Chiral Fermions on the Lattice:
A Flatlander's Ascent into Five Dimensions

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QCD on the Lattice

Quantumchromodynamics is formally described by the Lagrange density:

$$\mathcal{L}_{\text{QCD}} = \bar{\psi}(i\not{D} - m_q)\psi - \frac{1}{4} G_{\mu\nu} G^{\mu\nu}$$

- Non-perturbative, gauge invariant regularisation
- Lattice regularization: discretize Euclidean space-time
- Continuum limit $\Rightarrow a \to 0$
  - Poincaré symmetries are restored automatically
  - Naive discretisation of Dirac operator introduces doublers $\Rightarrow$ restoration of chiral symmetry requires fine tuning

On-shell chiral symmetry

- It is possible to have chiral symmetry on the lattice without doublers if we only insist that the symmetry holds on-shell
- Such a transformation should be of the form

$$\psi \to e^{i\alpha\gamma_5(1-aD)}\psi; \quad \overline{\psi} \to \overline{\psi}e^{i\alpha(1-aD)\gamma_5}$$

and the Dirac operator must be invariant:

$$D \to e^{i\alpha(1-aD)\gamma_5} D e^{i\alpha\gamma_5(1-aD)} = D$$

- For an infinitesimal transformation this implies that

$$(1 - aD)\gamma_5 D + D\gamma_5(1 - aD) = 0$$

which is the Ginsparg-Wilson relation

$$\gamma_5 D + D\gamma_5 = 2aD\gamma_5 D$$

Overlap Dirac operator I

- We can find a solution D_{GW} of the Ginsparg-Wilson relation as follows:
  - Let the lattice Dirac operator be of the form

$$aD_{GW} = \frac{1}{2}(1 + \gamma_5 \hat{\gamma}_5); \quad \hat{\gamma}_5^\dagger = \hat{\gamma}_5; \quad aD_{GW}^\dagger = \gamma_5 aD_{GW} \gamma_5$$

    This satisfies the GW relation if $\hat{\gamma}_5^2 = 1$
  - And it must have the correct continuum limit

$$D_{GW} \to \not{\partial} \Rightarrow \hat{\gamma}_5 = \gamma_5(2a\not{\partial} - 1) + O(a^2)$$

  - Both conditions are satisfied if we define

$$\hat{\gamma}_5 = \gamma_5 \frac{D - \rho}{\sqrt{(D-\rho)^\dagger (D-\rho)}} = \text{sgn}\left[\gamma_5 (D - \rho)\right]$$

Overlap Dirac operator II

- The resulting overlap Dirac operator:

$$D(H) = \frac{1}{2}(1 + \gamma_5 \mathrm{sgn}\,[H(-\rho)])$$

  - has exact zero modes with exact chirality $\Rightarrow$ index theorem
  - no additive mass renormalisation, no mixing
- Three different variations:
  - Choice of kernel
  - Choice of approximation:
    - polynomial approximations, e.g. Chebyshev
    - rational approximations $\mathrm{sgn}(H) \simeq R_{n,m}(H) = \frac{P_n(H)}{Q_m(H)}$
  - Choice of representation:

    $\Rightarrow$ continued fraction, partial fraction, Cayley transform

Kernel choices

- Simplest choice is the Wilson kernel $H_W = \gamma_5 D_W(-\rho)$
- Domain wall fermion kernel is

$$H_T = \gamma_5 D_T; \quad D_T = \frac{D_W(-\rho)}{2 + aD_W(-\rho)}$$

- The generic Moebius kernel interpolates between the two:

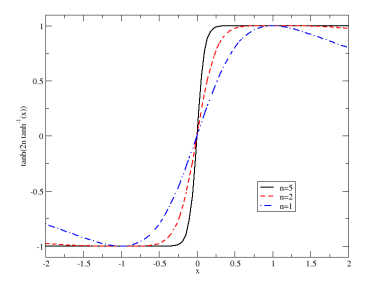
$$H_M = \gamma_5 D_M; \quad D_M = \frac{(b+c)D_W(-\rho)}{2 + (b-c)aD_W(-\rho)}$$

- Use UV-filtered covariant derivative:
  - overlap operator becomes more local
  - no tuning of ρ, better scaling, cheaper,. . .

