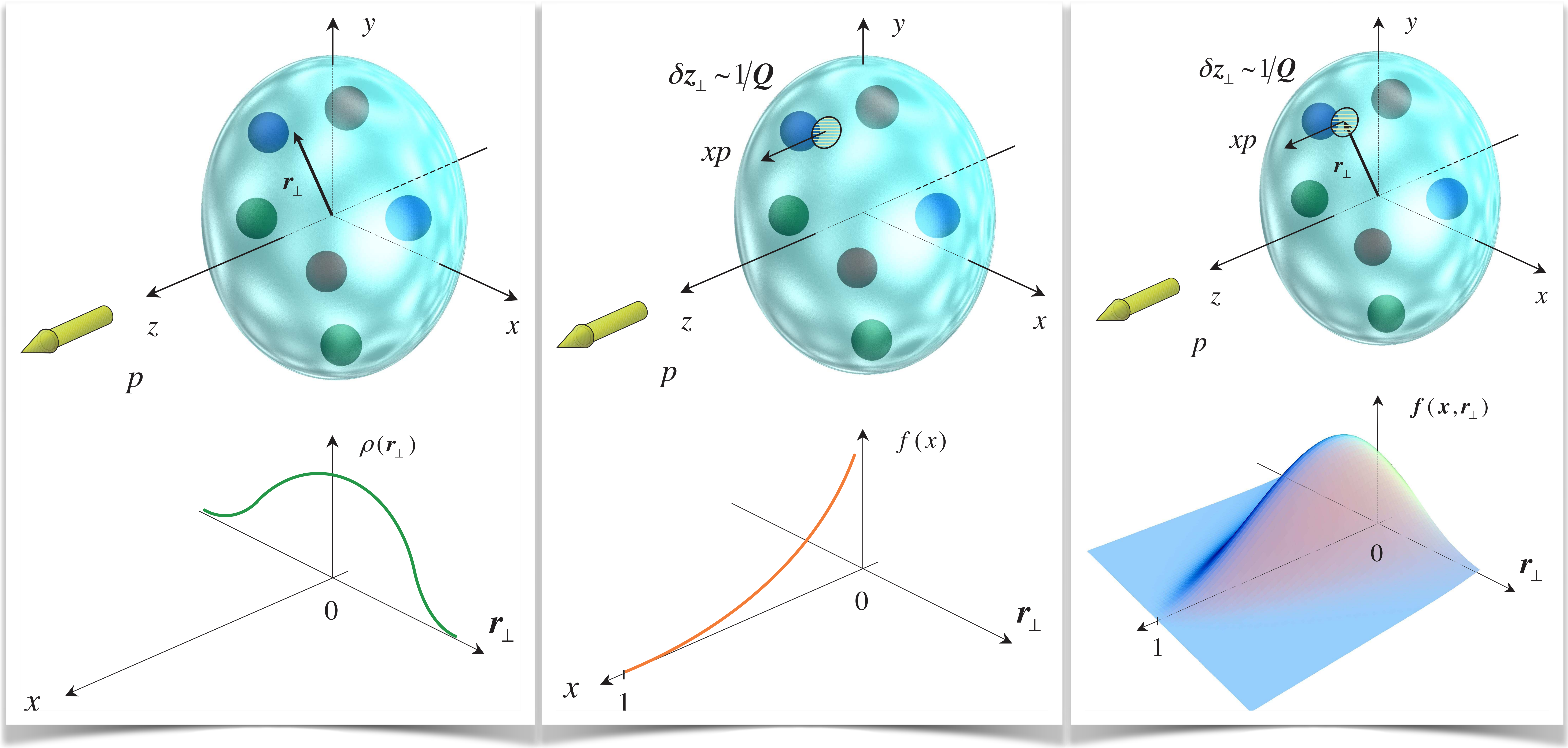
Hierarchical HMC

SciDAC 5 — Dec 1-2, 2022, JLab

Kostas Orginos

X. Ji, D. Muller, A. Radyushkin (1994-1997)



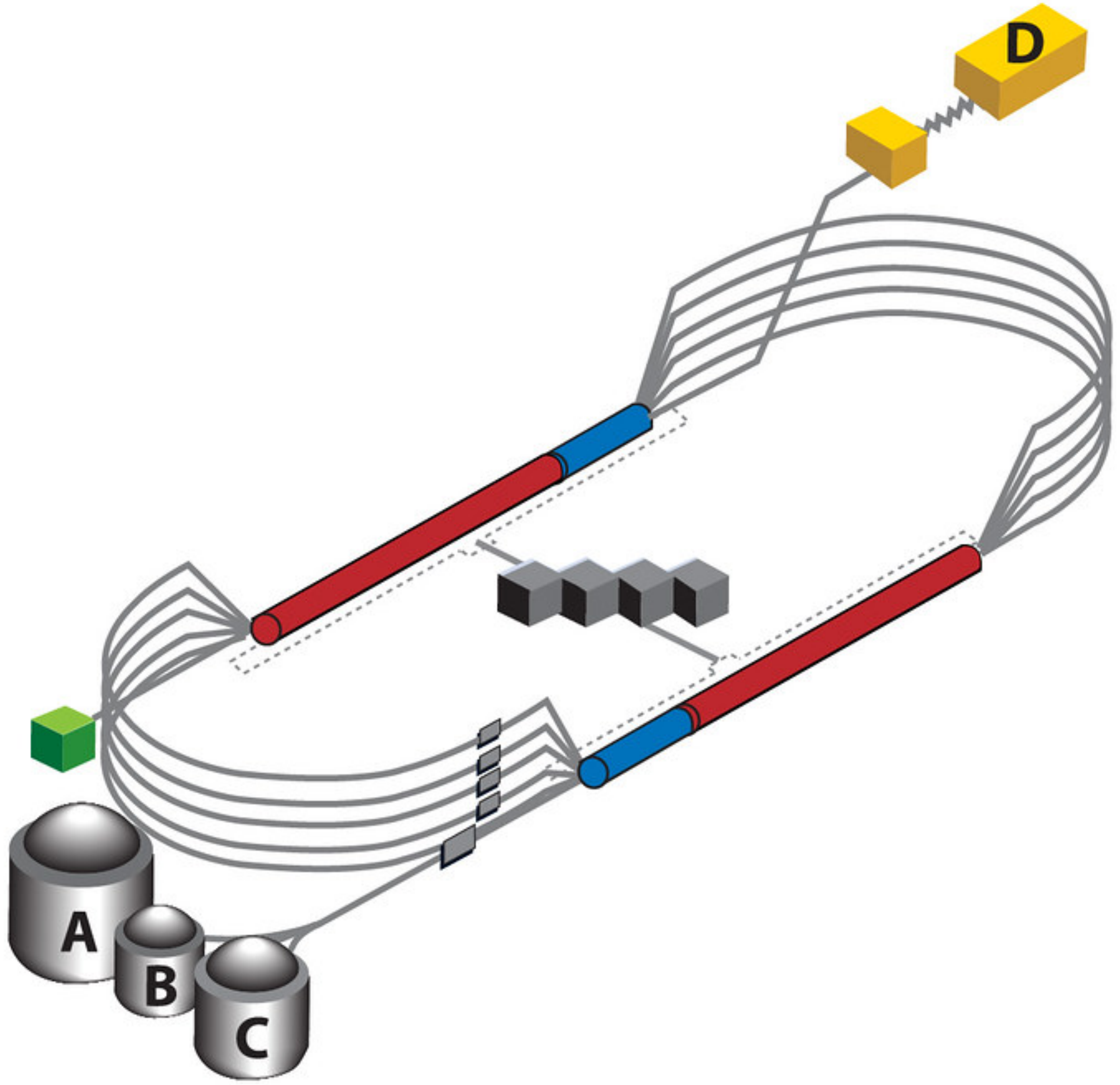
Form Factors

Parton Distribution functions

Generalized Parton Distribution functions

JLab 12 GeV

Generalized Parton Distributions



The Electron-Ion Collider

A machine that will unlock the secrets of the strongest force in Nature

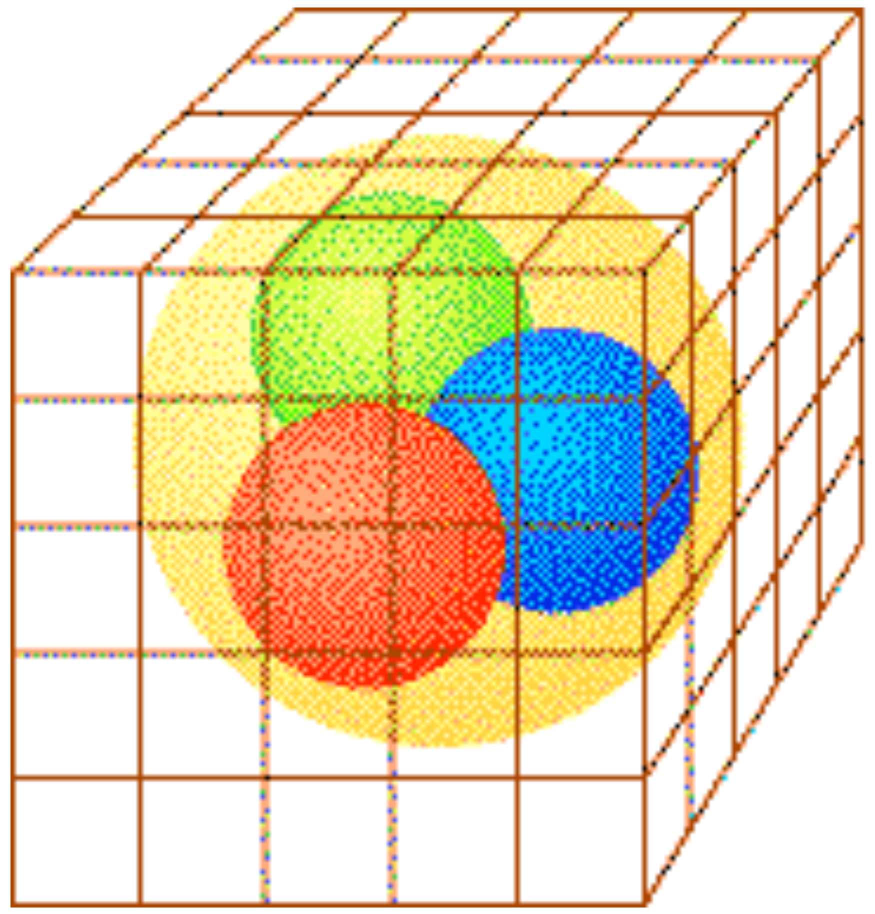
The computers and smartphones we use every day depend on what we learned about the atom in the last century. All information technology—and much of our economy today—relies on understanding the electromagnetic force between the atomic nucleus and the electrons that orbit it. The science of that force is well understood but we still know little about the microcosm within the protons and neutrons that make up the atomic nucleus. That's why Brookhaven Lab is building a new machine—an Electron-Ion Collider, or EIC—to look *inside* the nucleus and its protons and neutrons.

The EIC will be a particle accelerator that collides electrons with protons and nuclei to produce snapshots of those particles' internal structure—like a CT scanner for atoms. The electron beam will reveal the arrangement of the quarks and gluons that make up the