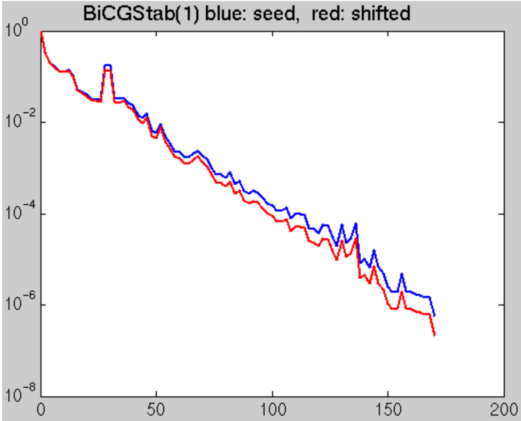
'colinear residual' approach:

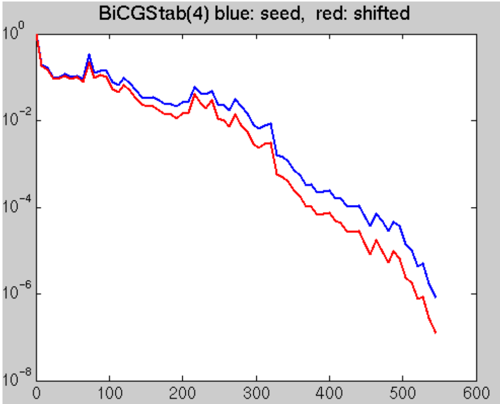
- shifted GMRES(k) (F. and Glässner)
- shifted BiCGstab (Jegerlehner)
- shifted BiCGstab(ℓ) (F.)

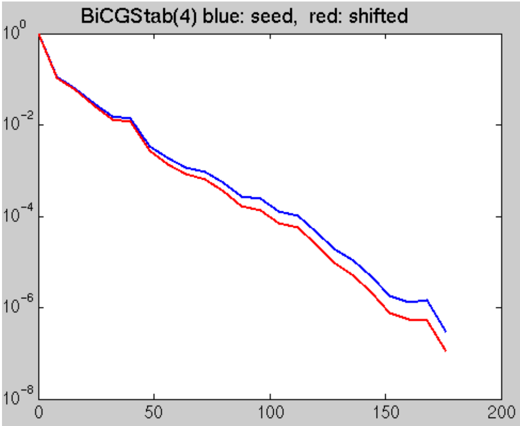
Example theorem [F., Glässner 98, F. 03]:
Perform true GMRES(k) for largest $\kappa < \kappa_c$
$\longrightarrow$
shifted method converges faster for all other values of κ.

Example: shifted BiCGstab(1), BiCGStab(4)









$\kappa_1 = 0.180, \kappa_2 = 0.176$ $\kappa_1 = 0.176, \kappa_2 = 0.170$

Back
Close

Restarted GMRES: Deflation becomes important
(Baglama, Calvetti, Golub, Reichel; Morgan)

Preconditioning

For Wilson fermion matrix M:

SSOR-preconditioning = ILU(0)-preconditioning

since $(I + \gamma_\mu)(I - \gamma_\mu) = 0$.

SSOR preconditioning of the odd-even ordered matrix is standard.
('Odd-even reduced system')

$$\left(I - \kappa^2 D_{eo} D_{oe}\right) \psi_e \;=\; \widetilde{\varphi}_e$$

Parallelizes well, no cost $\rightarrow$ factor 2-3 improvement.

Overlap Fermions

Chiral symmetry is an important physical property which should be reflected in the discretized operator N.

- Ginsparg-Wilson relation (= algebraic Riccati equation) is sufficient condition
- **Wilson fermion matrix:** No chiral symmetry
- **Overlap fermions (Neuberger, 1998):** fulfill Ginsparg-Wilson relation.
- Chiral symmetry breaking is related to non-normality of operator

