Some ideas for WP2

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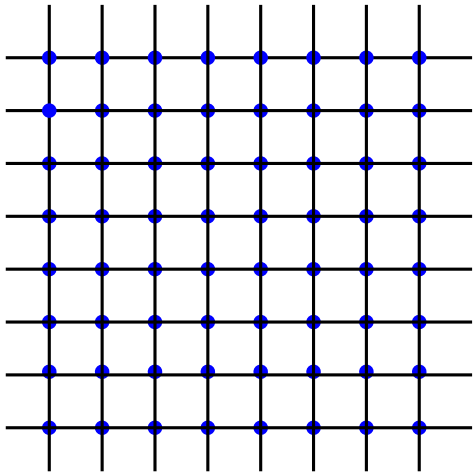
Lattice QCD in a Nutshell

Formulate QCD on a hypercubic lattice in Euclidean space-time

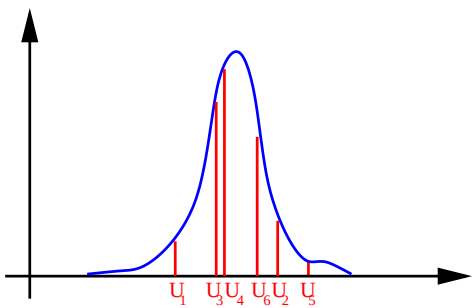
$$\langle O \rangle = \frac{1}{Z} \int dU \, e^{-S[U]} O[U]$$

Numerical evaluation of this integral.



Very high dimensional
$\rightarrow$ Monte Carlo method

$$\frac{1}{Z} \int e^{-S[U]} [dU] O[U] \rightarrow \frac{1}{N} \sum_{i=1}^{N} O[U_i]$$



Lattice QCD in a Nutshell

Markov Chain Monte Carlo

Generate series of gauge fields

$$U_1 \to U_2 \to \cdots \to U_N$$

Molecular dynamics

Transitions by solving classical mechanics system

Dirac equation

Force computation needs solution of Dirac equation = sparse linear system
Largest fraction of cost in simulations.

Lattice QCD in 2001

Talk by Ukawa at Lattice 2001

Cost of a simulation (Ukawa Lattice 2001)

$$\text{Cost} = C \left[\frac{\#conf}{1000}\right] \cdot \left[\frac{m_\pi}{4 \times 135\,\text{MeV}}\right]^{-6} \cdot \left[\frac{L}{3\text{fm}}\right]^{5} \cdot \left[\frac{a}{0.1\text{fm}}\right]^{-7}$$

$C \approx 2.8$ Tflops year

Small lattice by today's standard
96×32^3, 250MeV, $a \approx 0.09$fm $\rightarrow$ few TFlops$\times$ years

With the methods of 2001: 250 TFlops$\times$ years

FERMI installation @ CINECA 2.1 PFlops $\approx$ 6 weeks

Need many of such lattices

Sources of progress

Determinant factorizations

Hasenbusch mass factorization, DD-HMC, RHMC
Reduce force fluctuations in equations of motion

Solvers for Dirac equation

Locally deflated / multi-grid solvers
Large reduction of cost of solution at small quark mass

Integrators for Molecular Dynamics

Force gradient integrators, 4th order, ...

Better methods for observables

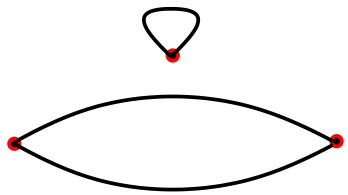
Point sources $\rightarrow$ noise sources

Future progress?

Difficult to predict → need something we can deliver

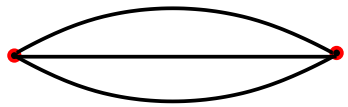
Observables with large noise

Disconnected diagrams
A lot known → very scattered



Baryons
Severe signal/noise problem at physical distances.

Accurate physics virtually impossible.



Collection of known methods — development of new methods

Reference implementations?

Linear solvers

$$D(m)\,\psi = \phi$$

Sparse linear system of equations

Classical iterative methods: cost increase with $(am)^{-1}$.

Large improvement by locally deflate / multi-grid solvers.

First production ready method Lüscher **2007** for Wilson fermions

Increasing activity

- **Improvements** $\leftrightarrow$ applied math
- Application to **other Dirac operators**

There seems to be room for improvement

Determinant factorizations

Hasenbusch's mass factorization

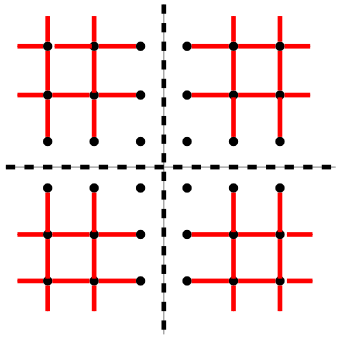
$$\det Q^2 = \det \frac{Q^2}{Q^2+\mu^2} \det(Q^2+\mu^2)$$

RHMC

$$\det Q^2 = \prod_{i=1}^{n} \det \sqrt[n]{Q^2}$$

Domain decomposition

$$\det Q = \prod_{\Lambda} \det Q_\Lambda \times \det R$$



Understand how they work and differences in performance $\rightarrow$ road to further improvement

Future Update Algorithms

New architectures

Computer architectures get more diverse

Accelerators (GPU, Phi) are a reality.

Are our **algorithms** adapted?

Seems relatively quiet area in recent years.

Wrong impression? Should this be changed?

Large volume

Global acceptance step in HMC makes large volumes expensive.

Improvements needed in the mid to long term.

Finite chemical potential

Finite chemical potential
$\rightarrow$ action not real

With a lot of effort, approximate solutions found
- reweighting
- Taylor expansion
- analytic continuation

Approaches under current investigation
- complex Langevin
- dual variables
- Lefschetz thimble
- ...

Problem highly challenging — with high potential reward

What are the approaches that fit into HPC?
Project that can deliver within set timeframe?

Summary

Conservative

Disconnected diagrams

Multi-grid

Determinant factorizations

Algor. & new machines

Higher Risk

Baryon correlation functions

Large volume

Algor. & new machines

Finite μ

Theories beyond QCD?
$\rightarrow$ Specialized methods/adaption of QCD methods?

Data analysis?