USING LOCALITY IN LATTICE QCD
THE DOMAIN-DECOMPOSED MULTIBOSON ALGORITHM

Stefan Schaefer

John von Neumann Institute for Computing
DESY

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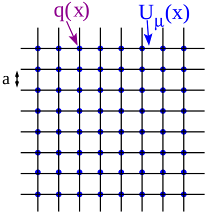
Cè, Giusti, S.S, PRD93 (2016) 094507 , PrdD95 (2017), 034503
EPJ WC 175 (2018) 01003, EPJ WC 175 (2018) 11005

Motivation

Definition of QCD on a Euclidean space-time lattice with lattice spacing a



$$\langle A[\bar{\psi}, \psi, U] \rangle = \frac{1}{Z} \int [dU][d\psi][d\bar{\psi}] e^{-S[\bar{\psi}, \psi, U]} A[\bar{\psi}, \psi, U]$$

We start out with a nicely local action.

Goal: Numerical evaluation evaluation of the discretized path integral.

$$S_{\mathrm{f}} = \sum_f \bar{\psi}_f D_{\mathrm{w}}(m_f) \psi_f \quad \text{with} \quad D_{\mathrm{w}} = \sum_{\mu=0}^{3} \frac{1}{2} \{ \gamma_\mu (\nabla_\mu^* + \nabla_\mu) - \nabla_\mu^* \nabla_\mu \}$$

$$S_{\mathrm{g}} = \frac{1}{g_0^2} \sum_p \mathrm{tr}\{1 - U_p\}$$

Wick contractions

Grassmann variables not suitable for numerical calculations

First step is to remove them from the problem

Use Wick's theorem to integrate them out in observable

$$\langle P^{\mathrm{ud}}(x) P^{\mathrm{du}}(0) \rangle = -\langle \mathrm{tr}\{\gamma_5 D_u^{-1}(x,0) \gamma_5 D_d^{-1}(0,x)\}\rangle$$

and also from the action with Dirac operator D

$$\int [d\psi][d\bar{\psi}] e^{\bar{\psi} D \psi} = \det D \; .$$

Left with integral over gauge variables

$$\langle P(x) P(0) \rangle = -\frac{1}{Z} \int [dU] \{ \prod_f \det D(U, m_f) \} e^{-S_g[U]} \mathrm{tr}\,\{\gamma_5\, D^{-1}(x,0) \gamma_5 D^{-1}(0,x)\}$$

Local action and operators → non-local determinant and propagators

Locality

Is giving up locality a good idea?

Yes

- Makes numerical computations possible
- Particularly successful in pseudo-scalar sector
  $\rightarrow$ no signal-to-noise problem

No

- Unnatural
- Local updates have cost $\propto V$
- Leads to global operations
- Hinders use of multilevel strategies

Multilevel strategies: Classical examples I

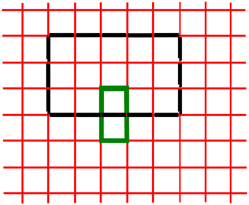
Pure gauge theory

$$S_g = \beta \sum_p [1 - \frac{1}{N} \mathrm{Re\,tr} U_p]$$

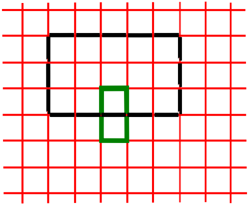
Multi-hit algorithm Parisi,Petronzio,Rapuano'83

$$\begin{aligned}\langle \mathrm{tr} W \rangle &= \frac{1}{Z} \int [dU] e^{-S_g[U]} \mathrm{tr}\, W \\ &= \frac{1}{\tilde{Z}} \int \overline{[dU]} e^{-\bar{S}_g} \frac{1}{Z_1} \int dX e^{-\beta \mathrm{Re\,tr} VX} \mathrm{tr} \tilde{W} X\end{aligned}$$

with V the staple attached to link X.
Keep fixed all links outside of loop.



Multi-hit



Efficient because action has only contributions from the vicinity of the updated link.