The Overlap Operator

$$
\begin{aligned}
N &= I + (1-\mu)\cdot M \cdot (M^H M)^{-1/2} \\
&= I + (1-\mu)\cdot \Gamma_5 \mathrm{sign}(Q)
\end{aligned}
$$

where

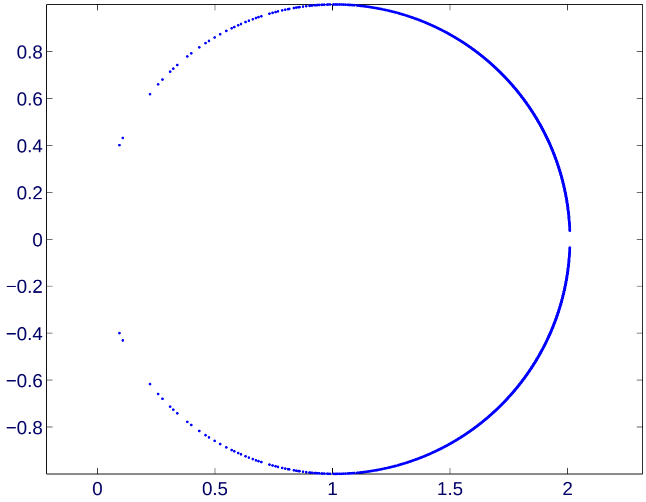
$Q = \Gamma_5 \cdot M \quad \Rightarrow Q^H = Q$

κ in Q significantly larger

$\mathrm{sign}(Q) = V \mathrm{sign}(\Lambda) V^H$ where $Q = V \Lambda V^H$

$\mathrm{sign}(Q) = Q \cdot \left(Q^2\right)^{-1/2}$

$0 \leq \mu << 1$



spectrum of $N = I + 0.99 * (\Gamma_5 \cdot \mathrm{sign}(Q))$

Back
Close

The overlap operator $N = I + (1 - \mu) \cdot \Gamma_5 \text{sign}(Q)$:

- respects chiral symmetry
- is represented by a dense matrix
  $\Rightarrow$ cannot be determined explicitly
- nested iteration for

$$(I + (1 - \mu) \cdot \Gamma_5 \text{sign}(Q))\, \psi = \phi$$

  – outer iteration: MVM with N
  – inner iteration: approximate $\text{sign}(Q)b$ in Nb

Krylov Subspace Approx. for sign$(Q)b$

$$K_m(Q,b) = \text{span}\{b, Qb, Q^2b, \ldots, Q^{m-1}b\}$$

Lanczos Based Methods

- **[van der Vorst 99]** Let P_m be orthogonal projection on $K_m(Q,b)$:

$$x^m = P_m^H \cdot \text{sign}(P_m Q P_m^H) \cdot P_m b \ \ (= p_m(Q)b)$$

  [Borici 99] Put

$$x^m = QP_m^H \cdot \left(P_m Q^2 P_m^H\right)^{-1/2} \cdot P_m b \ \ (= p_{m+1}(Q)b)$$

- **[Borici 99]** Let P_m be orthogonal projection on $K_m(Q^2, b)$

$$x^m = QP_m^H \cdot \left(P_m Q^2 P_m^H\right)^{-1/2} \cdot P_m b \ \ (= p_{2m+1}(Q)b)$$

Stopping Criterion

Lanczos for $K_m(Q^2, b)$variant:

Theorem [van den Eshof et al. 02]: We have

$$\begin{aligned}\|QP_m^H \cdot \left(P_m Q^2 P_m^H\right)^{-1/2} \cdot P_m b - \mathsf{sign}(Q) b\|_2 &\leq \|r_k\|_2 \\ &\leq 2\kappa \left(\frac{\kappa - 1}{\kappa + 1}\right)^k \cdot \|b\|_2,\end{aligned}$$

where

$$\kappa = \frac{b}{a}, \quad \mathsf{spec}(Q) \subseteq [-b, -a] \cup [a, b]$$

r_k k-th residual of CG for $Q^2 x = b$, $x^0 = 0$.

Rational Approximations

Idea: Approximate

$$\text{sign}(t) \approx r(t) = \sum_{i=1}^{m} \omega_i \frac{t}{t^2 + \tau_i} \in R_{2m-1,2m}.$$

Then

$$\text{sign}(Q)b \approx r(Q)b = \sum_{i=1}^{m} \omega_i Q \left(Q^2 + \tau_i I\right)^{-1} b.$$

Solve all these m systems in one stroke
('Multishift CG') since

$$K_m(Q^2, b) = K_m(Q^2 + \tau_i I, b), \; i = 1, 2, \ldots, m.$$

Theorem [Zolotarev]: The (l_∞-) best approximation to $\operatorname{sign}(t)$ on $[-b/a, -1] \cup [1, b/a]$ from $R_{2m-1,2m}$ is

$$r(t) = ts(t^2) \quad \text{where} \quad s(t) = D\frac{\prod_{i=1}^{m-1}(t + c_{2i})}{\prod_{i=1}^{m}(t + c_{2i-1})},$$

and

$$c_i = \frac{\mathrm{sn}^2\left(iK/(2m); \sqrt{1-(b/a)^2}\right)}{1 - \mathrm{sn}^2\left(iK/(2m); \sqrt{1-(b/a)^2}\right)},$$