protons and neutrons of nuclei. The force that holds quarks together, carried by the gluons, is the strongest force in Nature. The EIC will allow us to study this "strong nuclear force" and the role of gluons in the matter within and all around us. What we learn from the EIC could power the technologies of tomorrow.

taken from https://www.bnl.gov/eic/

Lattice QCD

Defined on a Euclidean Lattice



- Lattice QCD: QCD on discrete Euclidean space time
    - The lattice regulates UV divergences
- QCD: the continuum limit of Latice QCD
- Provides a numerical, non-perturbative method for computing correlation functions : Monte Carlo evaluation of integrals

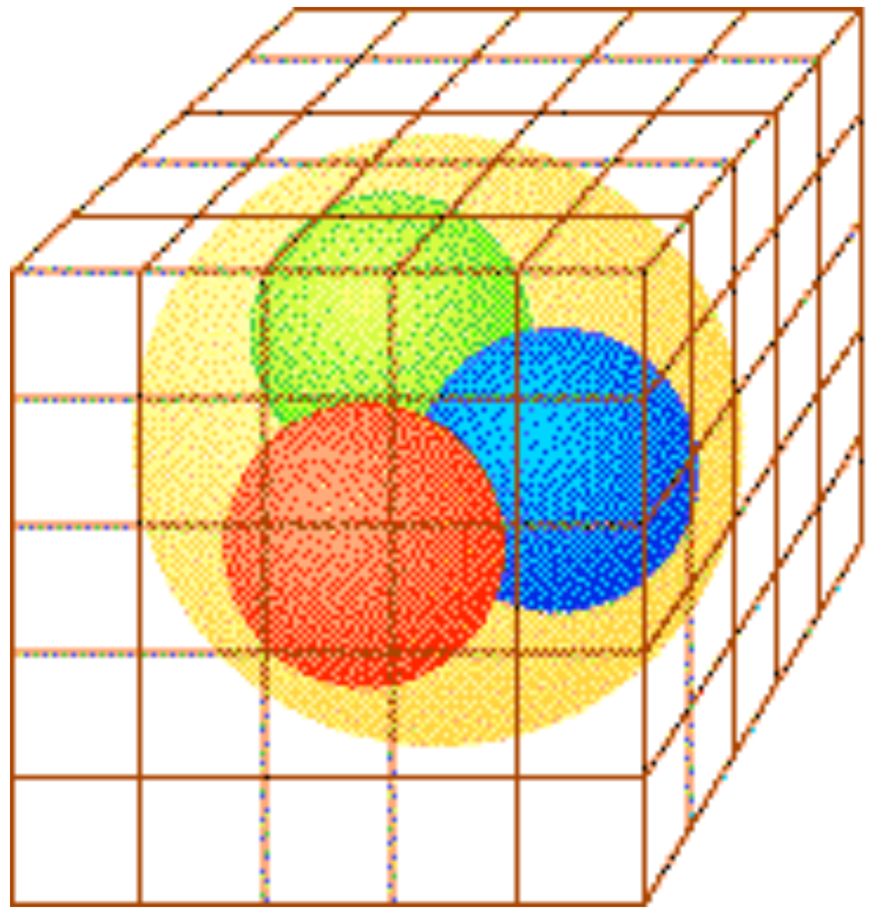
$$\mathcal{Z} = \int \mathcal{D}[U]\mathcal{D}[\bar{\psi}]\mathcal{D}[\psi] \; e^{-\bar{\psi}D(U)\psi - S_g(U)}$$

$$\langle \mathcal{O} \rangle = \frac{1}{\mathcal{Z}} \int \mathcal{D}[U]\mathcal{D}[\bar{\psi}]\mathcal{D}[\psi] \; \mathcal{O}(\bar{\psi}, \psi, U) \; e^{-\bar{\psi}D(U)\psi - S_g(U)}$$

Monte Carlo calculation

LQCD

$$\langle \mathcal{O} \rangle = \frac{1}{\mathcal{Z}} \int \prod_{\mu,x} dU_\mu(x) \;\; \mathcal{O}[U, D(U)^{-1}] \;\; \det \left(D(U)^\dagger D(U) \right)^{n_f/2} \;\; e^{-S_g(U)}$$



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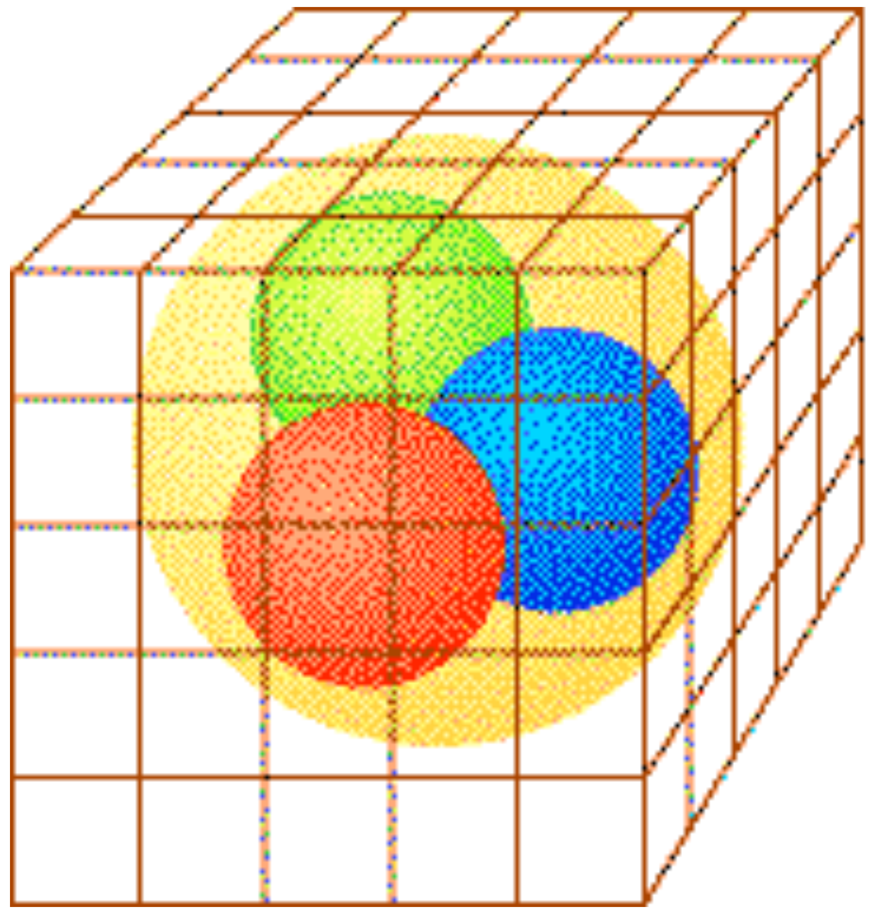

