Advances in the Hybrid Monte Carlo algorithm for Lattice QCD

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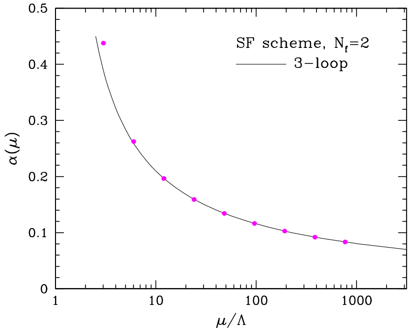
Excited QCD Workshop, Peniche

QCD: Problems not accessible by PT

Two extremal regimes:

- high energy $\rightarrow$ quarks essentially free: asymptotic freedom
- low energy $\rightarrow$ quarks confined into hadrons



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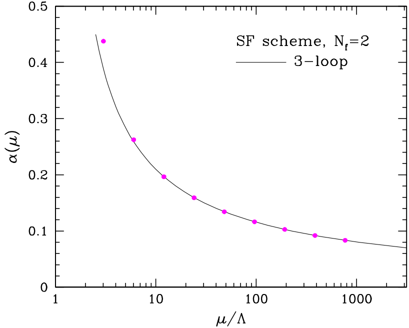

At low energy/momentum transfer: perturbation theory methods fail!

QCD: Problems not accessible by PT

Chiral symmetry breaking

- Explicit: Not-zero quark masses
- Spontaneous: The pion is a Goldstone boson

Confinement and the low energy properties of hadrons

- Hadron masses
- Low energy parameters (decay constants, LEC of ChPT)

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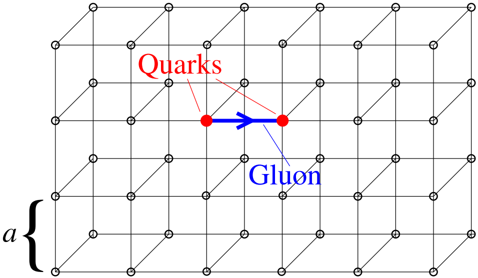
Non-perturbative methods needed: lattice QCD

Quark and Gluon fields on the lattice

$S_{QCD}[\psi, \bar{\psi}, A] = S_G[A] + S_F[\psi, \bar{\psi}, A]$



Quarks $\sim \overline{\psi}(x), \psi(x)$

Gluons $\sim$ "Link variables" $\sim$ Parallel transporter $\sim$ $U_\mu(x) = e^{iagA_\mu}$

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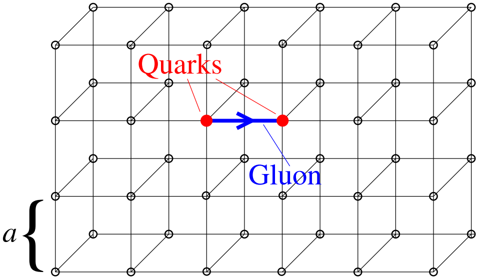

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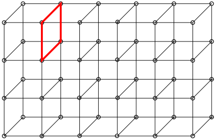
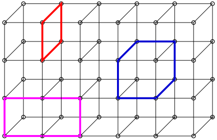
Extracting observables on the lattice

- $\langle O[\psi, \overline{\psi}, U] \rangle = \frac{1}{Z} \int DU\mathcal{D}\psi\mathcal{D}\overline{\psi} e^{-S_G[U]-S_f[U,\psi,\overline{\psi}]} O[\psi, \overline{\psi}, U]$

- S_G





- S_F

$$\int \mathcal{D}\ \psi \mathcal{D}\ \overline{\psi}\ e^{-\overline{\psi}\ (\gamma_\mu D_\mu + m_q)\ \psi} \quad \approx \quad det\ (\gamma_\mu D_\mu + m_q)$$

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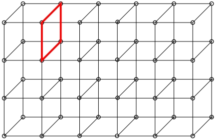

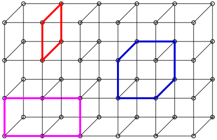

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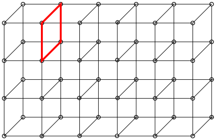
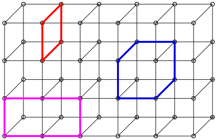
- Non-local object on the lattice → impossible to compute exactly!
- Contributions from quark loops to $\langle O[\psi, \overline{\psi}, U] \rangle$

