Lattice Gauge Theory and High Performance Computing

Karl Jansen

- **Introduction**
- **Static potential**
  - why quarks are not free
  - what happens when they try to escape
- **How it works**
  discretizing, simulating and back to the continuum
- **More to compute**
  α_s, m_{quark}, $\langle x \rangle$, ...
- **Why we are not happy**
  - chiral symmetry
  - Algorithms and machines
- **Outlooks and Needs**

Why Lattice Gauge Theory had to be invented

→ QuantumChromoDynamics

asymptotic freedom	confinement
distances $\ll 1\mathrm{fm}$	distances $\gtrsim 1\mathrm{fm}$
world of quarks and gluons	world of hadrons and glue balls
perturbative description	non-perturbative methods

non-perturbative methods: Lattice
(in combination with e.g. chiral perturbation theory)

- conquering the challenge K.G. Wilson 1974
- demonstrating practicability M. Creutz 1980

Spreading the news around ...

using lattice methods in many areas
different from QCD

- rigorous mathematical definition of field theories
  e.g. QCD, chiral gauge theories

- Electroweak physics
  e.g. Higgs mass bounds, strength of finite temperature phase transition

- spin models
  e.g. precise critical exponents

- Supersymmetry
  e.g. phase diagram, mass spectrum

- Quantum gravity
  e.g. matrix models, contruction of quantum gravity

What Lattice Gauge Theory can provide

- test of theory and validity of analytical methods
  → overlap with
  - *perturbation theory*
  - *chiral perturbation theory*
  - *large-N expansion*
  - *sum rules*

- precise values of many physical observables
  → overlap with
  - *phenomenology*
  - *experiment*

- understanding of strong interaction
  - *semi-classical picture*
  - *monopoles, instantons*

Example: electroweak phase transition

→ test of perturbation theory

exciting possibility: *baryon-asymmetry* of the universe is generated in an early stage of the universe at the *electroweak phase transition* at $T_c \approx 250\text{GeV}$

Condition Sakharov;Kuzmin,Rubakov,Shaposhnikov

– rate of baryon generation $\neq$ rate of baryon annihilation

→ out of equilibrium phenomena

→ strong enough *first order* phase transtion

$\frac{v_T}{T_c} > 1$	jump of order parameter v_T large enough
v_T	*Higgs vacuum expectation value*
T_c	*critical temperature*

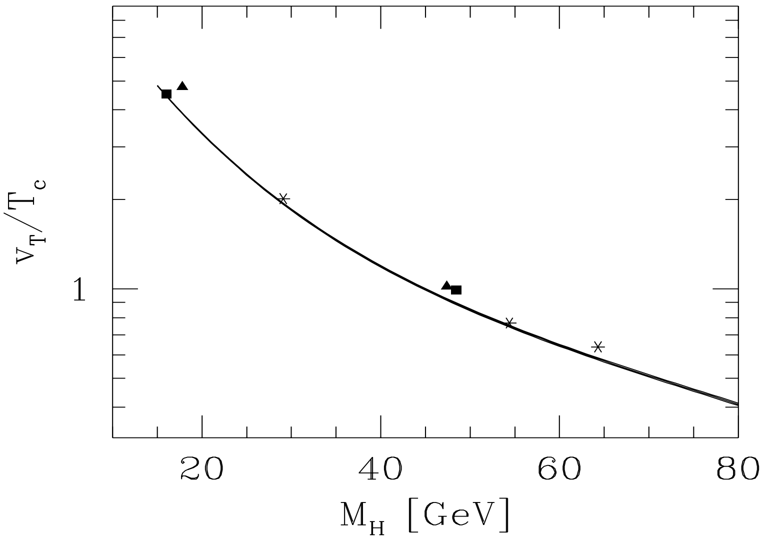
electroweak physics $\Rightarrow$ use perturbation theory

Buchmüller, Fodor, Hebecker

uncertainty in perturbation theory triggered
numerical lattice simulations of the electroweak sector
(SU(2)-Higgs model)

- 4-dimensional simulations at finite temperature
  Fodor, Hein, Jansen, Jaster, Montvay

- 3-dimensional effective field theory simulations
  Kajantie, Laine, Shaposhnikov, Rummukainen

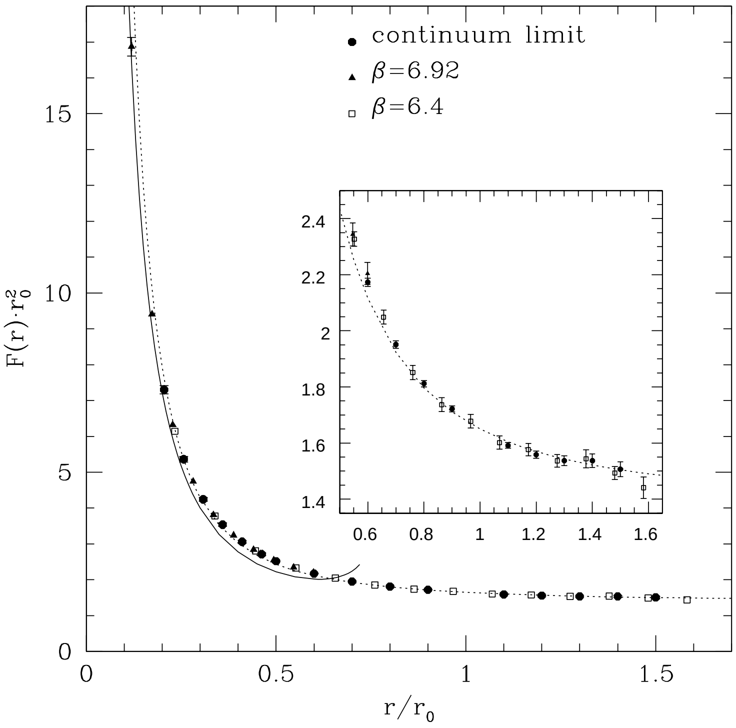


Other examples

- $g-2$: contribution of light by light scattering
- parton distributions at small momentum transfer
- matrix elements for (indirect) CP-violation
- Kaon decay matrix elements
- $\vdots$