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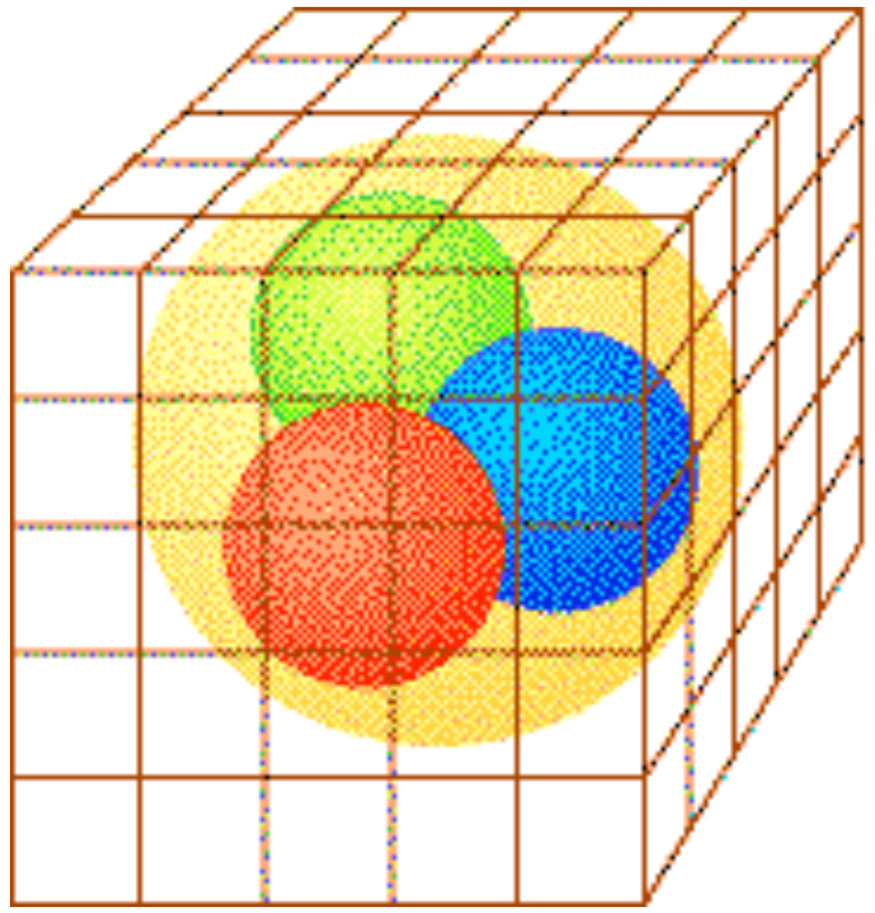

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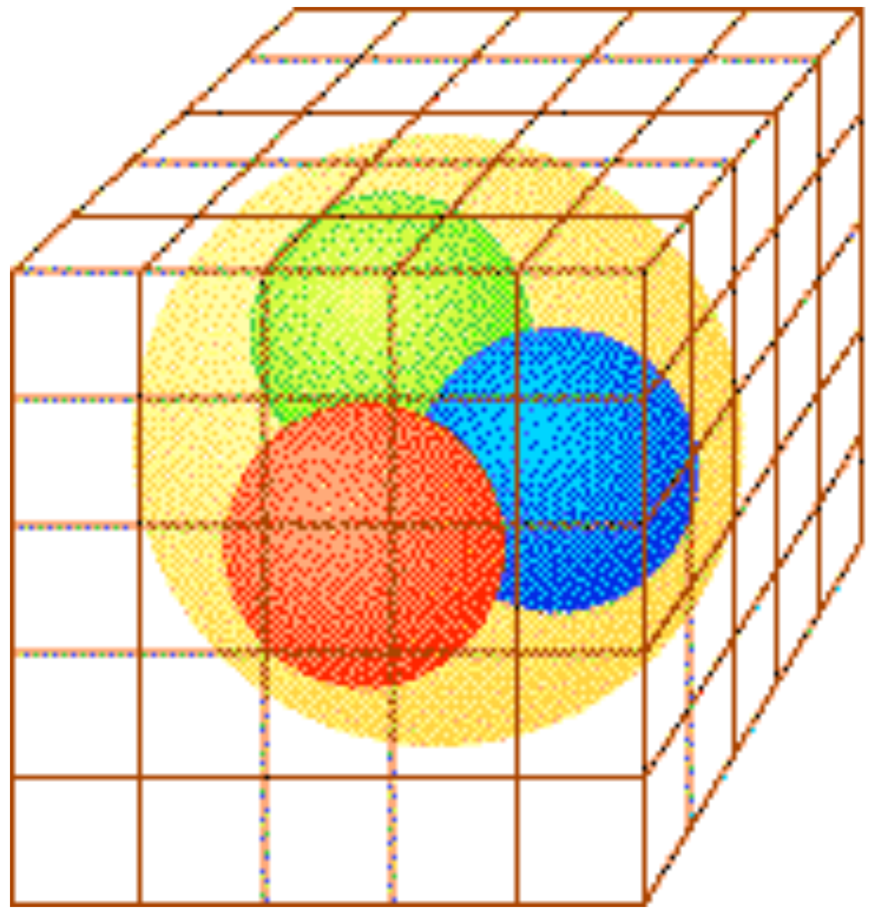

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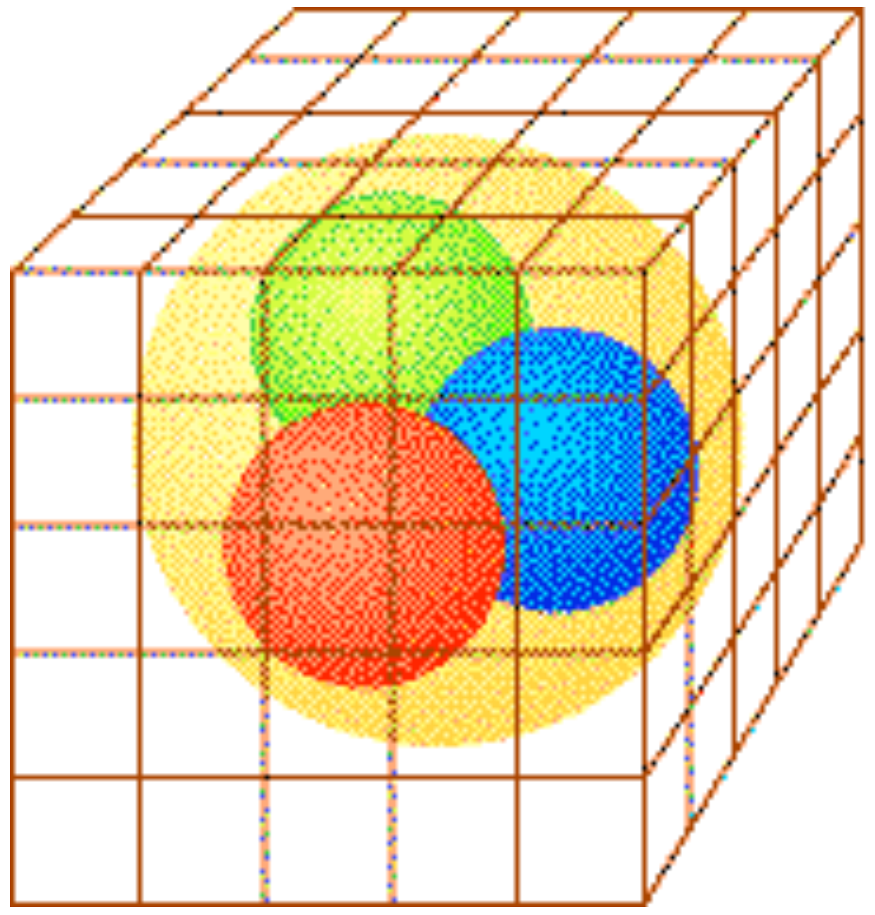

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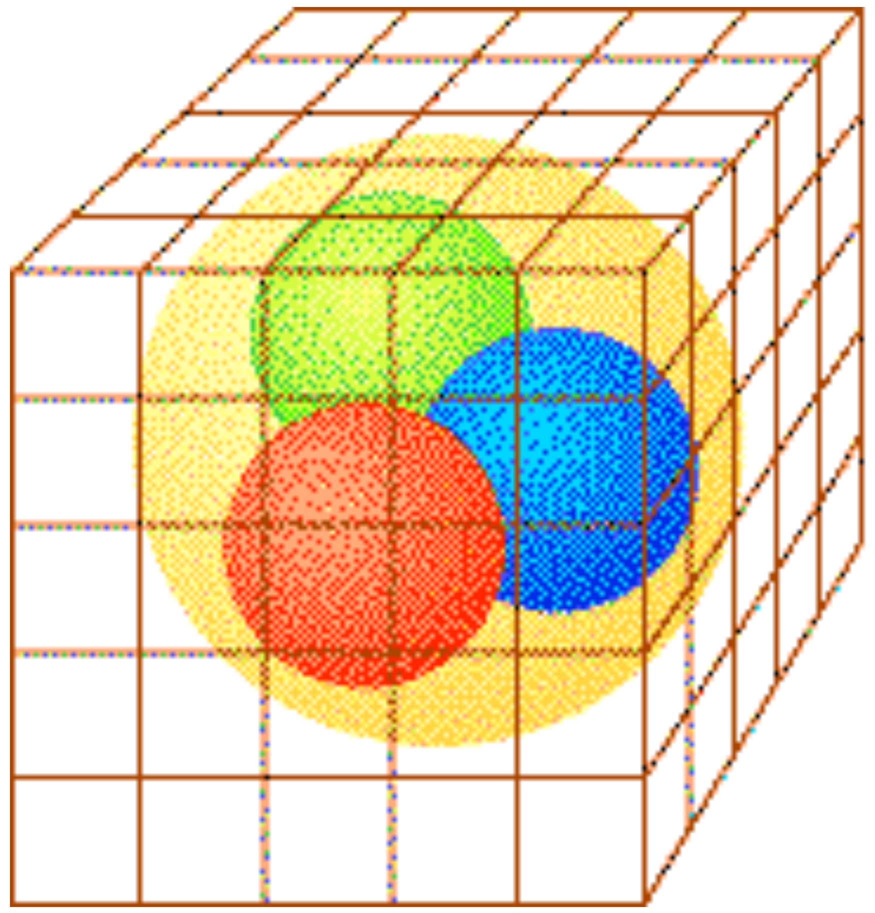
- Gauge field configuration generation