For each link use N_1 hits $\Rightarrow$ corresponds to $N_1^{\#\mathrm{links}}$ configurations.

Larger loops $\rightarrow$ more configurations.

BUT: more configurations $\neq$ more independent configurations.

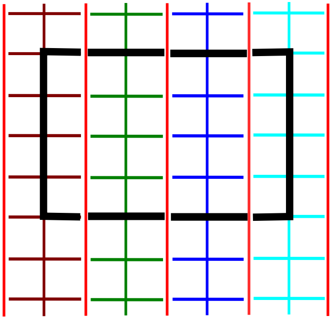
Classical examples II

Multilevel for Wilson loops `Lüscher & Weisz '01`

Introduce two-link building blocks

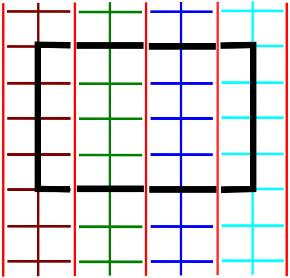
Keep links between (thick) time slices fixed

Independent updates possible.



Classical examples II

Multilevel for Wilson loops Lüscher & Weisz ’01



$$\langle W \rangle = \langle\, \langle [\rangle_1 \otimes \langle = \rangle_2 \otimes \langle = \rangle_3 \otimes \langle] \rangle_4 \,\rangle_{U_B}$$

$$= \langle L_1(U_1) \otimes \langle\langle T_2(U_1, U_2)\rangle_1 \otimes \langle T_2(U_2, U_3)\rangle_2 \otimes \langle L_3^*(U_3)\rangle_{1,3}$$

Multilevel!

Use hierarcy of thickness of time slices to reduce effect of fixed links.

Can essentially solve exponential signal-to-noise problem.

Remarks

Exponential signal-to-noise problems get more severe with the separations in the n-point function

Multilevel strategies can effectively increase the statistics with the extension of the objects

With the right setup, they can solve the s-to-n problems

Locality is an essential requirement

Fermions

Gauge actions are typically local
$\to$ terms involving only links on one (or a few) plaquette

For fermions such a formulation involves Grassmann variables

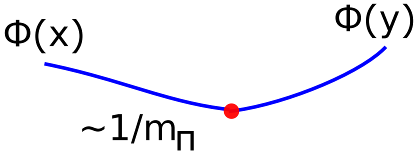
$$\int [d\psi][d\bar{\psi}] e^{\bar{\psi} D \psi} = \det D \, .$$

Represented by bosonic *pseudofermion* fields `Weingarten'81`

$$\det(D^\dagger D) = \frac{1}{Z_\phi} \int [\phi][\phi^\dagger] \exp(-|D^{-1}\phi|^2)$$

This action is rather non-local for the ϕ fields.

Empirical observation: $D^{-1}(x,y) \propto e^{-|x-y| m_\pi}$ for large $|x-y|$



Multi-boson algorithm

A New Approach to the Problem of Dynamical Quarks in Numerical Simulations of Lattice QCD

Martin Lüscher

Deutsches Elektronen-Synchrotron DESY
Notkestrasse 85, D-22603 Hamburg, Germany

Abstract

Lattice QCD with an even number of degenerate quark flavours is shown to be a limit of a local bosonic field theory. The action of the bosonic theory is real and bounded from below so that standard simulation algorithms can be expected to apply. The feasibility of such calculations is discussed, but no practical tests have yet been made.

Source: Title page of hep-lat/9311007

Multi-boson algorithm

Use a polynomial which approximates $f(x) = \frac{1}{x}$ in a suitable range $[0, 1)$.

$$P(x) = \sum_{k=0}^{n} (1-x)^k = \prod_{k=1}^{n/2} (x - z_k)(x - z_k^*) \overset{n\to\infty}{\to} \frac{1}{x}$$

Then we get

$$\det Q^2 = \prod_{k=1}^{n/2} \frac{1}{\det[(Q^2 - z_k)(Q^2 - z_k^*)]} = \prod_{k=1}^{n} \frac{1}{\det[(Q - \mu_k)^2 + \nu_k^2]}$$

which can easily be represented by bosonic fields ϕ_k

$$S_{\mathrm{mb}} = \sum_k |(Q - \mu_k)\phi_k|^2 + \nu_k^2 |\phi_k|^2$$

with $\sqrt{z_k} = \mu_k + i\nu_k$.
Local action $\to$ local update algorithm

Approximation $\to$ number of MB fields depends on conditioning number of Q^2.