Test of the pieces

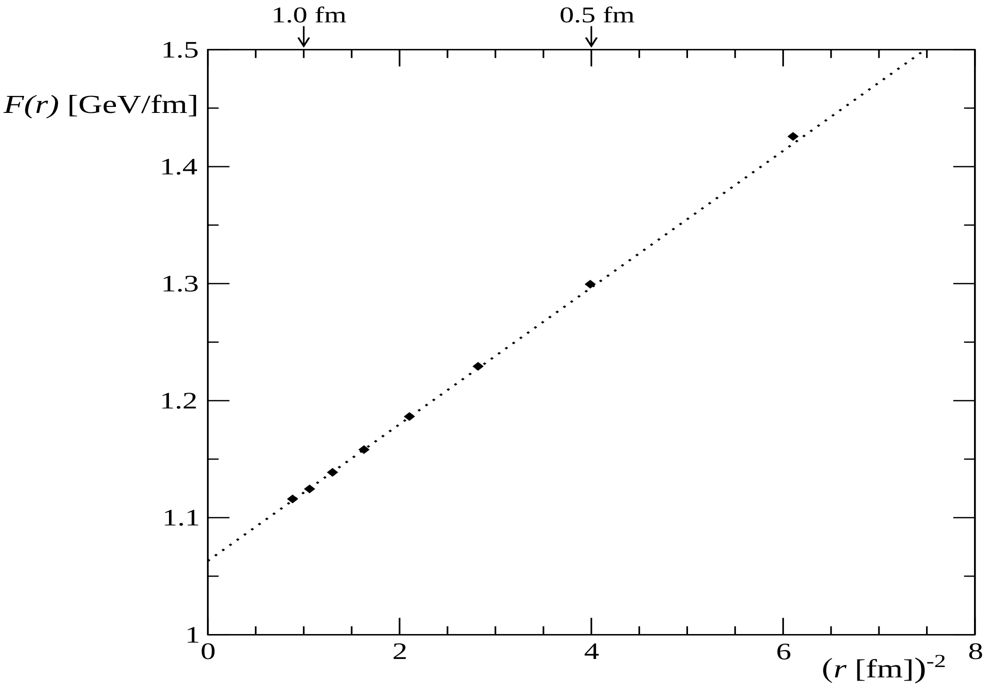
- short to intermediate ranges (Necco and Sommer)



$r_0 \approx 0.5\text{fm}$

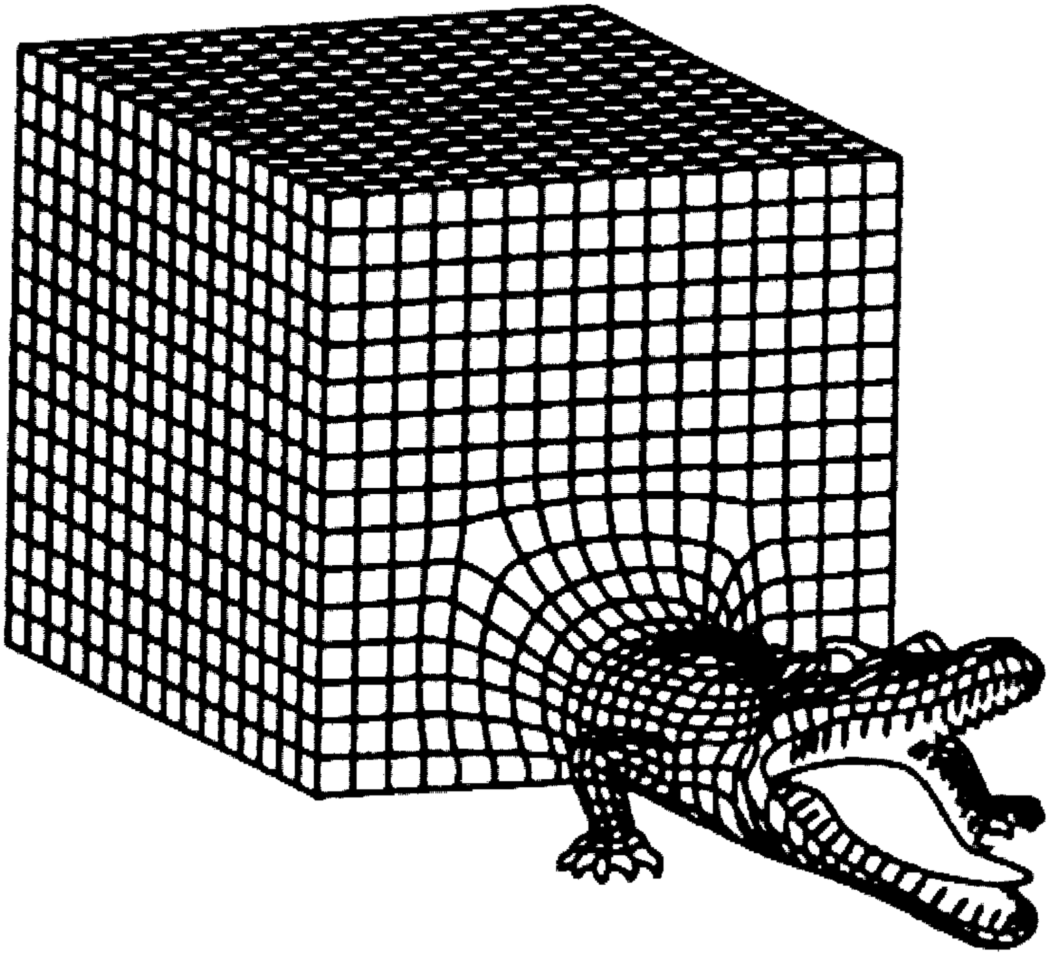
$F(r) = \alpha \cdot 1/r^2 + \sigma$

- long range (Lüscher and Weisz)