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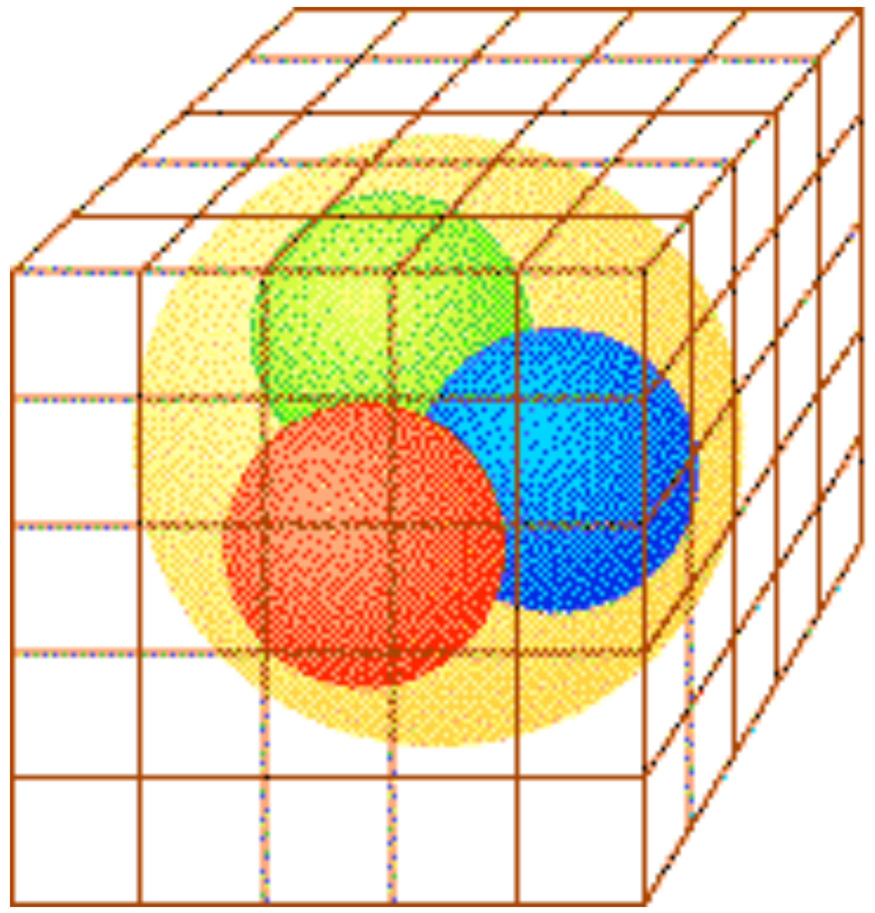
- Gauge field configuration generation
  - Can be used for several observables



Monte Carlo calculation

LQCD

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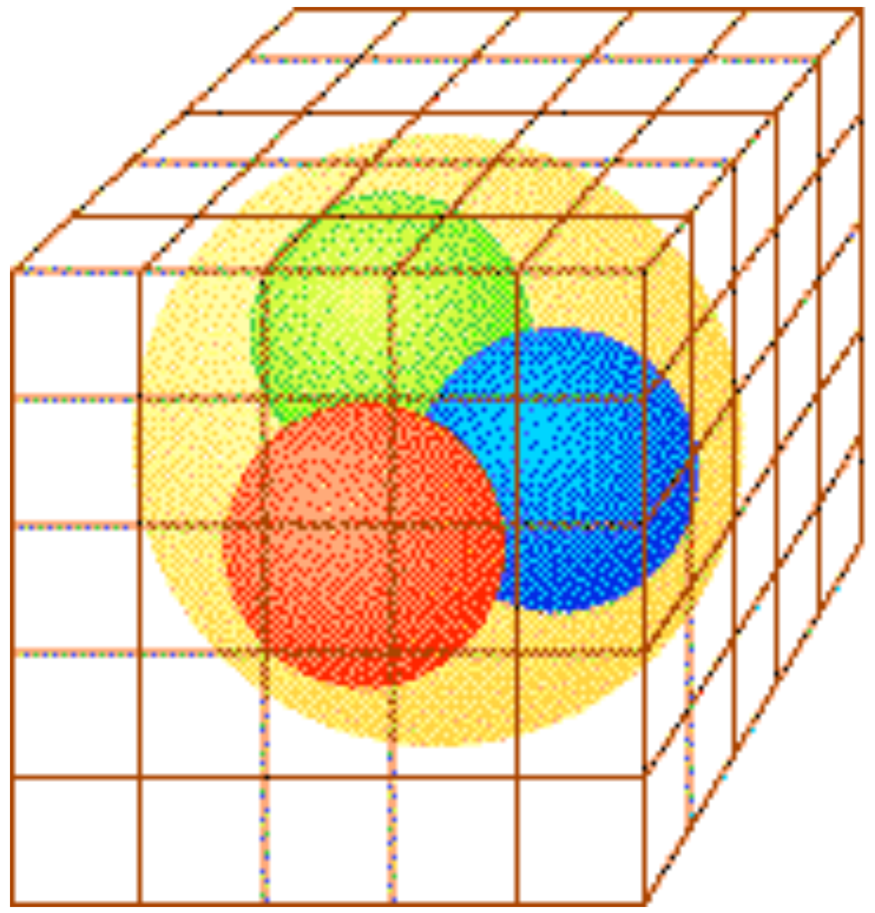
- Gauge field configuration generation
  - Can be used for several observables
- Correlation function calculation



Monte Carlo calculation

LQCD

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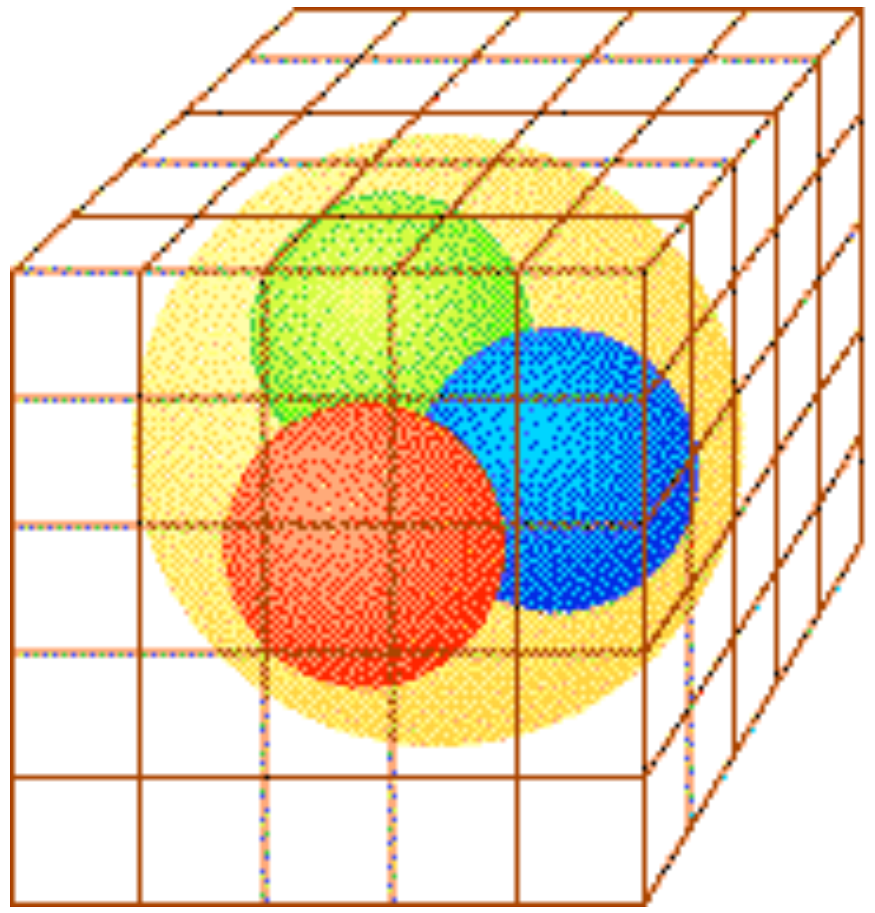
- Gauge field configuration generation
  - Can be used for several observables
- Correlation function calculation
  - Observable specific