Multi-boson algorithm

Why is this currently not used?

Light fermions might need n in the hundreds for a good approximation.

With increasing n, system becomes stiff

Autocorrelation times rise $\propto n$ `Jegerlehner'95`

$\rightarrow$ Problem traced back to $U_{x,\mu} U^{\dagger}_{x,\mu}$ terms in eff. action

Further developements, but currently no longer in use

`de Forcrand, Montvay, Scholz,...`

Advantage of a local formulation

$\leftrightarrow$

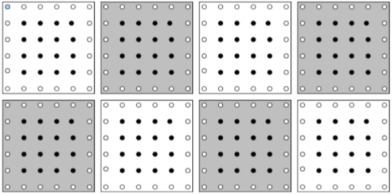
Disadvantage of sum over many terms

Maybe asking for a nearest neighbor interaction is asking too much?

Domain decomposition

Feasibility of domain decomposition is intimately linked to locality

Again proposal by Lüscher DD-HMC



Source:hep-lat/0409106

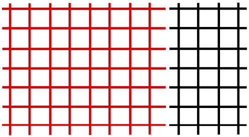
Divide lattice in two regions: Ω and Ω^* Lüscher '04

$$Q = Q_\Omega + Q_{\Omega^*} + Q_{\partial\Omega} + Q_{\partial\Omega^*}$$

from which follows a decomposition of the determinant

$$\det Q = \det Q_\Omega \det Q_{\Omega^*} \det(1 - P_{\partial\Omega^*} Q_\Omega^{-1} Q_{\partial\Omega} Q_{\Omega^*}^{-1} Q_{\partial\Omega^*})$$

Reminder: Schur complement



$$Q = \begin{pmatrix} Q_\Gamma & Q_{\partial\Gamma} \\ Q_{\partial\Gamma^*} & Q_{\Gamma^*} \end{pmatrix}$$

For the Wilson Dirac operator, $Q_{\partial\Gamma}$ and $Q_{\partial\Gamma^*}$ act on the boundaries.

$$Q = \begin{pmatrix} 1 & Q_{\partial\Gamma} Q_{\Gamma^*}^{-1} \\ 0 & 1 \end{pmatrix} \begin{pmatrix} S_\Gamma & 0 \\ 0 & Q_{\Gamma^*} \end{pmatrix} \begin{pmatrix} 1 & 0 \\ Q_{\Gamma^*}^{-1} Q_{\partial\Gamma^*} & 1 \end{pmatrix}$$

with the **Schur complement**

$$S_\Gamma = Q_\Gamma - Q_{\partial\Gamma} Q_{\Gamma^*}^{-1} Q_{\partial\Gamma^*}$$

For the determinant follows

$$\det Q = \det S_\Gamma \cdot \det Q_{\Gamma^*}$$

Can also be used to factorize propagator.

Domain decomposition

$$\det Q = \det Q_\Omega \det Q_{\Omega^*} \det(1 - P_{\partial\Omega^*} Q_\Omega^{-1} Q_{\partial\Omega} Q_{\Omega^*}^{-1} Q_{\partial\Omega^*})$$

Each determinant represented by pseudofermions

Used in $N_f = 2$ flavor CLS simulations, a variant also by PACS-CS

Actual implementation very much geared towards cluster computing (at the time)

Turned out to be inferior to/less flexible than standard HMC w/ Hasenbusch spliting

Large "correction term"

Locality on a block level seems a great idea.

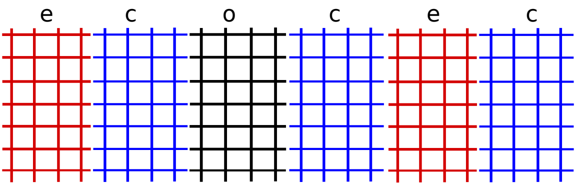
Can maybe be recast with different guiding principles.