$$F(r) = \pi/12 \cdot 1/r^2 + \sigma$$

Dangerous lattice Animals



→ discretization errors

→ finite volume effects

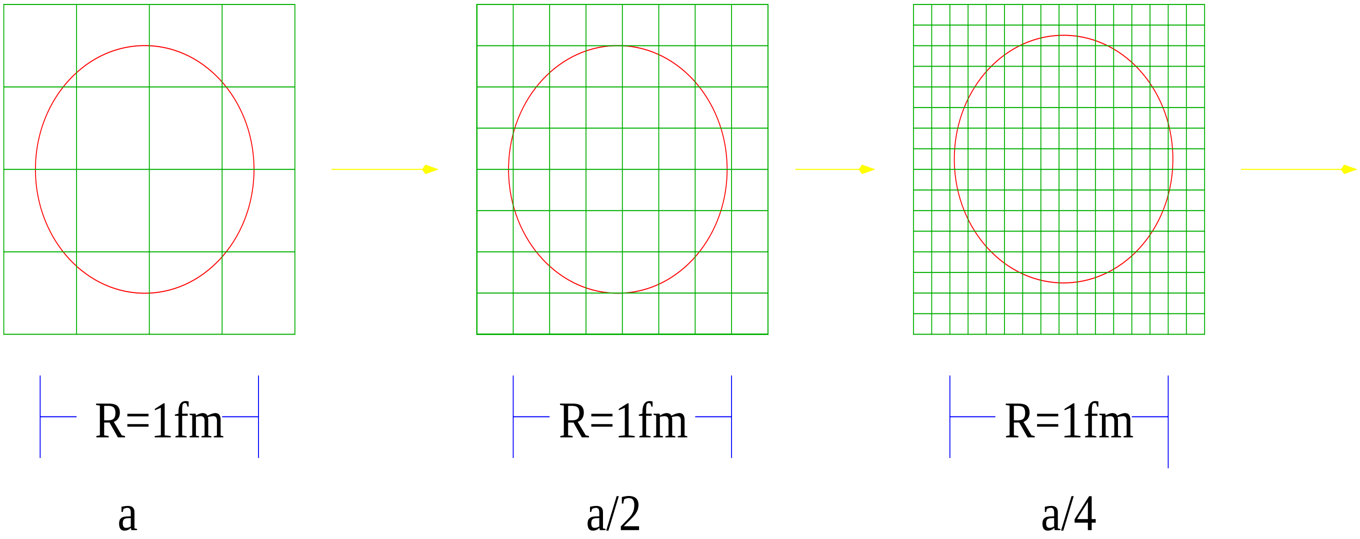
A look at the continuum limit

the general idea of the continuum limit:

we keep fixed values of physical quantities such as a particle mass $m^{\mathrm{phys}} = m^{\mathrm{lattice}}/a$

$\Rightarrow$ for $a \rightarrow 0 \Rightarrow m^{\mathrm{lattice}} \rightarrow 0$

since $m^{\mathrm{lattice}} = 1/\xi^{\mathrm{lattice}}$ in the contunuum limit
the *lattice correlation length diverges*



$\xi^{\mathrm{lattice}} \approx 2.5$ $\quad$ $\xi^{\mathrm{lattice}} \approx 5.0$ $\quad$ $\xi^{\mathrm{lattice}} \approx 10.0$

a fixed physical size of a particle (e.g. the proton) receives a finer and finer resolution as $\xi^{\mathrm{lattice}} \rightarrow \infty$

The continuum limit

fixed *physical* length $L = Na = 1\mathrm{fm}$ means

$a = 0.1\mathrm{fm} \Rightarrow N = 10$

$a = 0.05\mathrm{fm} \Rightarrow N = 20$

$a = 0.01\mathrm{fm} \Rightarrow N = 100$

number of lattice points: N^4
easily running out of computertime and memory

solutions (?)

- keep $a \gg 0 \Rightarrow$ lattice artefacts
- keep $L < 1\mathrm{fm} \Rightarrow$ finite size effects

modern approach through theoretical advances

→ accelerate continuum limit: improvement programme

→ do not be afraid of finite size effects: make use of them

Acceleration to the continuum limit

(old) standard lattice action of QCD is

$$S_{\mathrm{old}} = \underbrace{S_{\mathrm{G}}}_{\mathrm{O}(a^2)} + \underbrace{S_{\mathrm{wilson}}}_{\mathrm{O}(a)}$$

⇒ expectation values of physical observables

$$\langle O \rangle = \langle O \rangle_{\mathrm{cont}} + \mathrm{O}(a)$$

employing all lattice symmetries, equations of motions

⇒ only one more term in $\mathrm{O}(a)$ possible

(improved) standard lattice action

Skeikoleslami and Wohlert

$$S_{\mathrm{new}} = S_{\mathrm{old}} + \underbrace{S_{\mathrm{sw}}}_{\mathrm{O}(a)}$$

$$S_{\mathrm{sw}} = a^5 \sum_x c_{\mathrm{sw}} \bar{\psi}(x) \tfrac{i}{4} \hat{F}_{\mu\nu}(x) \Psi(x)$$

with c_{sw} a *tunable* parameter

⇒ compute non-perturbatively c_{sw} such that $\mathrm{O}(a)$ cancel

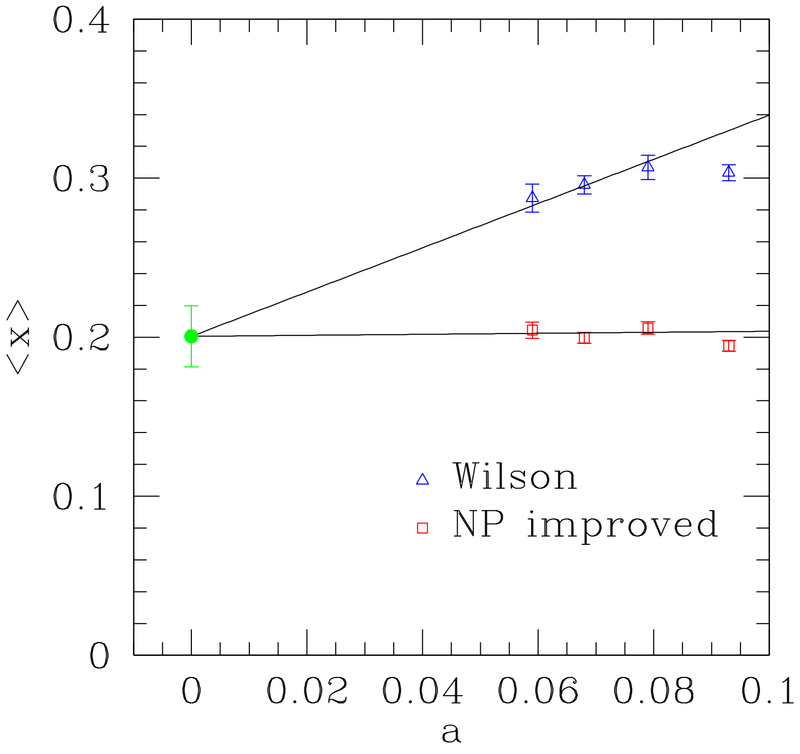
$\Rightarrow$ (nota bene: if also the operator is improved)

$$\langle O \rangle = \langle O \rangle_{\rm cont} + {\rm O}(a^2)$$

succesful *Symanzik improvement programme* of the

ALPHA
Collaboration

Example of physical quantity: *avererage momentum* $\langle x \rangle$ *of non-singlet, twist-2 operator in a pion*