Extracting observables on the lattice

- $\langle O[U] \rangle = \frac{1}{Z} \int DU \; e^{-S_G[U]} \; det\; (\gamma_\mu D_\mu + m_q) \; O[U]$

- S_G





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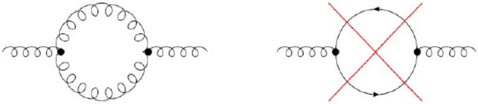
Dynamical quark effects

- **Quenched approximation:** $det\ (\gamma_\mu D_\mu + m_q) = 1$

  $\longrightarrow$ Quark loops are completely supressed



- Success of lattice QCD: confinement in strong coupling [Wilson, '74]
- Right order of scales: $m_\pi / f_\pi = O(10)$
- With the technology from the 1980's!

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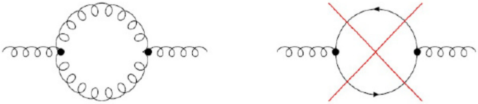
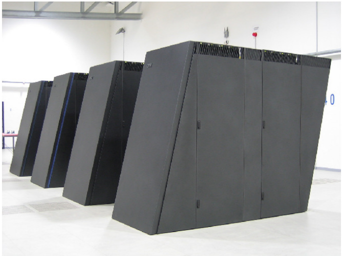
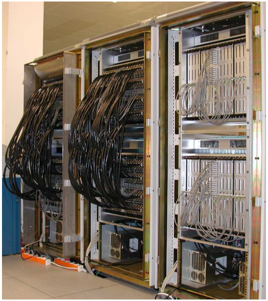


- Success of lattice QCD: confinement in strong coupling [Wilson, '74]
- Right order of scales: $m_\pi / f_\pi = O(10)$
- With the technology from the 1980's!
- But: **Making it a precision tool is very hard!**

Lattice QCD as a precision tool





- Requirements:
  - **Physical quark masses**
  - **Fine lattice spacings**
  - **Good control over many details of the simulations**
- Typical lattice sizes: ~ 3 *fm*
- 64ˆ3 x 128 lattice $\longrightarrow$ 34000000 points
- lattice spacings a: $0.04 - 0.08$ *fm*

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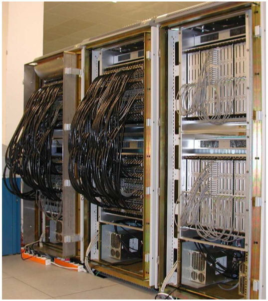

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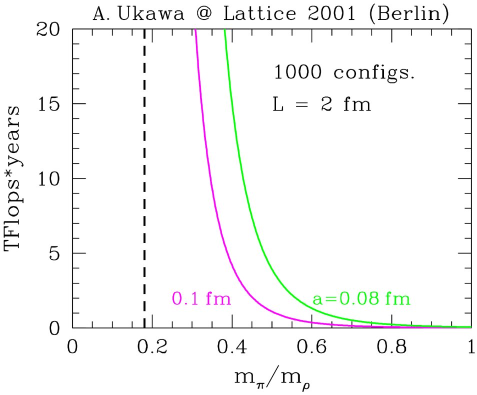
- Need for supercomputers and advanced algorithms

Cost of dynamical fermion simulations

- Panel discussion on Lattice 2001 in Berlin ("Berlin Wall plot")
- Estimated cost to generate 1000 independent fermion configurations



- Impossible to reach the domain of physical m_π

Why is simulating fermions so expensive?

- We need to compute:

$$det\ (\gamma_\mu D_\mu + m_q)$$

- Determinant can be represented by bosonic fields → "pseudofermions"

$$det\ (\gamma_\mu D_\mu + m_q) \propto \int \mathcal{D}\Phi^\dagger\ \mathcal{D}\Phi\ e^{\ \Phi^\dagger\ (\gamma_\mu D_\mu + m_q)^{-1}\ \Phi}$$

- Effective action:

$$S_{eff} = \Phi^\dagger\ (\gamma_\mu D_\mu + m_q)^{-1}\ \Phi$$

- Solving:

$$\chi = (\gamma_\mu D_\mu + m_q)^{-1}\ \Phi$$

very expensive for:

- small quark mass m
- large lattice extent $\frac{L}{a}$

Hybrid Monte Carlo

[Duane, Kennedy, Pendleton, Roweth, 1987]

- Most used algorithm for lattice QCD
- Introduce momenta $P_\mu(x)$ conjugate to fundamental fields $U_\mu(x)$ and the Hamiltonian:

$$\mathcal{H} = \frac{1}{2} \sum_{n,\mu} P^2_{n,\mu} + S[U]$$

- **Molecular dynamics (MD)** evolution of P and U

$\longrightarrow$ by numerical integration of the corresponding e. o. m.

$$(P, U) \quad \rightarrow \quad (P', U')$$

- **Metropolis accept/reject step**

$\longrightarrow$ to correct for discretization errors of the numerical integration

$$P_{acc} = min\{1, exp(-\Delta\mathcal{H} = \mathcal{H}(P', U') - \mathcal{H}(P, U))\}$$

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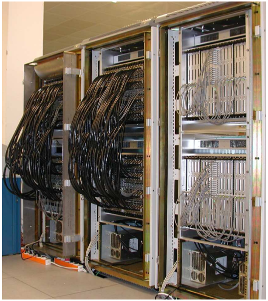

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Preconditioning

- Most expensive part: $det\ (\underbrace{\gamma_\mu D_\mu + m_q}_{Q})^2$

- Precondition by factorization (suitable C and E)

  $detQ^2 = det(C) \cdot det(E)$

  $\rightarrow$ C and E better "behaved" than Q^2

- Different preconditioning approaches:
  - Mass preconditioning [Hasenbusch '01]
  - Domain decomposition [Lüscher '04]
  - polynomial filtering [Peardon, Sexton '02]
  - n^{th}-root trick [Clark, Kennedy '06]
  - . . .

- Often is the case:
  - C is cheap
  - E is expensive

Hasenbusch trick (mass preconditioning)

- Precondition the fermion determinant

$$detQ^2 = det\left[Q^2 + \mu^2\right] \cdot det\left[\frac{Q^2}{Q^2 + \mu^2}\right]$$

- Corresponding effective action:

$$S_{eff} = S_G + \Phi_1^\dagger \frac{1}{Q^2 + \mu^2} \Phi_1 + \Phi_2^\dagger \frac{Q^2 + \mu^2}{Q^2} \Phi_2$$

- Can be extended to $N_{PF} > 2$ pseudo-fermion fields

- Saves large factors!

Domain Decomposition

- Blocking separate infrared from ultraviolet
- $\det D = \det D_\Omega \det D_{\Omega^*} \det \left\{ 1 - D_\Omega^{-1} D_{\partial\Omega} D_{\Omega^*}^{-1} D_{\partial\Omega^*} \right\}$

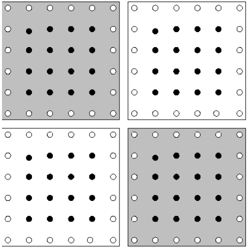
  $\Omega \ = \cup \ \{black \ \ blocks\}$

  $\Omega^* = \cup \ \{white \ \ blocks\}$

  $\partial\Omega = \cup \ \{\circ \ in \ white \ \ blocks\}$

  $\partial\Omega^* = \cup \ \{\circ \ in \ black \ \ blocks\}$

- Block fermion force + global inter-block interaction
- Multi-time scale integrator



Why does preconditioning *of the algorithm* help?

Tune preconditioner such that ($S = S_G + S_1 + S_2 + ...$)

- the most expensive part (S_j) contributes the least to the total force

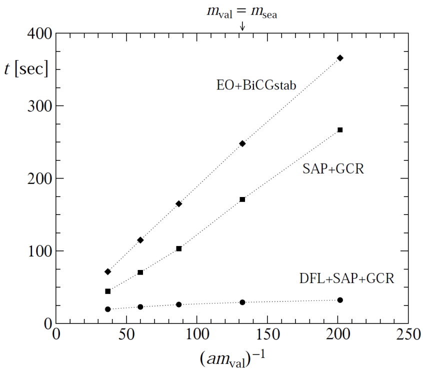
  $\rightarrow$ can be integrated with large $\Delta\tau$

- the cheaper the action part, the smaller $\Delta\tau_j$

- different parts can be integrated on different time scales

Efficient implementation in lattice QCD codes

- DD-HMC program package [M. Lüscher '06]
- MP-HMC program package [M.M, S.Schaefer '10]
- Based on the very efficient solver!