New factorization of the determinant

Ce, Giusti, S'16

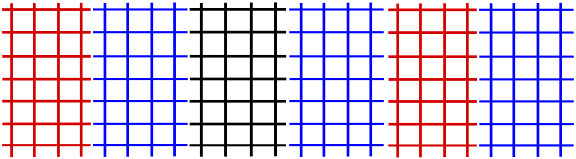
$$\langle A \rangle = \frac{1}{Z} \int [dU] \prod_f \det Q(m_f)\, e^{-S_g[U]} A$$

Sea quark contribution is given by **fermion determinant**



$$\det Q = \det \begin{pmatrix} Q_{e,e} & Q_{e,c} & 0 \\ Q_{e,c} & Q_{c,c} & Q_{c,o} \\ 0 & Q_{o,c} & Q_{o,o} \end{pmatrix}$$

Basic steps



Pull out central contribution

$$\det\, Q = \det Q_{c,c} \det \begin{pmatrix} Q_{e,e} - Q_{e,c}Q_{c,c}^{-1}Q_{c,e} & -Q_{e,c}Q_{c,c}^{-1}Q_{c,o} \\ -Q_{o,c}Q_{c,c}^{-1}Q_{c,e} & Q_{o,o} - Q_{o,c}Q_{c,c}^{-1}Q_{c,o} \end{pmatrix} ,$$

Factor diagonal terms

$$\det\, Q = \det Q_{c,c} \det\, S_e \,\det\, S_o \det \begin{pmatrix} 1 & -S_e^{-1}Q_{e,c}Q_{c,c}^{-1}Q_{c,o} \\ -S_o^{-1}Q_{o,c}Q_{c,c}^{-1}Q_{c,e} & 1 \end{pmatrix} ,$$

with Schur complements

$$S_e = Q_{e,e} - Q_{e,c}Q_{c,c}^{-1}Q_{c,e}$$
$$S_o = Q_{o,o} - Q_{o,c}Q_{c,c}^{-1}Q_{c,o}$$

Decomposition

$$\det Q = \det Q_{c,c} \det S_0 \det S_2 \det(1 - P_{\partial 0} Q^{-1}_{\Omega^*_0} Q_{1,2} Q^{-1}_{\Omega^*_1} Q_{1,0})$$

Loops in 0 and 1, passing through 0

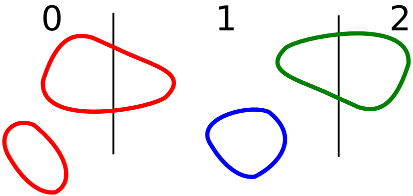
$$\det S_e = \det(Q_{e,e} - Q_{e,c} Q^{-1}_{c,c} Q_{c,e})$$

Loops in 1 and 2, passing through 2

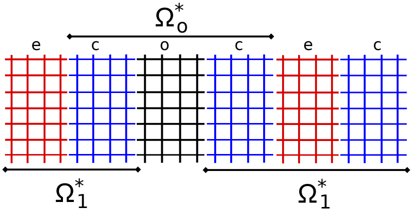
$$\det S_o = \det(Q_{o,o} - Q_{o,c} Q^{-1}_{c,c} Q_{c,o})$$

Loops in 1 $\det Q_{\Lambda_{1,1}}$

Loops stretching 0, 1, 2 $\det(1 - P_{\partial \Lambda_0} Q^{-1}_{\Omega^*_e} Q_{\Lambda_{1,2}} Q^{-1}_{\Omega^*_o} Q_{\Lambda_{1,0}})$



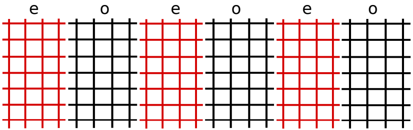
Comparison with DD-HMC



$$\det Q = \det Q_{c,c} \ \det S_e \ \det S_o \det(1 - P_{\partial\Lambda_e} Q^{-1}_{\Omega_e^*} Q_{c,o} Q^{-1}_{\Omega_o^*} Q_{\Lambda_{c,e}})$$

