QCD su reticolo

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IFAE20*10* - Roma 7-9 Aprile 2010

1 – OUTLINE

- **Breve panoramica della QCD su reticolo**

- **Alcuni risultati recenti (termodinamica e diagramma di fase)**

- **Il problema della potenza di calcolo**

2 – QCD on a lattice: main ideas and difficulties

There is a large range of energies for which perturbation theory is not usable for QCD computations. No other first principle analytic tool is presently known

A possible first principle approach is to compute numerically the theory discretized on a space-time lattice, as first proposed by Wilson more than thirty years ago

K. G. Wilson, "CONFINEMENT OF QUARKS," Phys. Rev. D 10, 2445 (1974).

Key ingredients: **path integral formulation and Monte-Carlo techniques**

Essential requirement: **enough computer power to solve a very complex system**

Only in the last few years resources have become powerful enough that we can hope to really "compute" QCD

The starting point is the QCD lagrangian

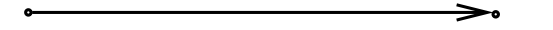
$$\mathcal{L}_{QCD} = \sum_f \bar{\psi}_i^f \left(i D_{ij}^\mu \gamma_\mu - m_f \delta_{ij} \right) \psi_j^f - \frac{1}{4} F_{\mu\nu}^a F_a^{\mu\nu}$$

ψ_i^f **are quark fields of flavor (color) index** f **(**i**) ;** A_μ^a **are gluon fields of color index** a

$F_{\mu\nu}^a = \partial_\mu A_\nu^a - \partial_\nu A_\mu^a - g f^{abc} A_\mu^b A_\nu^c$ **is the field strength tensor**

$D_{\mu\, ij} = \partial_\mu \delta_{ij} + i g T_{ij}^a A_\mu^a$ **is the covariant derivative** g **is the color gauge coupling**

An elegant gauge invariant discretization (Wilson 1974) is given in terms of elementary parallel transports, corresponding to the non-Abelian phases (rotations in color space) which a quark picks up moving from one lattice site to the other:



$$U_\mu(n) \simeq \mathcal{P} \exp(i \int_n^{n+\mu} A_\mu dx_\mu)$$ **(link variable)**

$\int d^4x F_{\mu\nu}^a F_a^{\mu\nu} \Rightarrow S_G =$ **sum on closed loops of elementary links (e.g. plaquettes)**

$\int d^4x \bar{\psi}_i^f \left(i D_{ij}^\mu \gamma_\mu - m_f \delta_{ij} \right) \psi_j^f \Rightarrow S_F = \bar{\psi}_n M[U]_{n,m} \psi_m$ **(M** $\equiv$ **fermion matrix)**

Different discretizations are possible, leading to different cutoff effects

The thermal QCD partition function is rewritten in terms of an Euclidean path integral

$$Z(V,T) = \mathrm{Tr}\left(e^{-\frac{H_{\mathrm{QCD}}}{T}}\right) \Rightarrow \int \mathcal{D}U\mathcal{D}\psi\mathcal{D}\bar{\psi}e^{-(S_G[U]+\bar{\psi}M[U]\psi)} = \int \mathcal{D}U e^{-S_G[U]} \det M[U]$$

$$T = \frac{1}{\tau} = \frac{1}{N_t a(\beta, m)}$$

where τ is the extension of the compactified time

Dynamical fermion contributions are encoded in the fermion determinant $\det M[U]$

$a \longrightarrow 0$ as the bare coupling $g_0 \longrightarrow 0$ $\Rightarrow$ we can take the continuum limit

(a gift from asymptotic freedom)

As long as $\mathcal{D}U e^{-S_G} \det M[U]$ is positive, it can be interpreted as a probability distribution $\mathcal{D}U\mathcal{P}[U]$ over gauge link configurations.