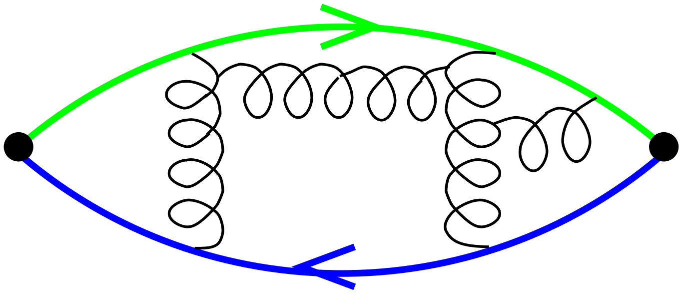
Simulations so far mostly done in

The quenched approximation

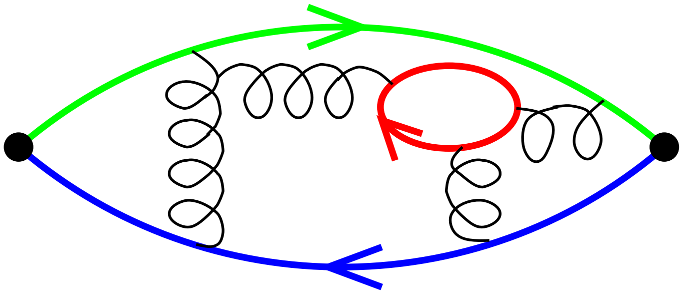
→ truncation of the theory

→ simulations much cheaper

→ surprisingly close to experimental values
O(20%) deviation for many quantities



(A) Quenched QCD: no internal quark loops



(B) full QCD

mass spectrum

one of the major goals of lattice QCD

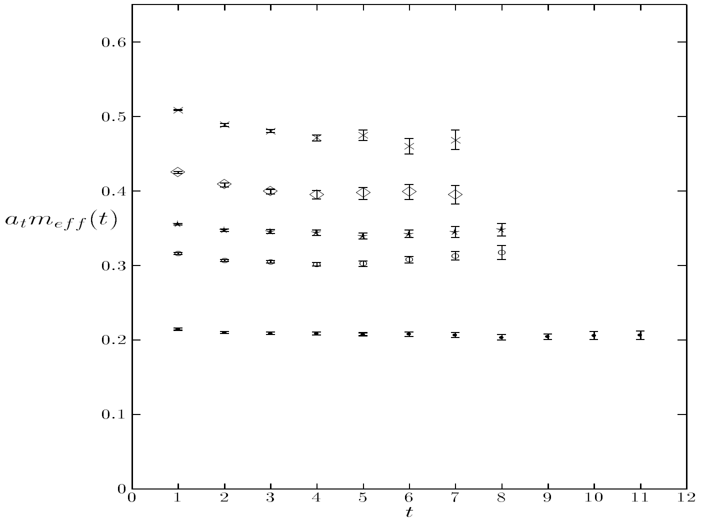
$\longrightarrow$ compute hadron masses from first principles

define appropriate operators at zero momentum

$$O(t) = \sum_{\mathbf{x}} O(\mathbf{x}, t)$$

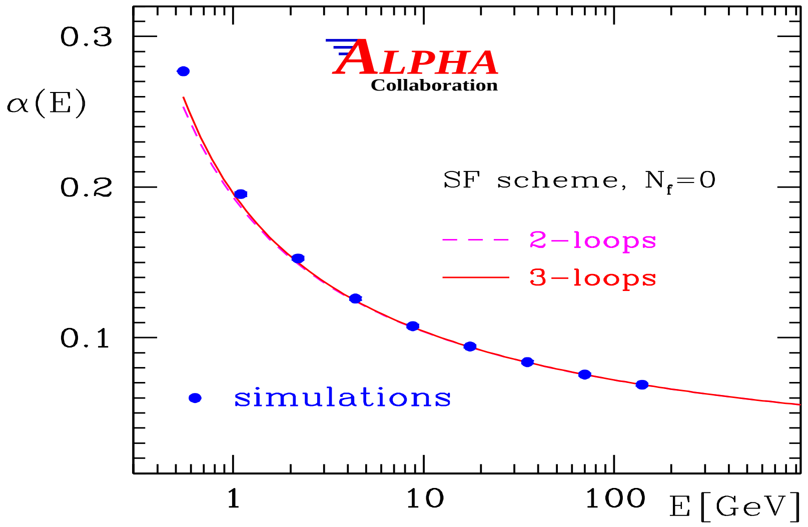
$$\begin{aligned} \langle O(0)O(t)\rangle &= \frac{1}{\mathcal{Z}} \sum_n \langle 0|O(0)e^{-\mathbb{H}t}|n\rangle\langle n|O(0)|0\rangle \\ &= \frac{1}{\mathcal{Z}}\sum_n |\langle 0|O(0)|n\rangle|^2 e^{-(E_n-E_0)t} \end{aligned}$$

$\longrightarrow$ effective masses $\quad m_{\text{eff}}(t) = -\ln\frac{\Gamma(t+1)}{\Gamma(t)}$