Propagators between separated boundaries

Handle to make them small



$$\det Q = \det Q_{e,e} \ \det Q_{o,o} \det(1 - P_{\partial\Lambda_e} Q^{-1}_{e,e} Q_{\Lambda_{e,o}} Q^{-1}_{o,o} Q_{\Lambda_{o,e}})$$

Propagators in correction term “loop back” $\rightarrow$ no suppression

No reason why last term should be small.

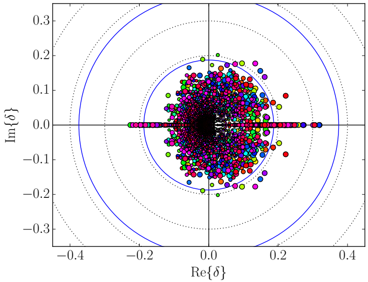
Reincarnation of the MB algorithm

$$\det(1 - w) = \det(1 - P_{\partial\Lambda_e} Q^{-1}_{\Omega^*_e} Q_{\Lambda_{c,o}} Q^{-1}_{\Omega^*_o} Q_{\Lambda_{c,e}})$$

This operator is quite well conditioned.

Contains propagators over distance Δ
$\rightarrow$ exponential suppression with $e^{-\Delta m_\pi}$.

Using multibosons leads to a factorization of the action.



Plot: Eigenvalues of w in complex plane.

Multiboson action

$$\det\{1-w\} \approx \prod_{k=1}^{n/2} (u_k - w)^{-1} (u_k^* - w^\dagger)^{-1}$$

Let us go one step back in the derivation

$$\det(u_k - w) = \det(u_k - P_{\partial\Lambda_e} Q_{\Omega_e^*}^{-1} Q_{c,o} Q_{\Omega_o^*}^{-1} Q_{c,e}) = \det W_{\sqrt{u_k}}$$

$$W_z = \begin{pmatrix} z\,P_{\partial\Lambda_e} & P_{\partial\Lambda_e} Q_{\Omega_e^*}^{-1} Q_{\Lambda_{c,o}} P_{\partial\Lambda_o} \\ P_{\partial\Lambda_o} Q_{\Omega_o^*}^{-1} Q_{\Lambda_{c,e}} P_{\partial\Lambda_e} & z\,P_{\partial\Lambda_o} \end{pmatrix} .$$

This leads to a contribution to the action which is local in the blocks

$$S_k = |W_{\sqrt{u_k}}\phi|^2 = \left|\sqrt{u_k}\phi_e + Q_{\Omega_e^*}^{-1} Q_{\Lambda_{c,o}} \phi_o\right|^2 + \left|\sqrt{u_k}\phi_o + Q_{\Omega_o^*}^{-1} Q_{\Lambda_{c,e}} \phi_e\right|^2$$

Note: Works flavor by flavor.

Full action

Fermion action

$$\frac{\det QQ^\dagger}{\det\{1-R_{n+1}(1-w)\}^2}$$
$$= C' \int [d\phi_e d\phi_e^\dagger] e^{-|P_{\Lambda_e} Q^{-1}_{\Omega_e^*} \phi_e|^2} \int [d\phi_c d\phi_c^\dagger] e^{-|Q^{-1}_{c,c} \phi_o|^2} \cdot$$
$$\int [d\phi_o d\phi_o^\dagger] e^{-|P_{\Lambda_o} Q^{-1}_{\Omega_o^*} \phi_o|^2} \cdot \prod_{k=1}^{n} \left\{ \int [d\chi_k d\chi_k^\dagger] e^{-|W_{\sqrt{u_k}} \chi_k|^2} \right\} ,$$

with

$$W_z = \begin{pmatrix} z P_{\partial\Lambda_e} & P_{\partial\Lambda_e} Q^{-1}_{\Omega_e^*} Q_{\Lambda_{c,o}} P_{\partial\Lambda_o} \\ P_{\partial\Lambda_o} Q^{-1}_{\Omega_o^*} Q_{\Lambda_{c,e}} P_{\partial\Lambda_e} & z P_{\partial\Lambda_o} \end{pmatrix} .$$

At fixed fields ϕ, the gauge field dependence of each term is local within the blocks.