K complete elliptic integral

D determined through

$$\max_{t\in[1,(b/a)^2]}\left(1 - \sqrt{t}s(t)\right) = -\min_{t\in[1,(b/a)^2]}\left(1 - \sqrt{t}s(t)\right).$$

[Kenny and Laub, van den Eshof et al. 02]

Comparison of methods

Conf.	1	2	3	4	5

Lanczos/PFE

MVs	2281	1969	1953	1853	1769
time/s	150	131	129	124	118

PFE/CG Zolotarev without removal

MVs	1141	985	977	927	885
time/s	154	125	125	116	102

PFE/CG Zolotarev with removal

MVs	1205	1033	1033	971	927
time/s	122	93	97	87	79

Nested Iteration

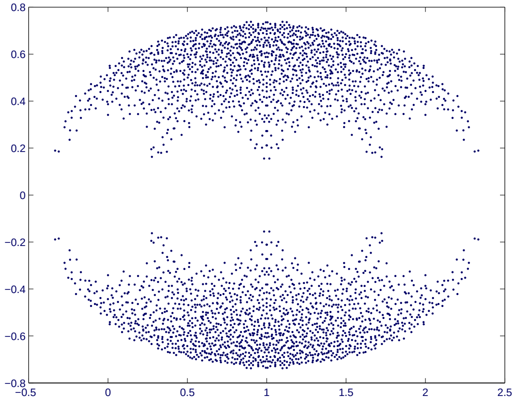
Solve

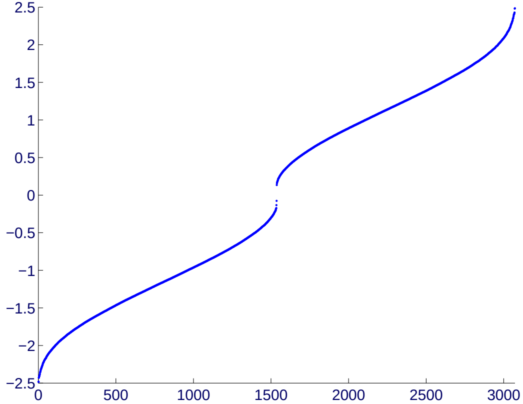
$$(I + (1-\mu)\cdot\Gamma_5\text{sign}(Q))x = b$$

Operators

- $N_u = I + (1-\mu)\cdot\Gamma_5\text{sign}(Q)$ shifted unitary
  SUMR (Jagels and Reichel)
- $N_h = \Gamma_5 + (1-\mu)\text{sign}(Q)$ hermitian indefinite
  MINRES, SYMMLQ
- $N_n = N_u N_u^H = N_h^2$ hermitian positive definite
  CGNE