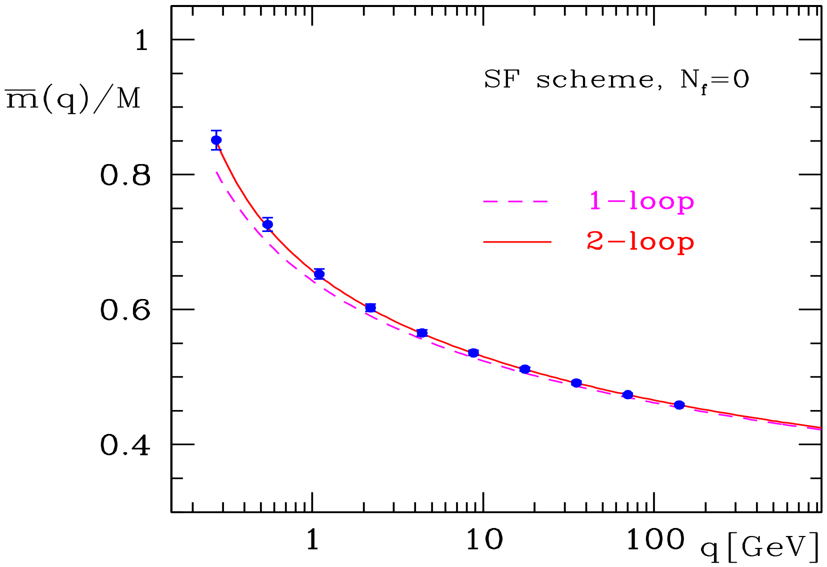


Fundamental Parameters of QCD

- running coupling $\alpha_s(E)$



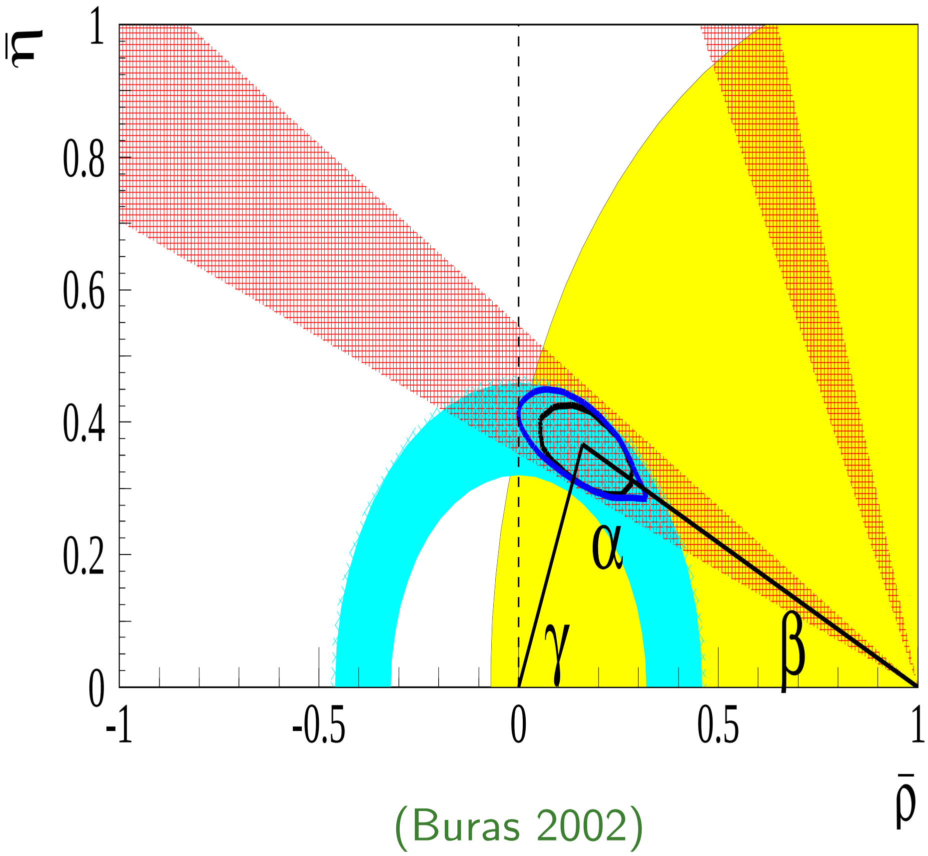
- running quark mass $m(q)$



non specialist introduction

R. Sommer and H. Wittig, physics/0204015

Unitarity triangle

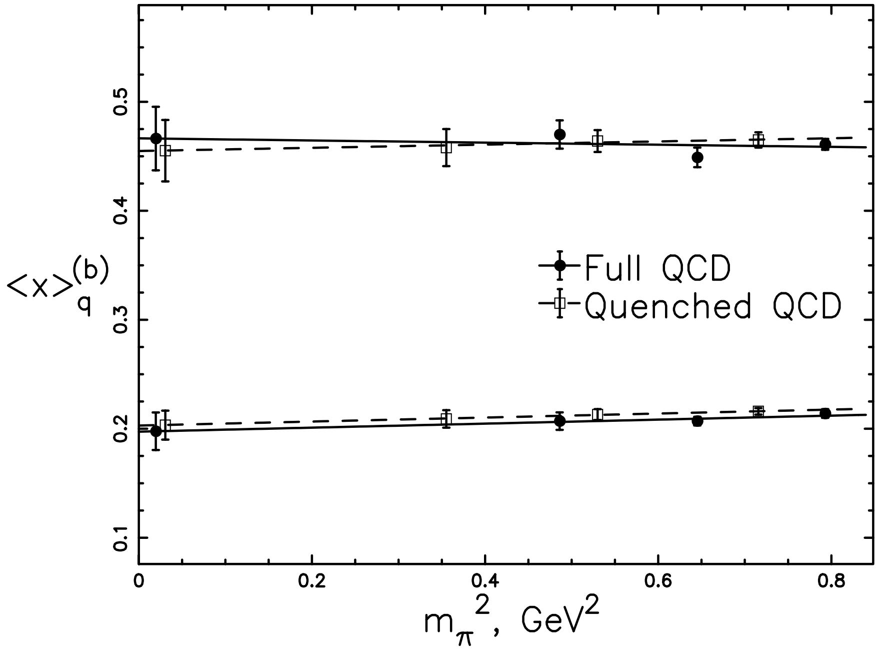


(Buras 2002)

→ sides of triangle constrained by results of lattice calculations

Moments of Parton distribution functions

example: lowest moment of twist-2, non-singlet operator in pion



LHPC, MIT-Wuppertal, QCDSF collaboration

quenched numbers:

Guagnelli,Jansen,Palombi,Petronzio,Shindler,Wetzorke

$$\langle x \rangle^{\text{experiment}}(\mu = 2.4\text{GeV}) \quad = \quad 0.23(2)$$

$$\langle x \rangle^{\text{quenched}}_{\overline{\text{MS}}}(\mu = 2.4\text{GeV}) \quad = \quad 0.30(3)$$