Lesser degree of locality, but sufficient for purpose of multilevel.

Practical test

$N_\mathrm{f} = 2$ flavors of non-perturbatively improved Wilson fermions

$m_\pi = 440\,\mathrm{MeV}$

lattice spacing $a = 0.065\,\mathrm{fm}$

64×32^3 lattice, open boundary conditions in time

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thickness of central time slice $\Delta = 12a$

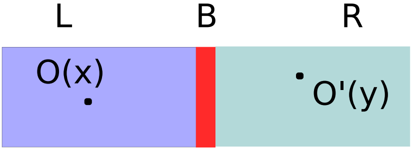
$N_b = 12$ multiboson fields

....much less than for in the original MB

Reweighting factor to correct for polynomial approximation negligible.

$\rightarrow$ practically exact action

Multilevel: Two active regions



Start with set of N_0 level-0 gauge field configurations

Define the boundary field U_B

$$\langle \{O(x) - \bar{O}\}\{O'(y) - \bar{O}'\}\rangle$$
$$= \frac{1}{Z_B}\int [dU_B] e^{-S_B[U_B]} [\{O(x) - \bar{O}\}]_L(U_B)[\{O'(y) - \bar{O}'\}]_R(U_B)$$

Estimate integrals over variables in L and R with N_1 configs per U_B

$$[O(x)]_L(U_B) = \frac{1}{Z_L}\int [dU_L] e^{-S(U_B,U_L)} O(x)$$
$$[O(y)]_R(U_B) = \frac{1}{Z_R}\int [dU_R] e^{-S(U_B,U_R)} O'(y)$$

Requirements

For multi-level to work we need two ingredients

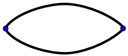
1) Factorized observable

2) Factorized action

Since we have used Wick's theorem, this is not obvious for observables and for the QCD action

Quark-line connected

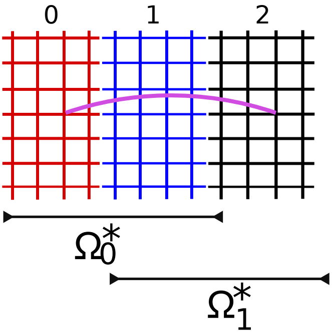
$$\langle P^{ud}(x) P^{du}(y) \rangle$$
$$= -\frac{1}{Z} \int [dU] \det D \, e^{-S_g[U]} \mathrm{tr}\left[\frac{1}{D_{m_u}}(x,y)\gamma_5 \frac{1}{D_{m_d}}(y,x)\gamma_5\right]$$



Quark-line disconnected

$$\langle P^{uu}(x) P^{dd}(y) \rangle$$
$$= \frac{1}{Z} \int [dU] \det D \, e^{-S_g[U]} \mathrm{tr}\left[\frac{1}{D_{m_u}}(x,x)\gamma_5\right] \mathrm{tr}\left[\frac{1}{D_{m_d}}(y,y)\gamma_5\right]$$

Factorizing propagators



$$P_{\Lambda_2} D^{-1} P_{\Lambda_0} = -P_{\Lambda_2} D^{-1}_{\Omega_1^*} D_{1,0} \frac{1}{1-w} D^{-1}_{\Omega_0^*} P_{\Lambda_0}$$

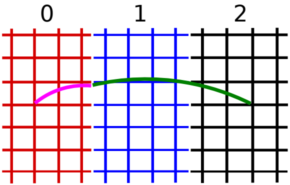
with

$$w = P_{\partial\Lambda_0} D^{-1}_{\Omega_0^*} D_{1,2} D^{-1}_{\Omega_1^*} D_{1,0}$$

For $\Delta\ O(0.5\text{fm})$, w is small $\sim e^{-\Delta M}$
$\rightarrow$ Neumann series converges well for $\Delta M \sim 1$.