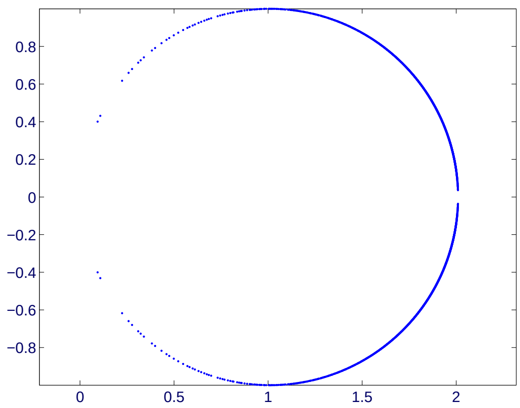
spectra of the operators

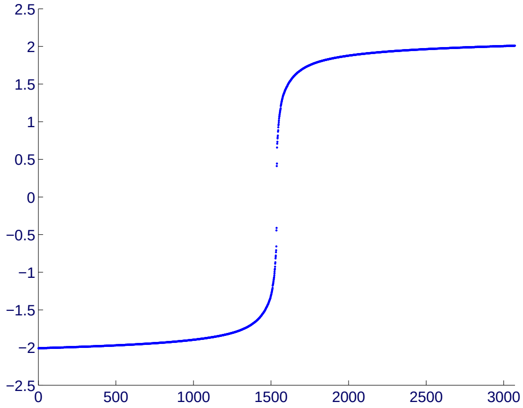




M Q

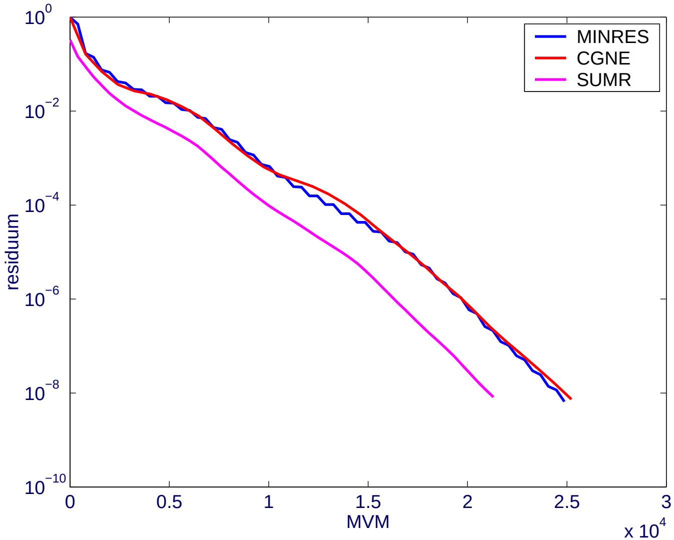
Back
Close


0.8
0.6
0.4
0.2
0
−0.2
−0.4
−0.6
−0.8
0
0.5
1
1.5
2


2.5
2
1.5
1
0.5
0
−0.5
−1
−1.5
−2
−2.5
0
500
1000
1500
2000
2500
3000

N_u N_h

Performance of methods on 4^4 lattice



Relaxation strategies:

- sign$(Q)b$ is required less accurately as iteration starts to converge
  [Fraysse and Bouras]
- Can be justified theoretically
  [Simoncini and Szyld, van den Eshof and Sleijpen]
- Can be implemented practically

Goal: (Outer) residual norm $\leq \varepsilon$.

Accuracy:

$$\|\text{sign}(Q)y_j - \hat{y}_j\| \leq \eta_j \varepsilon \|y_j\|$$

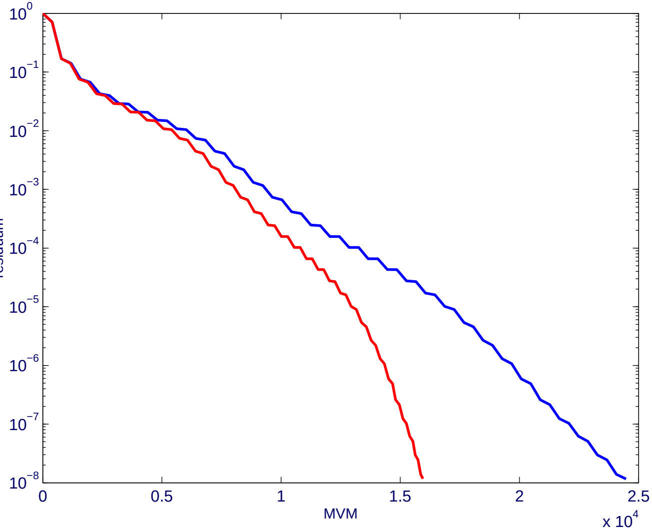
Analysis:

$$\|\underbrace{b - Ax_k}_{\text{true residual}}\| \leq \|\underbrace{r_k - (b - Ax_k)}_{\text{residual gap}}\| + \|\underbrace{r_k}_{\text{computed residual}}\|$$