Cost of numerical simulations

Quenched fermions

expensive part: fermion (quark) propagator D^{-1}

$$\langle\bar{\psi}(x)\psi(y)\rangle \propto D^{-1}b$$

b is external source vector

$\Rightarrow$ need to solve

$DX = b$ with D a complex matrix that is

- high-dimensional $O(10^6) \otimes O(10^6)$
- sparse (diagonal and a few subdiagonals)

example: quenched $16^3 \cdot 32$ lattice:
≈ 100Mflops for one fermion matrix times
vector multiplication

having a 50 Gflops (sustained) machine
$\Rightarrow$ about 10 hours for a physical result at one set of parameters

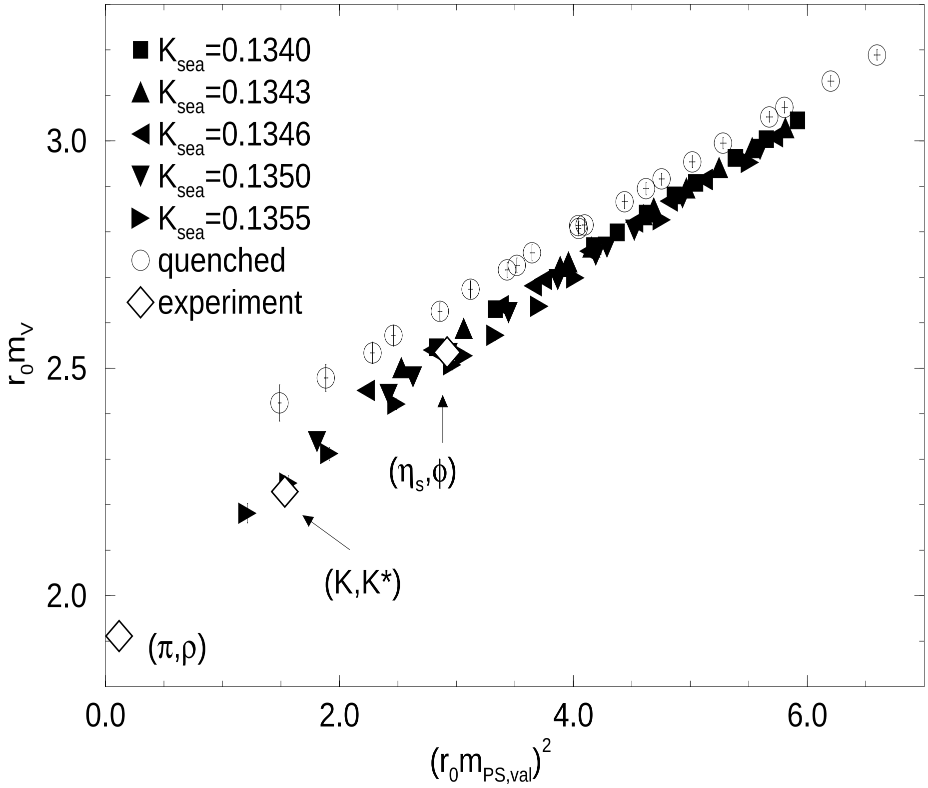
realistic lattices today: $32^3 \cdot 64$ or $48^3 \cdot 96$
$\rightarrow$ factor 10 to 100

Dynamical fermions

$\rightarrow$ additional factor of O(100)

First results with dynamical fermions

example: vector meson spectrum



JLQCD collaboration

- effects of dynamical quarks visible
- systematics not under control yet
  - *continuum limit*
  - *finite size effects*
  - *ρ-meson decay*

Dynamical fermions

generate new configuration by integrating the field equations in a *Monte Carlo time* τ

$$\begin{aligned} \delta\pi/\delta\tau &= -\delta S/\delta U \\ \delta U/\delta\tau &= \pi \end{aligned}$$

fields: *gauge fields* U
conjugate momenta π

numerical integration ⇒ non-vanishing step size $\delta\tau$

experience: $\delta\tau N_\tau = 1$, $\delta\tau \approx 0.01$

discrete integration step size ⇒ integration error
⇒ global *accept/rejection step*

The difficulty:

$\delta_U S \propto \left[D^\dagger D\right]^{-1}\Phi$, Φ Gaussian random vector

since $N_\tau \approx 100$
⇒ simulations are $O(100)$ more expensive than quenched approximation

Costs of dynamical fermion simulations

see panel discussion in Lattice2001, Berlin, 2001

Cost of 1000 dynamical $N_{\mathrm{F}} = 2$ configurations

$$\begin{aligned} C_{\mathrm{per}} &= F_{\mathrm{per}} \left(\frac{m_\pi}{m_\rho}\right)^{-z_\pi} \left(\frac{L}{a}\right)^{z_L} \left(\frac{r_0}{a}\right)^{z_a} \\ F_{\mathrm{per}} &= 6 \cdot 10^6 \mathrm{flops} \\ z_\pi &= 6, \quad z_L = 5, \quad z_a = 2 \end{aligned}$$

given a 10 Teraflops computer,
lattice spacing $a = 0.1$fm, physical volume of 2fm^4

- for $m_\pi/m_\rho = 0.5 \rightarrow$ 70 days
- for $m_\pi/m_\rho = 0.4 \rightarrow$ 270 days

- do not simulate directly at the physical point
- combine simulation results with analytical methods to extrapolate
  $\rightarrow$ *chiral perturbation theory*

question of overlap region of simulation and
chiral perturbation theory major research topic
is $m_\pi/m_\rho = 0.4$ sufficient?