The thermal expectation value of a physical operator, $\langle O \rangle_T$, is then given by

$$\langle O \rangle_T = \frac{\int \mathcal{D}U e^{-S_G[U]} \det M[U] O[U]}{\int \mathcal{D}U e^{-S_G[U]} \det M[U]} = \int \mathcal{D}U \mathcal{P}[U] O[U]$$

As the time extension $\tau \to \infty$ ($T \to 0$) we recover vacuum expectation values:

$$\lim_{\tau \to \infty} \langle O \rangle_T = \langle 0|O|0 \rangle$$

We take also an IR cutoff (finite lattice size) $\Rightarrow$ huge but finite number of stochastic variables, distribution peaked over a restricted set of "important" configurations. Importance sampling Monte-Carlo is the ideal numerical tool to evaluate the path integral on a finite spatial volume V

3 – What can be computed?

Zero temperature

- **Time correlators of suitable operators give the mass gap in a given channel**

$$\lim_{\tau\to\infty}\langle 0|\mathcal{O}(\tau)\mathcal{O}(0)|0\rangle = \lim_{\tau\to\infty}\sum_n |\langle n|\mathcal{O}(0)|0\rangle|^2 e^{-\tau(E_n-E_0)} \sim |\langle n_{\mathcal{O}}|\mathcal{O}(0)|0\rangle|^2 e^{-\tau\Delta M_{\mathcal{O}}}$$

  Glueball and hadron masses, as well as matrix elements (beware of renormalizations ...) relevant to SM phenomenology

- **Various relevant vacuum properties: topological properties, formation and properties of the confining flux tubes between static sources, confining potentials.**

Finite temperature

- **Chiral symmetry restoration and deconfinement. Location and order of the transition (also in presence of different conditions: external fields, finite density?)**
- **Thermodynamical and Transport Properties around and above the transition**

Beyond QCD

- **Non-perturbative properties of gauge theories possibly suitable for BSM physics**

4 – Computational difficulty

UV cutoff a^{-1} and IR cutoff $L^{-1} \Rightarrow$ total number of lattice sites $\sim (L/a)^4$. What are acceptable values for L and a to get reliable computations?

$L \gg$ largest length (m_π^{-1}) and $a \ll$ shortest length $\Rightarrow$ ideally L/a at least $O(100)$.

Most expensive task: evaluation of $\det M$ (strictly non-local), needs inversion of M, whose condition number rapidly worsens as $m_{\rm quark}$ (m_π) decreases

STATE OF THE ART: $a^{-1} \sim$ few GeVs and $L/a \sim 50$, m_π as low as $200 - 300$ MeV

$\Rightarrow$ we still need some help from effective theories (CPT or HQET) to extrapolate to physical light quark masses or to study B physics.

The choice of fermion discretization:

Wilson (no doubling, no chiral symmetry, $O(a)$ errors if not improved)

Staggered (residual chiral symmetry, $O(a^2)$ errors, doubling $\Longrightarrow$ needs rooting $(\det M)^{N_f/4}$

Ginsparg-Wilson (overlap or domain wall) (residual chiral symmetry, no doubling, not strictly local and much more expensive)

The goal of really computing QCD is closer nowadays. It is not simply a matter of increasing the computational power, but also of improving algorithms and adopting improved actions with less discretization effects.

An example: computational difficulty for QCD with 2 Wilson fermions

Numerical cost for 100 statistically independent gauge configurations:

Ukawa, Lattice 2001:

$$3.10 \left(\frac{L_s}{3\ \mathrm{fm}}\right)^5 \left(\frac{L_s}{2L_t}\right) \left(\frac{0.2}{\hat{m}/m_s}\right)^3 \left(\frac{0.1\ \mathrm{fm}}{a}\right)^7 \mathrm{TFlop}\cdot\mathrm{year}$$

Del Debbio et al. 2006 **(after algorithmic and technical improvements)**

$$0.03 \left(\frac{L_s}{3\ \mathrm{fm}}\right)^5 \left(\frac{L_s}{2L_t}\right) \left(\frac{0.2}{\hat{m}/m_s}\right) \left(\frac{0.1\ \mathrm{fm}}{a}\right)^6 \mathrm{TFlop}\cdot\mathrm{year}$$