Required accuracy of inner iteration for outer precision ε

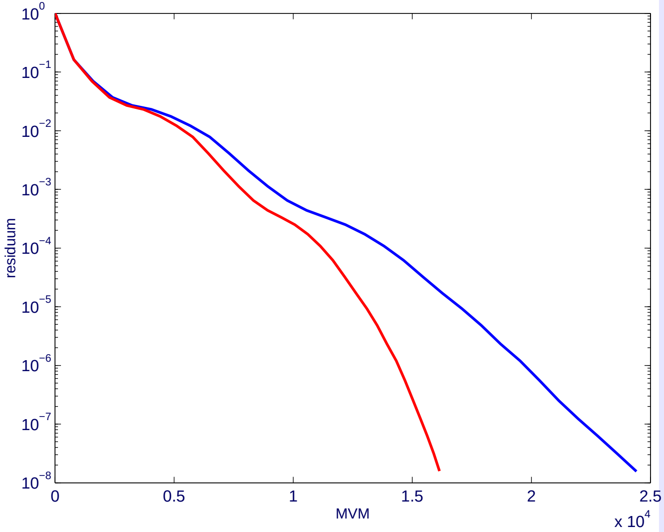
Matrix prop.	Proposed method	Tolerance η_j
herm. indefinite	MINRES	$\eta_j = \|r_j\|^{-1}$
	Rutishauser's CG	$\eta_j = \sqrt{\sum_{i=0}^{j} \|r_i\|^{-2}}$
shifted unitary	SUMR	$\eta_j = \|r_j\|^{-1}$
herm. pos. def.	CG	$\eta_j = \sqrt{\sum_{i=0}^{j} \|r_i\|^{-2}}$

[van den Eshof, Sleijpen]



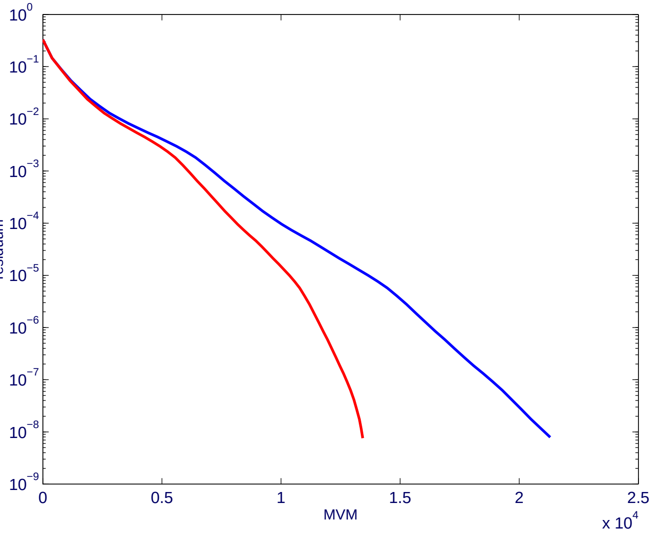
10^0
10^−1
10^−2
10^−3
10^−4
10^−5
10^−6
10^−7
10^−8
0
0.5
1
1.5
2
2.5
MVM
x 10^4

MINRES

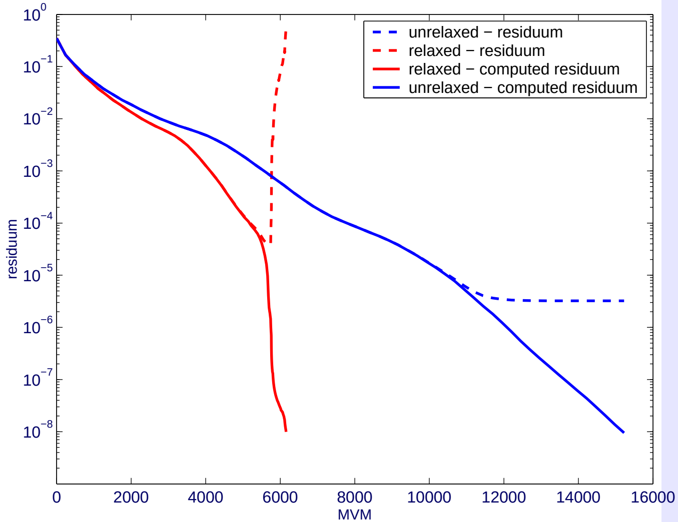


residuum
10^0
10^−1
10^−2
10^−3
10^−4
10^−5
10^−6
10^−7
10^−8
0
0.5
1
1.5
2
2.5
MVM
x 10^4

CGNE



SUMR



SUMR, wrong relaxation

Conclusions

- Lattice QCD requires enormous computations
- Petaflops computers
- Simulations become increasingly realistic
- Efficient iterative solvers are very important
- Problems are highly structured but/and stochastic
- Significant algorithmic improvements, but no breakthroughs
- Improve integrators?
- Lattice QCD physicists use new methods from numerical linear algebra

Last words:

- Solving the Wilson fermion matrix with BiCGstab is part of the SPEC98 high performance benchmark suite
- Some Wilson fermion matrices are available at the Matrix Market: math.nist.gov/MatrixMarket/data/misc/qcd/qcd.html