From enemies to friends:
Chiral symmetry on the lattice

chiral symmetry (exchange of massless left and right-handed fermions) very important to explain low-energy phenomena

in the continuum:
chiral symmetry expressed as $D_{\text{cont}}\gamma_5 + \gamma_5 D_{\text{cont}} = 0$

on the lattice: different anti-commutation relation

$$\boxed{\begin{array}{c} \gamma_5 D_{\text{latt}} + D_{\text{latt}}\gamma_5 = 2aD_{\text{latt}}\gamma_5 D_{\text{latt}} \\ \rightarrow \gamma_5^{\text{cont}} \rightarrow \gamma_5^{\text{latt}} = \gamma_5^{\text{cont}}(1 - aD_{\text{latt}}) \end{array}}$$

realizations of such a D_{latt}

- overlap operator (Neuberger)
- domain wall fermions (Kaplan, Shamir)
- fixed point action (Hasenfratz, Niedermayer, Wiese)

chiral invariant formulations of lattice QCD

↑ enjoy many properties of continuum theory

↑ can reach very small quark mass region

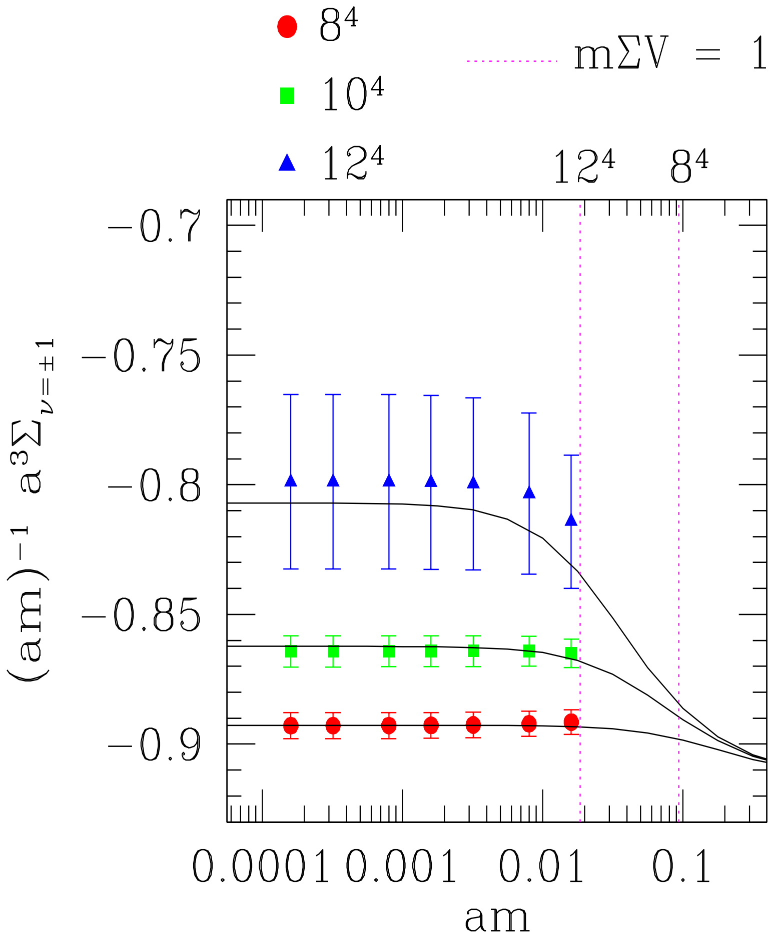
↓ are $O(100)$ more expensive than standard lattice fermions

Scalar condensate

data points at 7 masses on 3 volumes
attempt a fit according to chiral perturbation theory

$$\Sigma_{\nu=\pm 1} = m\Sigma^2 V + O((m\Sigma V)^2) + C/a^2$$

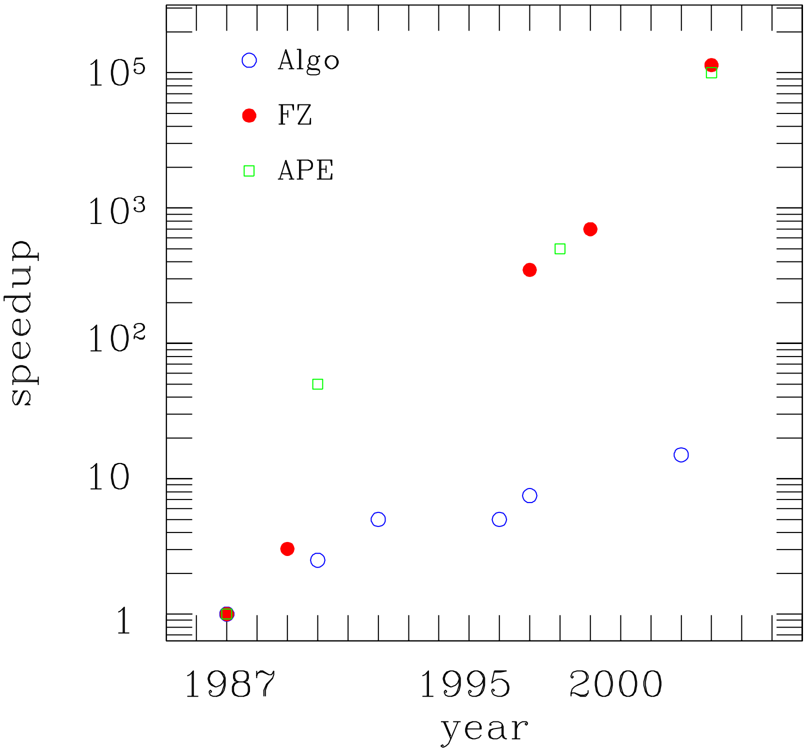
$\longrightarrow$ fixed topological sector $\nu = \pm 1$
$\longrightarrow$ only two free parameters infinite volume
scalar condensate Σ and divergence C



(Hernandéz, Lellouch, Jansen, hep-lat/0203029)

$\Rightarrow$ *find strong evidence for spontaneous chiral symmetry breaking in QCD!*

Algorithm and Machine Development



○ : algorithm development: factor 20

● : FZ CRAY at Research centre Jülich

□ : "Array Processor Experiment" (APE)

– machine development most important

– APE and CRAY equal performance
(following both Moore's law)

– cost(CRAY) $\approx 10\times$ cost(APE)

$\Rightarrow$ worthwhile to build machines
APE (*Europe*), QCDOC (*USA*), PC-Cluster

Japan

Computational Physics on Parallel Array Computer System
→ CPPACS

collaboration of lattice physicists from Tsukuba
+ industrial partner Hitachi

614 Gflops peak speed
128 Gbytes memory
2048 Processing units

future development → ?