Monte Carlo calculation

LQCD

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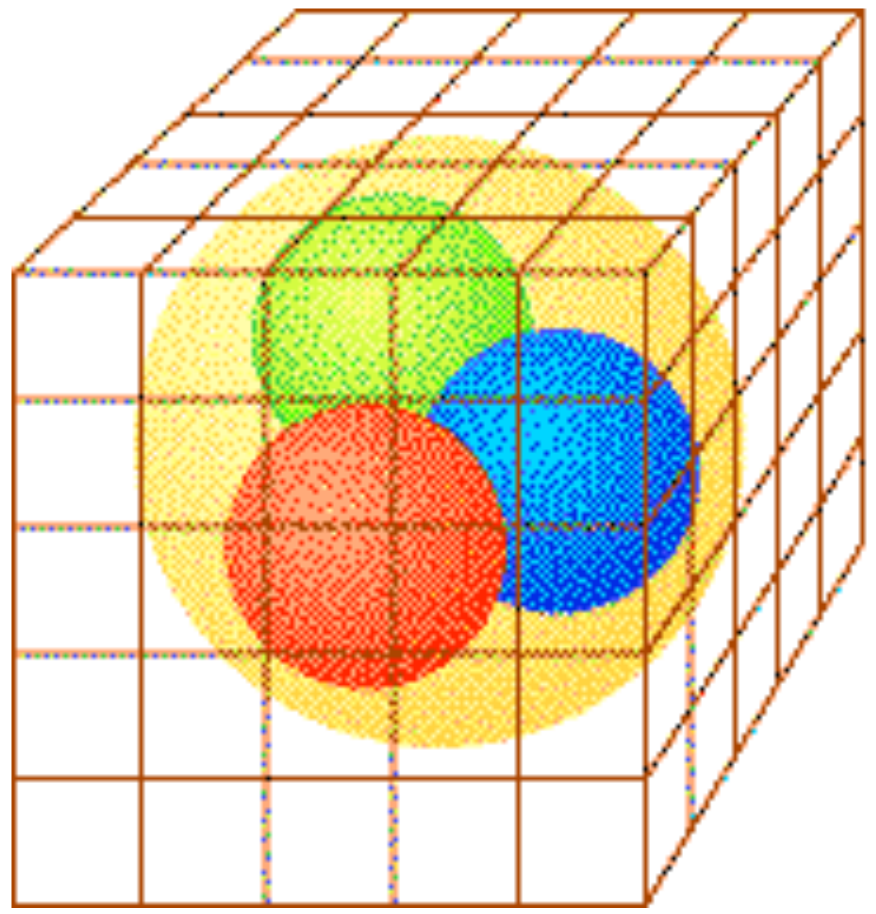
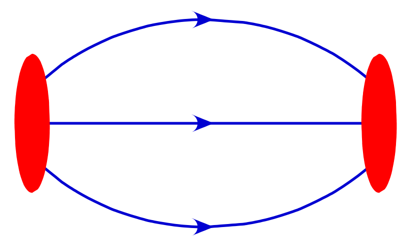
- Gauge field configuration generation
  - Can be used for several observables
- Correlation function calculation
  - Observable specific
- Allows for non-perturbative computations in QCD



Computation of equal time matrix elements
LQCD

At sufficiently large T and t we get

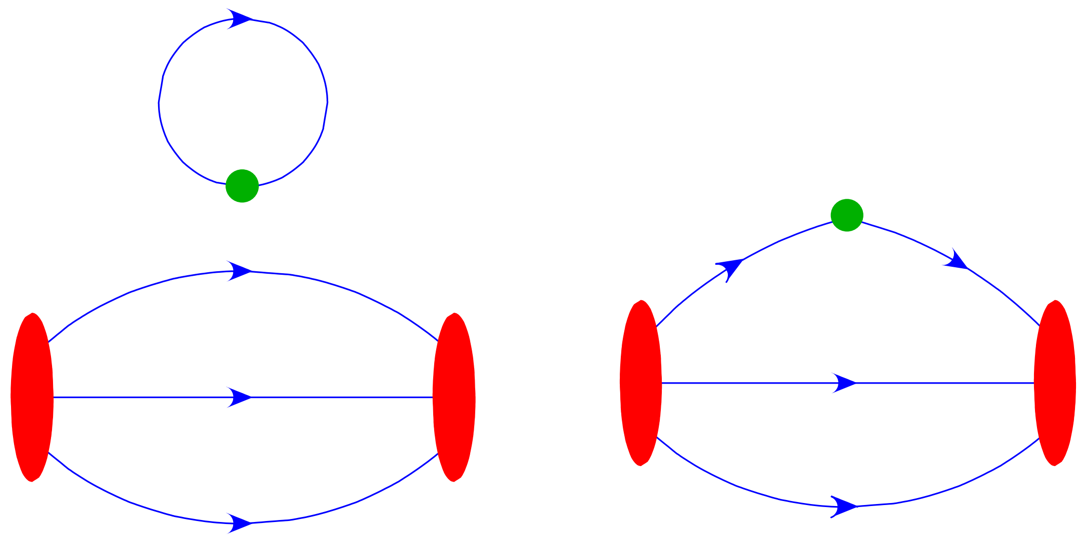
Two point function



$$C_{2pt} = \langle N(p,s,T)\bar{N}(p,s,0)\rangle = \langle 0|N,p,s\rangle \frac{e^{-E_p T}}{2E_p}\langle N,p,s,|0\rangle$$

Computation of ground state energy and overlap factors

Three point function



$$C_{3pt} = \langle 0|N,p,s\rangle \frac{e^{-E_p(T-t)}}{2E_p}\langle N,p,s|\mathcal{O}|N,p',s'\rangle \frac{e^{-E'_p t}}{2E'_p}\langle N,p',s',|0\rangle$$

Computation of ground state matrix elements

In practice we need to account for contributions from excited states

Energies and equal matrix elements are the same as those in Minkowski space

Briceno *et al* arXiv:1703.06072

Pseudo-PDFs

An alternative point of view

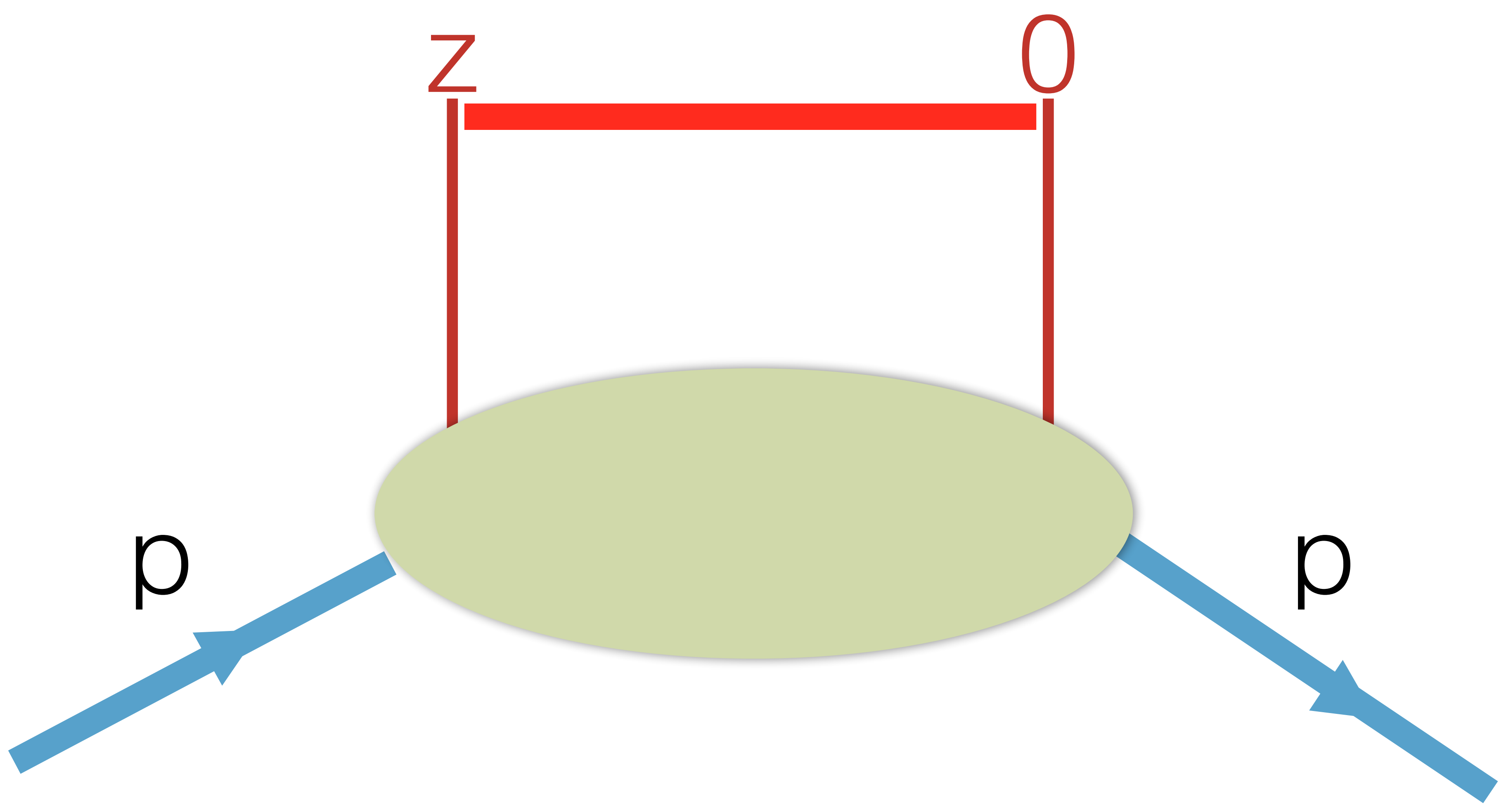
A. Radyushkin Phys.Lett. B767 (2017)