Factorizing propagators

$$P_{\Lambda_2} D^{-1} P_{\Lambda_0}$$
$$= -P_{\Lambda_2} D^{-1}_{\Omega_1^*} D_{1,0} \frac{1}{1-w} D^{-1}_{\Omega_0^*} P_{\Lambda_0}$$
$$w = P_{\partial\Lambda_0} D^{-1}_{\Omega_0^*} D_{1,2} D^{-1}_{\Omega_1^*} D_{1,0}$$



$P_{\Lambda_2} D^{-1}_{\Omega_1^*}(x,z) P_{\partial\Lambda_1}$
$\rightarrow$ all paths from x to boundary 1-0 which do not enter 0.

$P_{\partial\Lambda_0} D^{-1}_{\Omega_0^*}(z,y) P_{\partial\Lambda 0}$
$\rightarrow$ all paths to y from boundary 1-0 which do not enter 2.

Leading term in Neumann series represents all paths not looping back from 2 to 0

Higher orders in w generate additional loops.

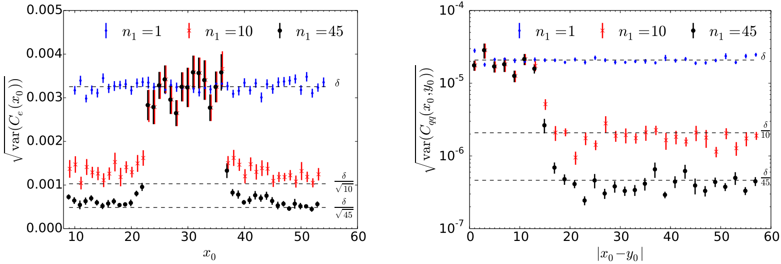
Multilevel

Test for gluonic observalbes

$$C_e(x_0, y_0) = \frac{1}{L^3} \langle \bar{e}(x_0) \rangle \quad ; \quad C_{qq}(x_0, y_0) = \frac{1}{L^3} \langle \bar{q}(x_0) \bar{q}(y_0) \rangle$$

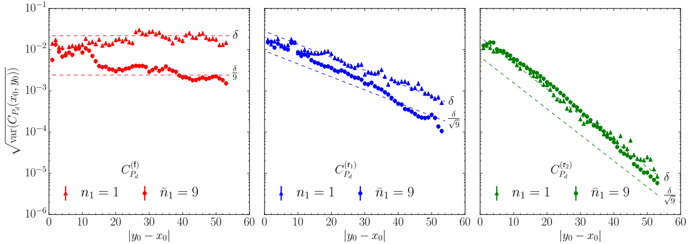
with

$$\bar{e}(x_0) = \frac{1}{4} \sum_{\vec{x}} F^a_{\mu\nu}(x) F^a_{\mu\nu}(x) \quad ; \quad \bar{q}(x_0) = \frac{1}{64\pi^2} \sum_{\vec{x}} \epsilon_{\mu\nu\rho\sigma} F^a_{\mu\nu}(x) F^a_{\rho\sigma}(x)$$



Quark-line disconnected

$$\langle P^{uu}(x_0)P^{dd}(y_0)\rangle$$



Nine independent level-1 configurations.

Fully factorized contribution profits as expected

Single correction term falls off with half pion mass, improves with $\sqrt{N_1}$.

Double correction term falls off with the pion mass.

Summary

Locality is an important property of quantum field theory.

It can be used to solve exponential signal to noise problem in n point functions.

See also Lüscher's "master field" $\rightarrow$ giant lattices can profit from local formulations

True locality is difficult to achieve for fermions.

Two-level methods work.

Demonstrated for quark-line disconnected graphs

Gluonic correlation functions $\langle q(x)q(y)\rangle$ Garcia Vera, SS, '16

Signal-to-noise require $\sqrt{N} \propto e^{mx_0} \longrightarrow N \propto e^{mx_0}$

Get twice as far with same effort. $\rightarrow$ **Generalize to multilevel.**