Tanh Approximation

- Use a tanh expressed as a rational function $\mathrm{sgn}(x) \simeq R_{2n-1,2n}(x)$:

$$\tanh\left(2n\tanh^{-1}(x)\right) = \frac{(1+x)^{-2n} - (1-x)^{-2n}}{(1+x)^{-2n} + (1-x)^{-2n}}$$



Properties:

$$\begin{aligned} f(x)|_{x=0} &= 0 \\ \lim_{x\to\infty} f(x) &= 0 \\ f(x) &= f(1/x) \end{aligned}$$

Zolotarev's Approximation I

- By means of Zolotarev's theorem we have:

$$\mathrm{sn}\left(\frac{u}{M},\lambda\right) = \frac{\mathrm{sn}(u,k)}{M} \prod_{r=1}^{[\frac{n}{2}]} \frac{1+\frac{\mathrm{sn}^2(u,k)}{c_{2r}}}{1+\frac{\mathrm{sn}^2(u,k)}{c_{2r-1}}}$$

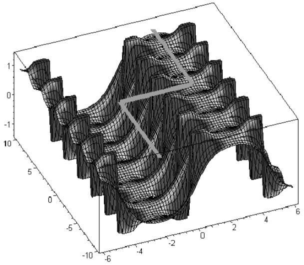
  - ◇ $c_r = \frac{\mathrm{sn}^2(\frac{rK'}{n},k'^2)}{1-\mathrm{sn}^2(\frac{rK'}{n},k'^2)}$
  - ◇ $\xi = \mathrm{sn}(u,k)$ is the Jacobian elliptic function defined by the elliptic integral

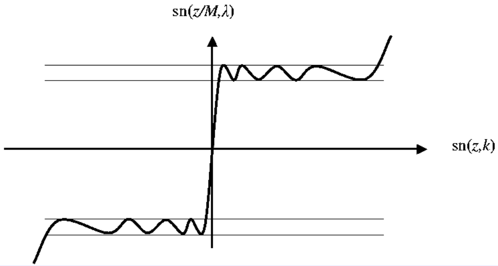
$$u = \int_0^{\xi} \frac{dt}{\sqrt{(1-t^2)(1-k^2t^2)}}, \; 0 < k < 1.$$

- Setting $x = k \cdot \mathrm{sn}(u,k)$ we obtain the best uniform rational approximation on $[-1,-k] \cup [k,1]$:

Zolotarev's Approximation II

$$\mathrm{sgn}(x) \simeq R_{n+1,n}(x) = (1-l)\frac{x}{kD}\prod_{r=1}^{[\frac{n}{2}]}\frac{x^2+k^2c_{2r}}{x^2+k^2c_{2r-1}}$$





Cayley Transform Representation

- Represent the rational function as a Euclidean Cayley transform:

$$R(x) = \frac{1 - T(x)}{1 + T(x)}$$

- It is an involutive automorphism,

$$T(x) = \frac{1 - R(x)}{1 + R(x)},$$

and the oddness of $R(x)$ translates into the logarithmic oddness of $T(x)$ and vice versa,

$$R(-x) = -R(x) \Longleftrightarrow T(-x) = T^{-1}(x)$$

- How do you evaluate this?

Continued Fraction Representation

- Continued fraction is obtained by applying Euclid's division algorithm:

$$\mathrm{sgn}(x) \simeq R_{2n+1,2n}(x) = k_0 x + \cfrac{1}{k_1 x + \cfrac{\cdots}{\cdots + \cfrac{1}{k_{2n-1} x + \cfrac{1}{k_{2n} x}}}}$$

where the k_i's are determined by the approximation.

- How do you evaluate this?

Partial Fraction Representation

- Partial fraction decomposition is obtained by matching poles and residues:

$$\mathrm{sgn}(x) \simeq R_{2n+1,2n}(x) = x\left(c_0 + \sum_{k=1}^{n} \frac{c_k}{x^2 + q_k}\right)$$

  - use a multi-shift linear system solver
- Physics requires inverse of $D(\mu)$ (propagators, HMC force)
  - leads to a *two level nested* linear system solution
- How can this be avoided?
  - introduce auxiliary fields $\Rightarrow$ extra dimension
  - five-dimensional representation of the *sgn*–function
  - nested Krylov space problem reduces to *single* 5d Krylov space solution