1 Tflop year $\sim 3 \cdot 10^{19}$ **floating point operations.**

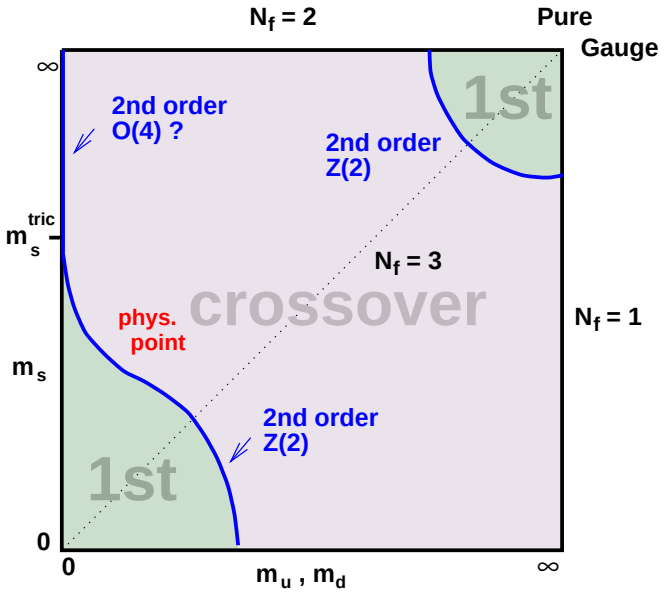
5 – What we have achieved so far (limited to finite T)

Order of the QCD phase transition

Large numerical difficulties:

- **compute susceptibilities (specific heat, order parameter) around the transition (simulations at different T) and check for divergences in the thermodynamical limit ($V \to \infty$)**
- **determine the universality class by a finite size scaling analysis**
- **keep UV cutoff effects under control**
- **Study flavor spectrum dependence**

In QCD with dynamical fermions no known exact symmetry changes its realization at deconfinement (apart from $m_q = 0$ or $m_q = \infty$), the "transition" can in principle be just a rapid analytic change (crossover).



This is the most commonly accepted diagram describing the order of the transition as function of light quark masses (Columbia plot).

Physical point consistent with crossover (Aoki et al., Nature 443, 675 (2006)): either the transition is extremely weak (hence not phenomenologically relevant) or absent.

An unsettled issue: the chiral limit of $N_f = 2$. Should be second order O(4) or first order (Pisarski, Wilczek; Basile, Pelissetto, Vicari) Data are not consistent with O(4), they are consistent with first order, but a clear signal of phase coexistence still not visible on the largest available lattices ($48^3 \times 4$). (C. Bonati, G. Cossu, M.D., A. Di Giacomo, C. Pica, 2005, 2007)

Very weak first order or very small scaling region around the chiral point?

One needs smaller masses, finer lattices and likely larger volumes to settle the issue

Thermodynamical quantities

energy density: $\epsilon = \frac{T^2}{V}\frac{\partial \ln Z}{\partial T}$

pressure: $p = T\frac{\partial \ln Z}{\partial V}$

interaction measure: $I = \epsilon - 3p$ **(= 0 for free massless particles).**

These quantities can be computed on the lattice in a well defined, sometimes not straightforward way. Derivatives must be expressed in terms of lattice parameters.

$$\frac{\partial}{\partial T} = \frac{\partial}{\partial (N_t a_t)^{-1}} = -N_t a_t^2 \frac{\partial}{\partial a_t}$$