Unpolarized PDFs proton:

$$\mathcal{M}^\alpha(z,p) \equiv \langle p|\bar{\psi}(0)\,\gamma^\alpha\,\hat{E}(0,z;A)\psi(z)|p\rangle$$

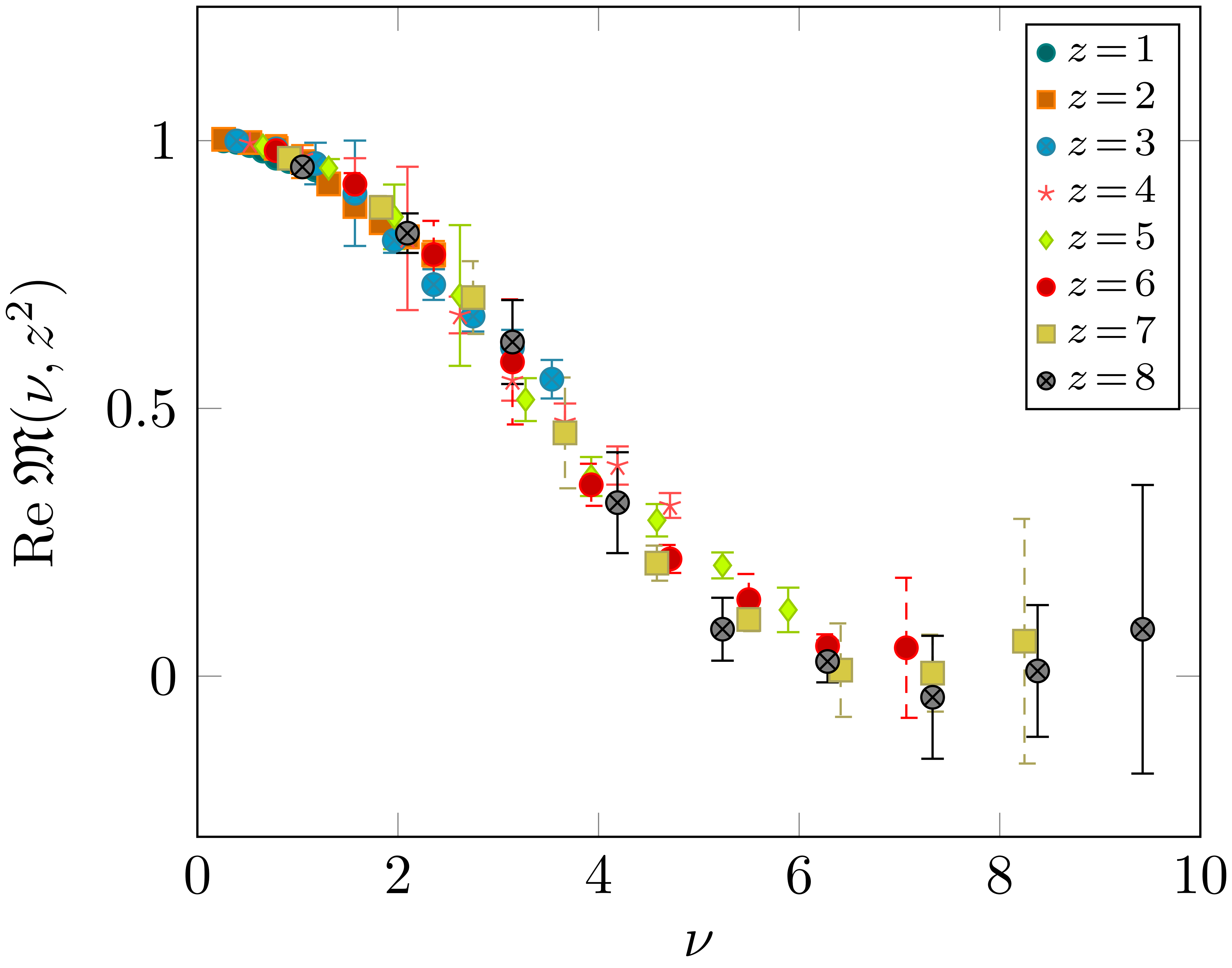
$$\hat{E}(0,z;A) = \mathcal{P}\exp\left[-ig\int_0^z \mathrm{d}z'_\mu\, A^\mu_\alpha(z')T_\alpha\right]$$

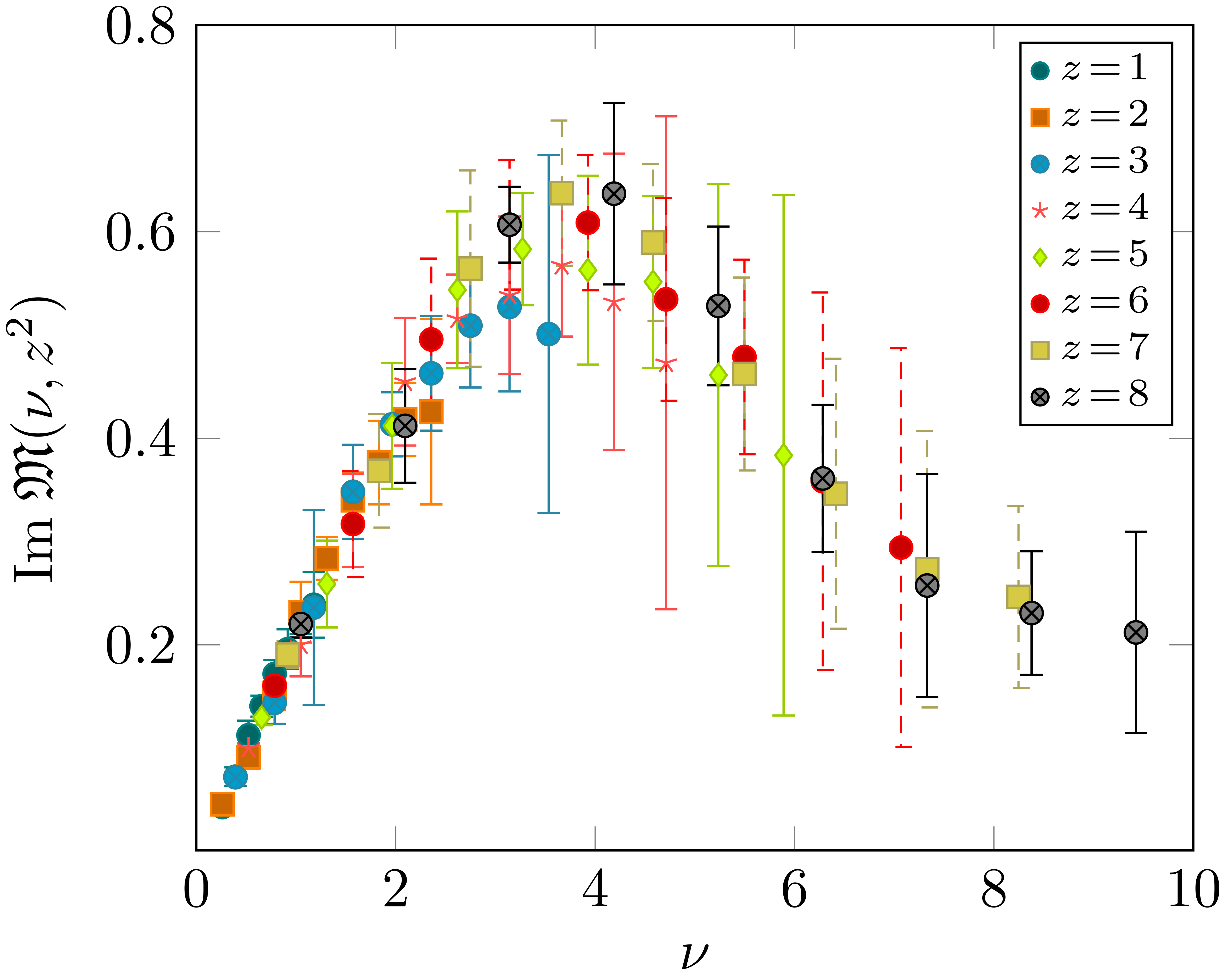
space-like separation of quarks



Lorentz decomposition:

$$\mathcal{M}^\alpha(z,p) = 2p^\alpha\mathcal{M}_p(-(zp),-z^2) + z^\alpha\mathcal{M}_z(-(zp),-z^2)$$