Schur Complement

- Consider the block matrix $\begin{pmatrix} A & B \\ C & D \end{pmatrix}$
  - It may be block diagonalised by a LDU decomposition (Gaussian elimination)

$$\begin{pmatrix} 1 & 0 \\ CA^{-1} & 1 \end{pmatrix} \cdot \begin{pmatrix} A & 0 \\ 0 & D - CA^{-1}B \end{pmatrix} \cdot \begin{pmatrix} 1 & A^{-1}B \\ 0 & 1 \end{pmatrix}$$

  - The bottom right block is the Schur complement
  - In particular we have

$$\det \begin{pmatrix} A & B \\ C & D \end{pmatrix} = \det(A) \det(D - CA^{-1}B)$$

Continued fractions I

- Consider a five-dimensional matrix of the form

$$\begin{pmatrix} A_0 & 1 & 0 & 0 \\ 1 & A_1 & 1 & 0 \\ 0 & 1 & A_2 & 1 \\ 0 & 0 & 1 & A_3 \end{pmatrix}$$

and its LDU decomposition where $S_0 = A_0; \; S_n + \frac{1}{S_{n-1}} = A_n$

$$\begin{pmatrix} 1 & 0 & 0 & 0 \\ S_0^{-1} & 1 & 0 & 0 \\ 0 & S_1^{-1} & 1 & 0 \\ 0 & 0 & S_2^{-1} & 1 \end{pmatrix} \begin{pmatrix} S_0 & 0 & 0 & 0 \\ 0 & S_1 & 0 & 0 \\ 0 & 0 & S_2 & 0 \\ 0 & 0 & 0 & S_3 \end{pmatrix} \begin{pmatrix} 1 & S_0^{-1} & 0 & 0 \\ 0 & 1 & S_1^{-1} & 0 \\ 0 & 0 & 1 & S_2^{-1} \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

- The Schur complement of the matrix is the continued fraction

$$S_3 = A_3 - \frac{1}{S_2} = A_3 - \frac{1}{A_2 - \frac{1}{S_1}} = A_3 - \frac{1}{A_2 - \frac{1}{A_1 - \frac{1}{A_0}}}$$

Continued fractions II

- We may use this representation to linearise our continued fraction approximation to the sign function:

$$\mathrm{sgn}_{n-1,n}(H) = k_0 H + \cfrac{1}{k_1 H + \cfrac{1}{k_2 H + \ddots + \cfrac{1}{k_n H}}}$$

as the Schur complement of the five-dimensional matrix

$$\begin{pmatrix} k_0 H & 1 & & & & \\ 1 & -k_1 H & 1 & & & \\ & 1 & k_2 H & & & \\ & & & \ddots & 1 & \\ & & & 1 & -k_n H \end{pmatrix}$$

Continued fractions II

- We may use this representation to linearise our continued fraction approximation to the sign function:

$$\mathrm{sgn}_{n-1,n}(H) = k_0 H + \cfrac{c_1}{c_1 k_1 H + \cfrac{c_1 c_2}{c_2 k_2 H + \ddots + \cfrac{c_{n-1} c_n}{c_n k_n H}}}$$

as the Schur complement of the five-dimensional matrix

$$\begin{pmatrix} k_0 H & c_1 & & & \\ c_1 & -c_1^2 k_1 H & c_1 c_2 & & \\ & c_1 c_2 & c_2^2 k_2 H & & \\ & & & \ddots & c_{n-1} c_n \\ & & & c_{n-1} c_n & -c_n^2 k_n H \end{pmatrix}$$

  - Class of operators related through equivalence transformations parametrised by c_i's

Partial fractions

- Consider a five-dimensional matrix of the form:

$$\begin{pmatrix} A_1 & 1 & 0 & 0 & 1 \\ 1 & -B_1 & 0 & 0 & 0 \\ 0 & 0 & A_2 & 1 & 1 \\ 0 & 0 & 1 & -B_2 & 0 \\ -1 & 0 & -1 & 0 & R \end{pmatrix}$$

  where $A_i = \frac{x}{p_i}$, $B_i = \frac{p_i x}{q_i}$
- Compute its LDU decomposition and find its Schur complement

$$R + \frac{p_1 x}{x^2 + q_1} + \frac{p_2 x}{x^2 + q_2}$$

- So we can use this representation to linearise the partial fraction approximation to the sgn-function:

$$\mathrm{sgn}_{n-1,n}(H) = H \sum_{j=1}^{n} \frac{p_j}{H^2 + q_j}$$

Partial fractions

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$$\left(\begin{array}{cc|cc|c} A_1 & 1 & 0 & 0 & 1 \\ 1 & -B_1 & 0 & 0 & 0 \\ \hline 0 & 0 & A_2 & 1 & 1 \\ 0 & 0 & 1 & -B_2 & 0 \\ \hline -1 & 0 & -1 & 0 & R \end{array}\right)$$