USA

QCD on digital Signal Processor System
→ QCDSP

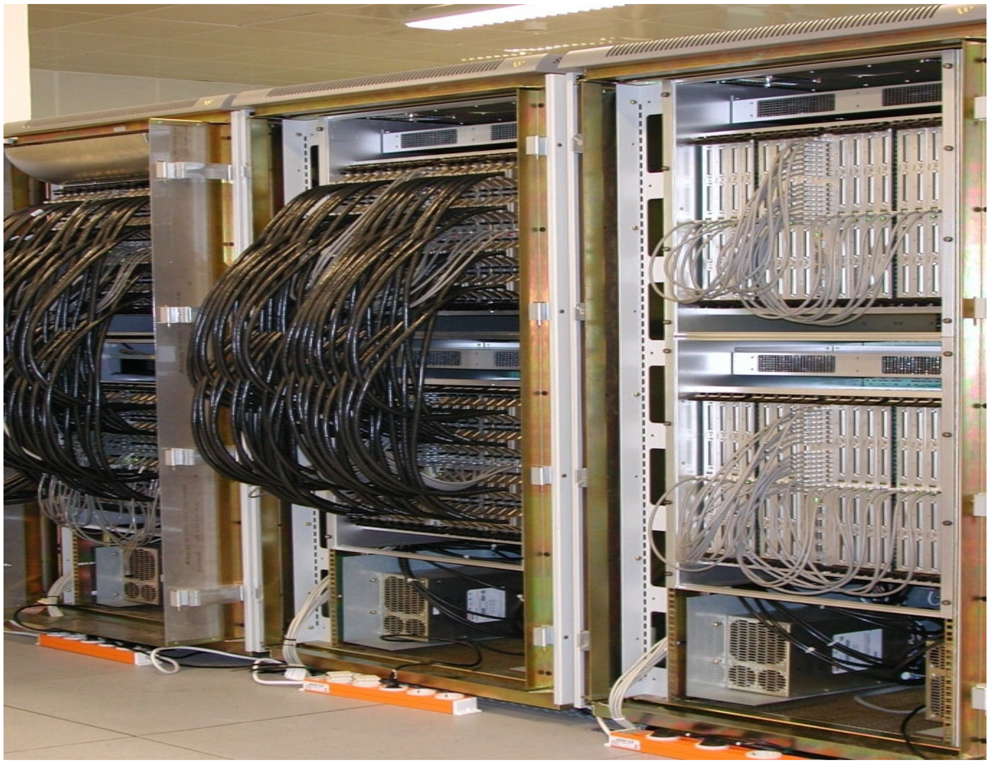
600 Gflops peak speed
50 Gbytes memory
12 288 Processing units

future development → QCDOC (QCD On Chip)
collaboration of lattice physicists from Columbia University, RIKEN, BNL and UKQCD + industrial partner IBM

10 Tflops peak speed
40Gbytes on chip + O(1) Tbytes external memory
O(10 000) Processing units
$1/Mflops sustained performance

Europe

Array Processor Experiment → APE



APEmille installation in Zeuthen

550 Gflops peak speed
32 Gbytes memory
1024 Processing units

future development → apeNEXT
collaboration of lattice physicists from INFN, DESY
and University of Paris Sud

10 Tflops peak speed
1-4 Tbytes memory
O(6 000) Processing units
1€/Mflops sustained performance

Future needs

large machines ⇒ collaborative efforts

USA

Scientific Discovery through Advanced Computing
SciDAC

demand of about 40 Teraflops realized by

- QCDOC
- large PC-Cluster installations

evaluation of needs in Europe

- ECFA Report
  Requirements for high performance computing for lattice QCD: report of the ECFA working panel
  F. Jegerlehner et.al., CERN 2000-002, ECFA/00/200
- NuPECC Report
  The NuPECC Working Group Computational Nuclear Physics
  M. Baldo et.al., June 2000

LATTICE FORUM LATFOR

→ special situation in Germany

Forum of German lattice physicists
\+ *association of groups in Austria & Switzerland*

- common initiative of lattice physicists
  Universities, GSI and NIC/DESY
  → rich and diverse spectrum of physics
  - *Fundamental parameters of QCD*
  - *Hadron spectrum*
  - *Structure functions*
  - *Physics of B-mesons*
  - *QCD thermodynamics*
  - *QCD at non-vanishing baryon density*
  - *Supersymmetry on the lattice*
  - *Algorithms*
  - *Chiral invariant lattice QCD*
- detailled definitions of milestones
  ⇒ integrated need of 25 Teraflops (peak)
- LATFOR evaluation group
  development of benchmark suite for evaluating platforms
  apeNEXT, QCDOC, PC-Cluster, CRAY, Hitachi, IBM

The **John von Neumann-Institute of Computing (NIC)**

coorporation between **DESY** and **research centre Jülich**

- **NIC** shall provide supercomputer resources

  Zeuthen: centre of LGT
  NIC research group
  +Theory
  +Universities HU,FU
  +APE100, APEmille

  Jülich: centre of general computational science
  Supercomputers: CRAY, IBM

- **NIC** research groups
  Many particle physics (P. Grassberger)
  Elementary particle physics (K.J.)

Numerical simulations

Monte Carlo integration

compute partition function (Feynman's pathintegral)

$$Z = \int_{\mathrm{fields}} e^{-S}$$

$$\int_{\mathrm{fields}} = \prod \int \text{degrees of freedom}$$

with degrees of freedom$= O(10^6)$ - $O(10^8)$

→ *Monte Carlo method with importance sampling*
(Metropolis, heatbath, over-relaxation, cluster, $\cdots$)

propagator measurement

$$\langle \bar{\psi}(x)\psi(y)\rangle \propto D^{-1}b$$

b is external source vector

⇒ need to solve

$DX = b$ with D a complex matrix that is

- high-dimensional $O(10^6) \otimes O(10^6)$
- sparse (diagonal and a few subdiagonals)

Final remarks

★ modern lattice computations

→ do not only want to have bigger computers

→ work hard on algorithmic improvements

→ incorporate theoretical progress:

- continuum limit $a \rightarrow 0$
  ← only acceleration of approach to the continuum limit
- have developed *exact chiral symmetry on the lattice:* important theoretical (numerical?) concept
- get rid of effects of finite physical boxlength L
  ⇐ use the finite extend of the box
  Finite Size Scaling technique

on the machine side:

- race between apeNEXT and QCDOC
- question: *role of PC-clusters*

big challenge is present transition towards
dynamical fermion simulations

- exciting → real physics
- powerful supercomputers are an essential ingredient
- combination with analytical methods are equally neccessary