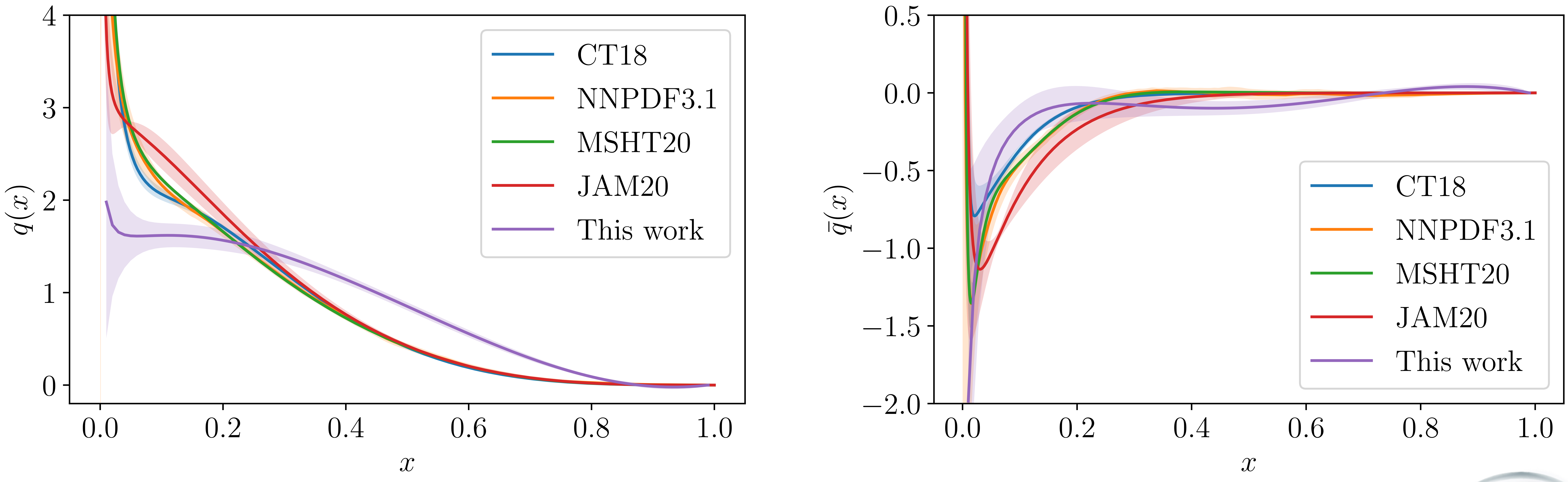
a= 0.048fm

arXiv:2105.13313 **[hep-lat] J. Karpie** *et. al.*

HadStruc

Isovector quark and anti-quark distributions

Comparison with phenomenology



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HadStruc

Statistical noise

Nucleon with momentum P two-point function:

$$C_{2p}(P,t) = \langle O_N(P,t) O_N^\dagger(P,0)\rangle \sim \mathcal{Z} e^{-E(P)t}$$

Variance of nucleon two-point function:

$$\mathrm{var}\left[C_{2p}(P,t)\right] = \langle O_N(P,t) O_N(P,t)^\dagger O_N(P,0) O_N^\dagger(P,0)\rangle \sim \mathcal{Z}_{3\pi} e^{-3m_\pi t}$$

Variance is independent of the momentum

$$\frac{\mathrm{var}\left[C_{2p}(P,t)\right]^{1/2}}{C_{ap}(P,t)} \sim \frac{\mathcal{Z}}{\mathcal{Z}_{3\pi}} e^{[E(P)-3/2 m_\pi]t}$$

Statistical accuracy drops exponentially with the increasing momentum limiting the maximum achievable momentum.

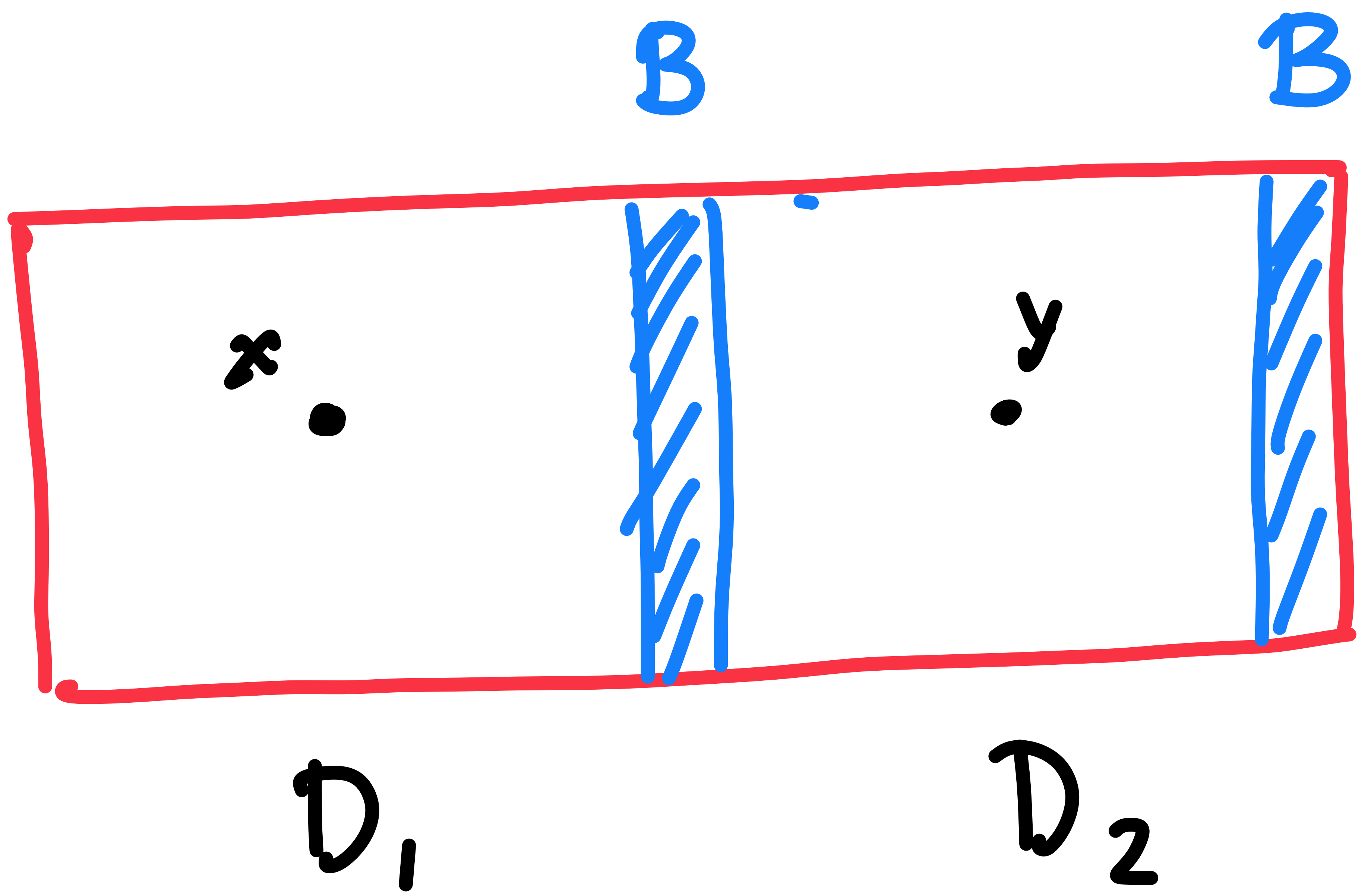
We need to find a way to increase statistics

Basic Idea

Let $Z = \int D\phi \; e^{-S(\phi)}$ $\qquad \phi$: a scalar field

$$\langle \phi_x \; \phi_y \rangle = \frac{1}{Z} \int D\phi \; \phi_x \, \phi_y \; e^{-S(\phi)}$$

S : contains only nearest neighbor couplings.



$$p(\phi) = \frac{e^{-S(\phi)}}{Z}$$

hep-lat/0209145 H. Meyer, 2002 : Pure Yang-Mills.

$$\langle \phi_x \phi_y \rangle = \int D\phi \; P[\phi] \; \phi_x \phi_y = \int D\phi_1 D\phi_2 D\phi_B \underbrace{P(\phi_B) P(\phi_1|\phi_B) P(\phi_2|\phi_B)}_{P[\phi]} \phi_x^{(1)} \phi_y^{(2)}$$

$$= \int D\phi_B \left[\int D\phi_1 \; \phi_x^{(1)} \; P(\phi_1|\phi_B) \right] \left[\int D\phi_2 \; \phi_y^{(2)} \; P(\phi_2|\phi_B) \right]$$