M. Lüscher, arXiv:1002.4232.

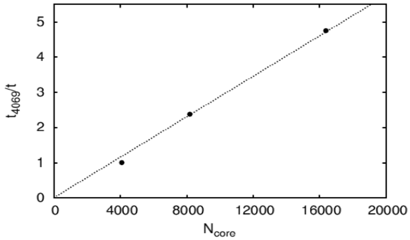
Computer time needed for the solution of the *O(a) improved Wilson Dirac* equation on a 64×32^3 lattice with spacing $a = 0.08\text{fm}$

Berlin Wall update after 2008

- Cost formula for domain decomposition

	$'01$ (HMC)	$'08$ (DD-HMC)
m_q	m_q^{-3}	m_q^{-1}
a	a^{-7}	a^{-6}
$Cost$	C	$\approx C/100$

- Similar for MP-HMC



- Mainly due to the usage of the deflated SAP-GCR solver
- Scaling of the quark mass significantly improved

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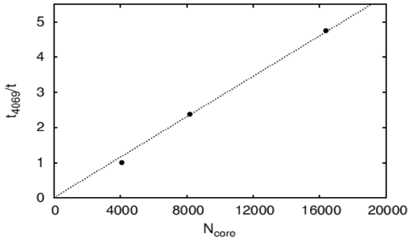
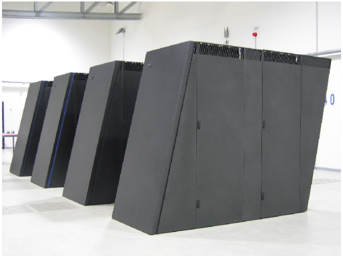
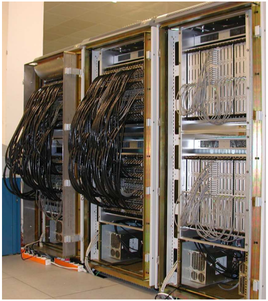


- Mainly due to the usage of the deflated SAP-GCR solver
- Scaling of the quark mass significantly improved
- **Precision computations are realistic!**

Lattice QCD as a precision tool





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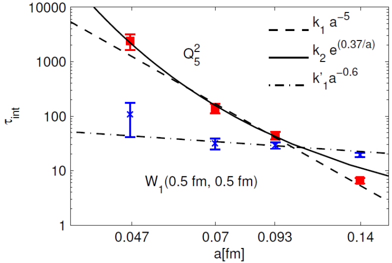
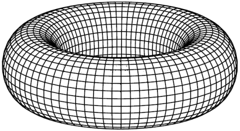
Critical slowing down for $a \to 0$

- continuum limit: varying a by a factor of 2 is not satisfactory
- $a < 0.5 fm$ needed for many observables, e.g. involving charm
- Autocorrelations: topological charge freezes as $a \to 0$

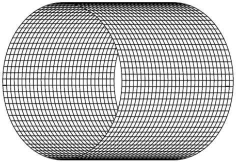


[Sommer, Schaefer, Virotta '10]

Open boundary conditions



- Periodic boundary conditions also in time
- Charge cannot flow out of the volume
- Simulations get stuck in one sector
- Cut-off effect!



- M.Lüscher and S. Schaefer [JHEP 1104 (2011) 104] and [JHEP 1107 (2011) 036]
- Open BC's in time direction
- Same transfer matrix
- Same spectrum (from the bulk)

Open boundary conditions

- Open boundaries let charge flow in and out of the volume
- Test on the pure gauge theory: ≈ 10 times smaller autocorrelations
- Will this also work including fermions?
- Needed for fine lattices

  (or some new solution to the tunneling problem)
- Test including fermions is (impatiently) expected soon!

Summary

- Entirely **non-perturbative** procedure: lattice QCD
- Quenched simulations(pure gauge): no physics information
- Including fermions: expensive calculations, many tricks in algorithms need to be applied
- Preconditioning of the HMC algorithm helps
- Efficient solver is essential(DFL-SAP-HMC)
- Critical slowing down for $a \to 0$: open boundary conditions
- Faster fermion algorithms ($+$ faster machines)

Thank you for your attention !