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where $A_i = \frac{x}{p_i}$, $B_i = \frac{p_i x}{q_i}$

- Compute its LDU decomposition and find its Schur complement

$$R + \frac{c_1 p_1 x}{c_1 (x^2 + q_1)} + \frac{c_2 p_2 x}{c_2 (x^2 + q_2)}$$

- So we can use this representation to linearise the partial fraction approximation to the sgn-function:

$$\mathrm{sgn}_{n-1,n}(H) = H \sum_{j=1}^{n} \frac{p_j}{H^2 + q_j}$$

Cayley Transform

- Consider a five-dimensional matrix of the form (transfer matrix form):

$$\begin{pmatrix} 1 & -T_1 & 0 & 0 \\ 0 & 1 & -T_2 & 0 \\ 0 & 0 & 1 & -T_3 \\ -T_0 & 0 & 0 & 1 \end{pmatrix}$$

  with its Schur complement $1 - T_0 T_1 T_2 T_3$

- So we can use this representation to linearise the Cayley transform of the approximation to the sgn-function:

$$\mathrm{sgn}_{n-1,n}(H) = \frac{1 - \prod_{j=1}^{n} T_j(H)}{1 + \prod_{j=1}^{n} T_j(H)}$$

- This is the standard Domain Wall Fermion formulation

What do we see . . .

- . . .each representation of the rational function leads to a different five-dimensional Dirac operator
- . . .they all have the same four-dimensional, effective lattice fermion operator

  $\Rightarrow$ the overlap Dirac operator
- . . .each five-dimensional operator has different symmetry properties

  $\Rightarrow$ different calculational behaviour

What do we see . . .

- . . .each five-dimensional operator can be even-odd preconditioned
- . . .lowest modes of the kernel can be projected out
- . . .lowest modes of the kernel can be suppressed:

$$\Rightarrow R'(x) \propto \frac{1}{R(x)}$$

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- . . .there is no physical significance to the standard Domain Wall formulation . . . is it?

Chiral symmetry breaking

- Ginsparg-Wilson defect $\gamma_5 D + D\gamma_5 - 2aD\gamma_5 D = \gamma_5 \Delta$:
  - it measures chiral symmetry breaking
  - for the approximate overlap operator $aD = \frac{1}{2}(1 + \gamma_5 R_n(H))$ it is $a\Delta_n = \frac{1}{2}(1 - R_n(H)^2)$
- The residual quark mass is $m_{res} = \frac{\langle G^\dagger \Delta_n G \rangle}{\langle G^\dagger G \rangle}$
  - G is the π propagator
  - it can be calculated directly in four and five dimensions
- m_{res} is just the first moment of Δ_n
  - higher moments might be important for other physical quantities

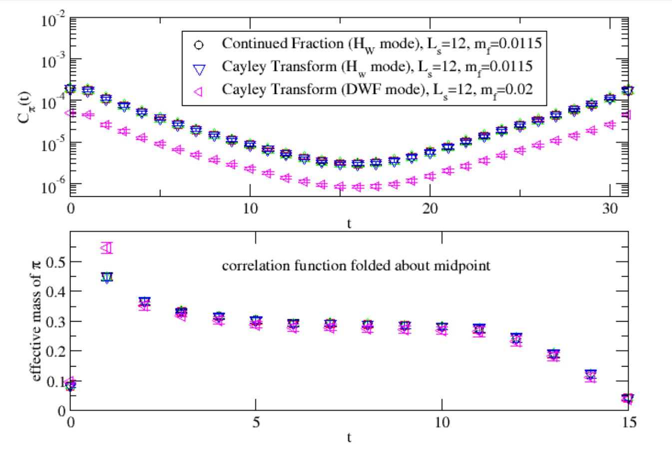
Setup

- We use 15 gauge field backgrounds from dynamical DWF dataset:

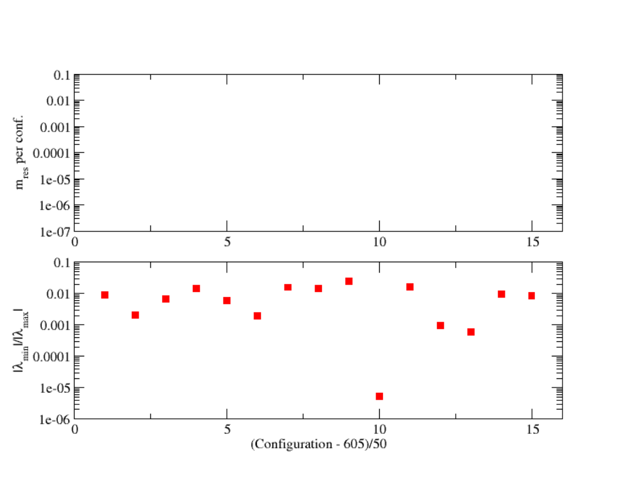
$$V = 16^3 \times 32, \quad L_s = 8, 12, 16, \quad N_f = 2, \quad \mu = 0.02$$

- Matched π mass for all representations
- All operators are even-odd preconditioned, no projection

Comparison of Representations



m_{res} per configuration



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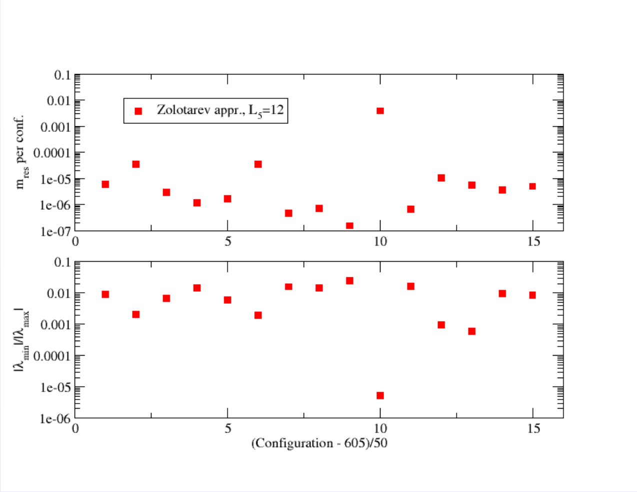

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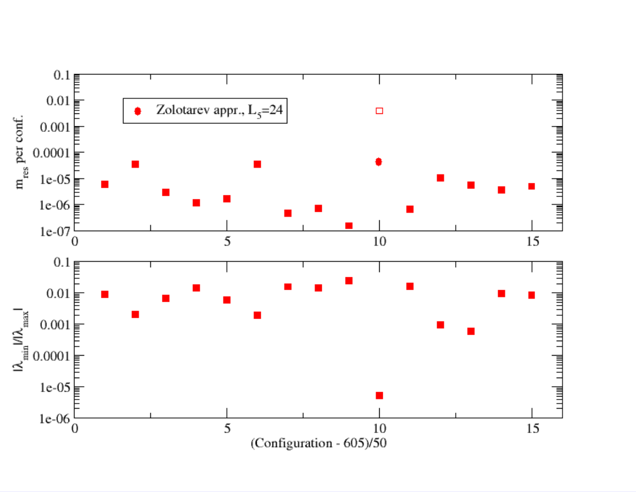

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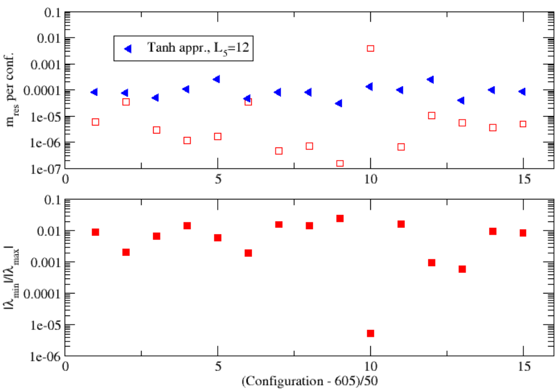