Task

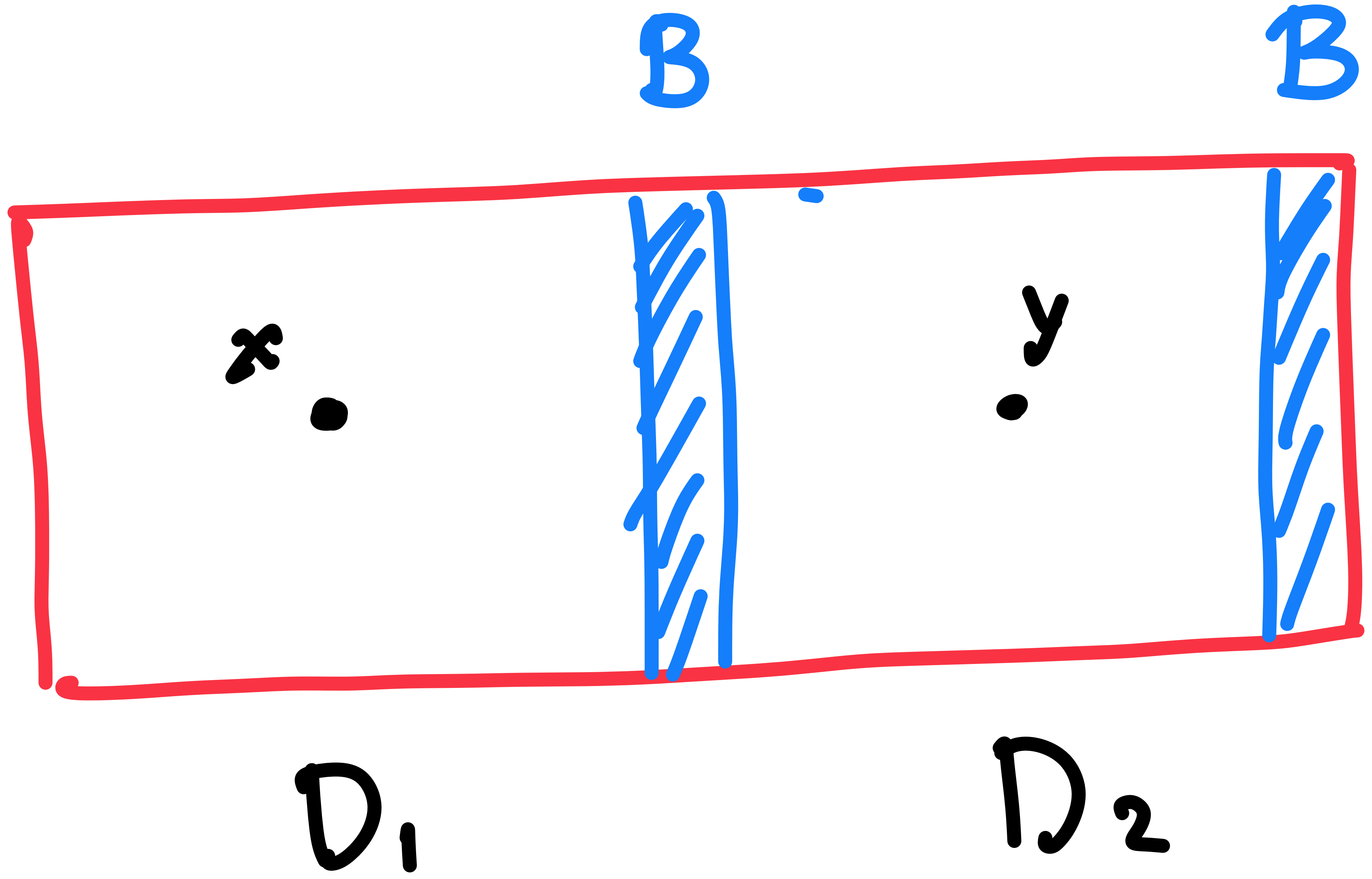
1) Perform Markov chain Montecarlo (MCMC) to generate thermalized configuration of $\{\phi\} \equiv \{ \{\phi_1\}, \{\phi_2\}, \{\phi_B\} \}$
   - standard global MCMC
2) Perform MCMC to generate $\{\phi_1\}_{\phi_B}, \{\phi_2\}_{\phi_B}$

$$P(\phi_i|\phi_B) \sim e^{-S(\phi_i) - S(\phi_i, \phi_B)}$$

3) Compute partial averages
4) Average over all Boundaries


N configs.
global MCMC
N_s configs
fixed boundary MCMC
partial averages
global averag
$\langle \phi_x \phi_y \rangle$

Cost



V: global volume

N: total global configurations

N_D: total configurations in each domain

$$\text{Cost} = VN + N N_d \frac{V}{2} \cdot 2 = NV(1+N_d) \simeq N N_d V$$

Statistics $\quad N_s = N_d^2 N$

Error $\quad E_2 \propto \frac{1}{\sqrt{N_s}} = \frac{1}{\sqrt{N}} \frac{1}{N_d}$, $\quad E_1 = \frac{1}{\sqrt{N N_d}}$

two level MC. $\qquad\qquad$ normal MC

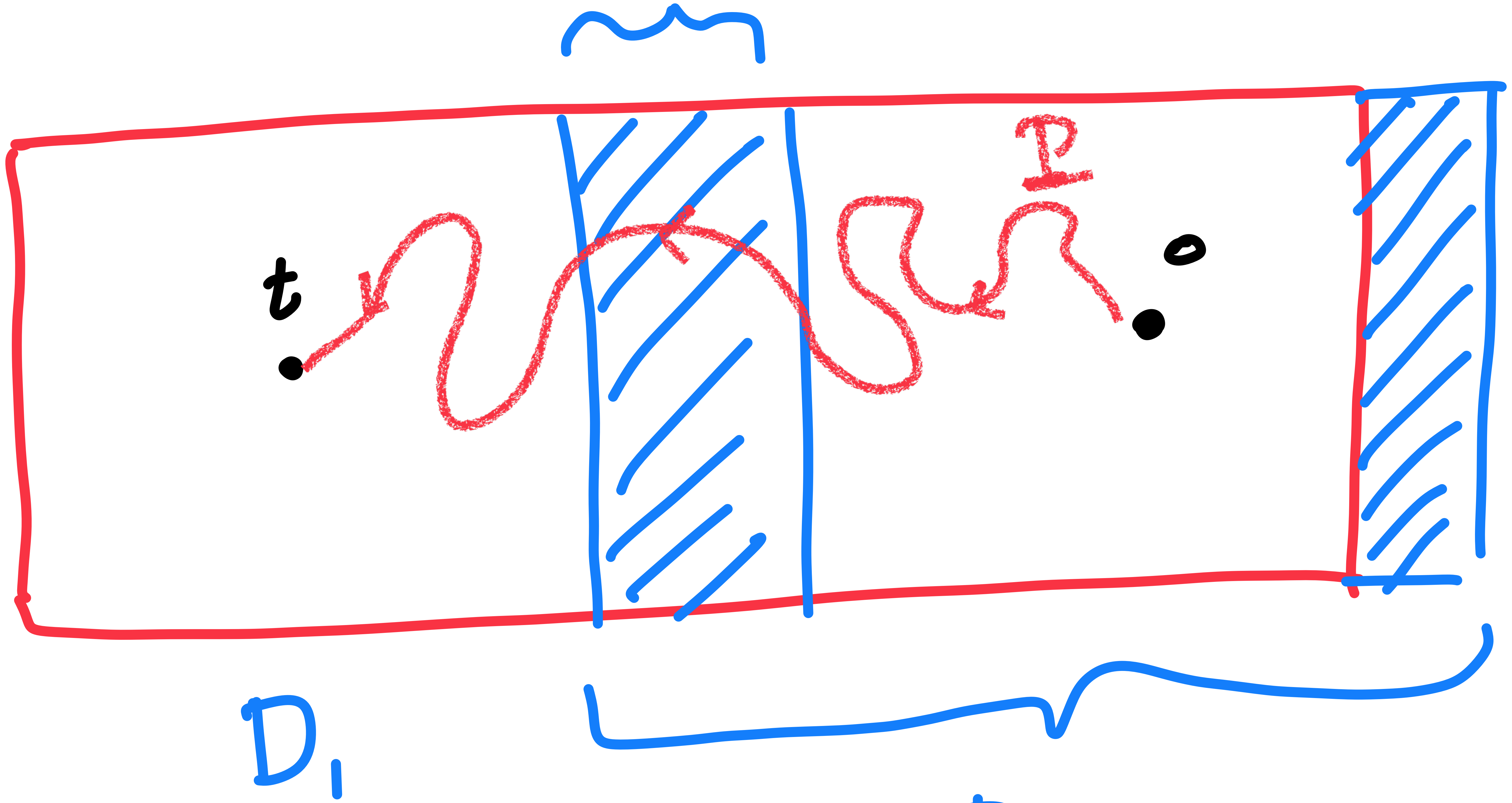
$\underline{QCD}$: problem with fermions !!

$$C_{2p}^{(N)} = \frac{1}{\mathcal{Z}} \int \mathcal{D}U \; B_t^{ijk} \underbrace{P_t^{ii'} P_t^{jj'} P_t^{kk'}}_{\text{non-local}} \bar{B}_0^{i'j'k'} \underbrace{\det(D^\dagger D)}_{\text{non-local}} \underbrace{e^{-S_g'(U)}}_{\text{local}}$$

$P = D^{-1}$ D : sparce matrix, depends on U

Solution:
- Approximate factorization of $\det D^\dagger D$
- Approximate factorization of D^{-1}
  - Drop all terms that couple the domains
  - Correct statistically the systematic error

Thick Boundary : essential for minimizing errors



D2

Schur decomposition,

Schur complement couples domains

- Drop coupling terms
- Correction through combination of reweighting and low statistics evaluation of the bias

M. Ce et al arXiv: 1601.04587

The Plan

1) Implement factorization of the D^{-1}
   - Incorporate distilation
   - Extend the method to 3-point functions
   - Preliminary test in Quenched QCD (i.e. $\det D^\dagger D = 1$)

- If succesfull

2) Implement $\det(D^\dagger D)$ factorization for 2 light and strange flavors.
   - Generate test ensemble
   - Test the effectiveness of the method.

- Can we improve our physics results with this approach?

Thank you!