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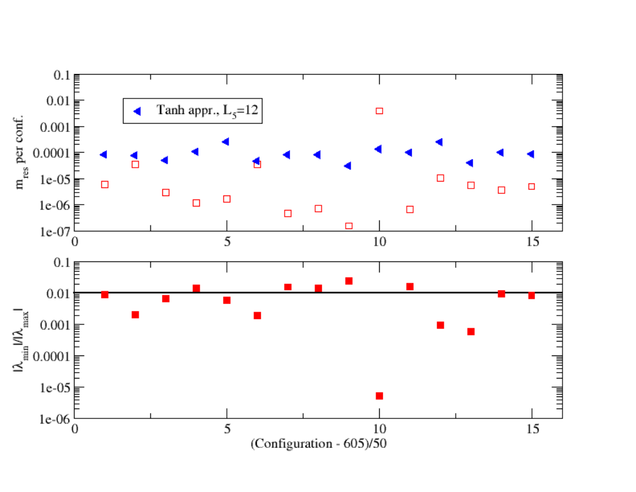

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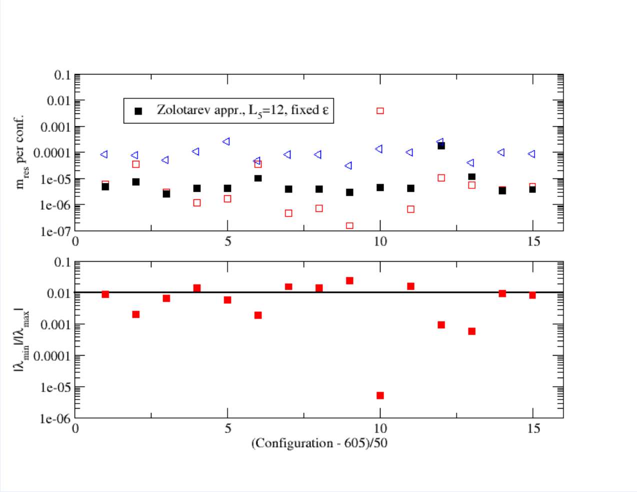
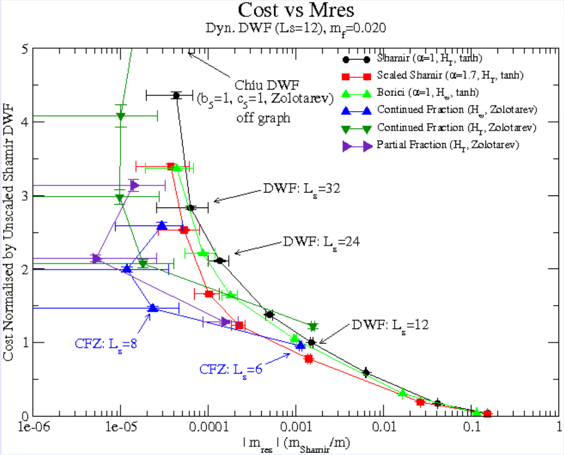


Cost versus m_{res}



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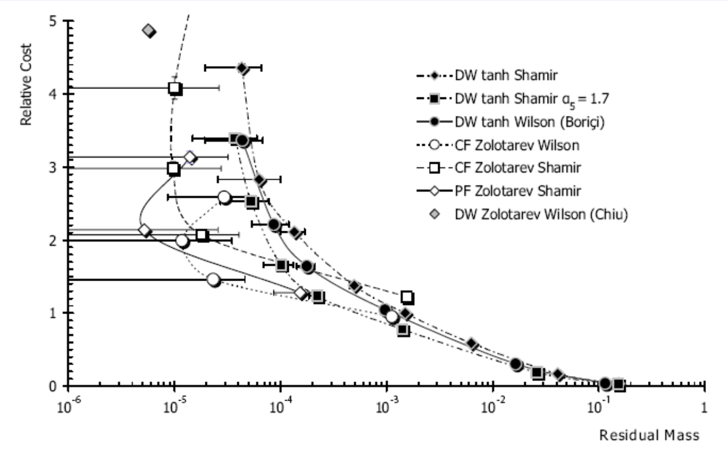

Conclusions

- We have a thorough understanding of various five dimensional formulations of chiral fermions
- More freedom and possibilities in 5 dimensions
- Physically they are all the same
- From a computational point of view there are better alternatives than the commonly used Domain Wall Fermions
- Hybrid Monte Carlo simulations:
  5 versus 4 dimensional dynamics?