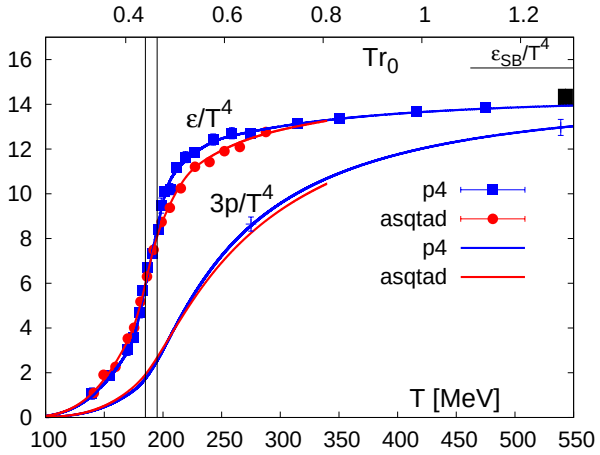
$$\epsilon = -T \left.\frac{\partial \ln g_0^2}{\partial \ln a_t}\right|_{a_s} \frac{\langle S_G \rangle}{V} + 3\beta T Re(\langle \mathrm{Tr}\Pi_s \rangle - \langle \mathrm{Tr}\Pi_t \rangle) \qquad \Pi_{s/t} = \textbf{spat./temp. plaquette.}$$

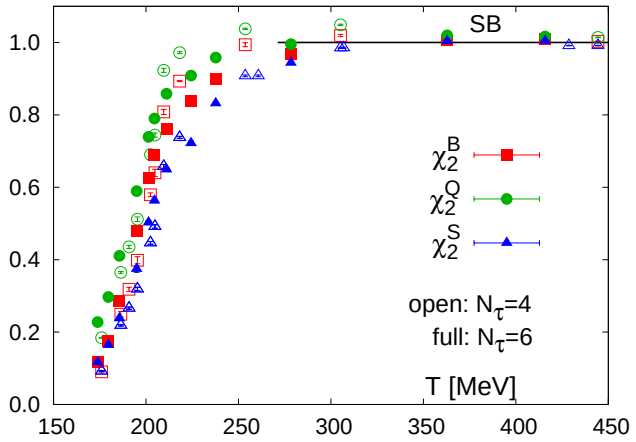
If the system is homogeneous (free energy $\propto V$**) then** $p = -f \equiv T\frac{\ln Z}{V}$

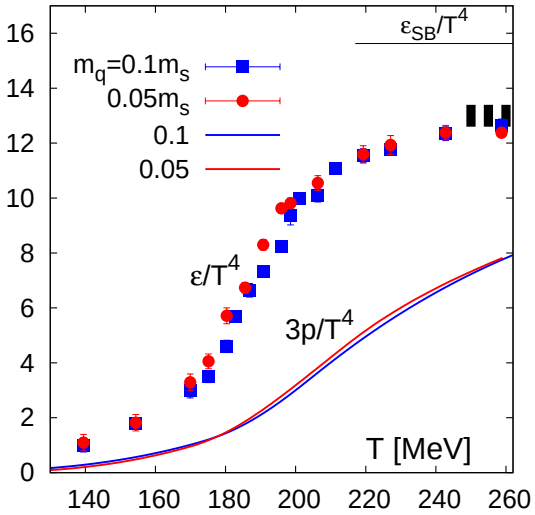
$$\frac{p(T) - p(0)}{T^4} = \frac{N_t^3}{N_x N_y N_z} \int_{\beta_0}^{\beta} \mathrm{d}\beta' \left(\langle S_G \rangle - \langle S_G \rangle_{T=0} \right) \quad .$$

$T = 0$ **subtractions are usually computed on a symmetric lattice** $N_x = N_y = N_z = N_t$

Latest state of the art results (improved staggered $N_f = 2 + 1$)







- up-left: **HotQCD, arXiv:0903.4379,** $N_t = 8$ **,** $m_q = m_s/10$**,** ϵ **and** $3p$

- right: **RBC-Bielefeld, arXiv:0811.1006,** $N_t = 6$**,** $m_q = m_s/10$**,** B, Q, S **charge fluctuations**

- down-left: **RBC-Bielefeld, arXiv:0911.2215,** $N_t = 8$**,** $m_q = m_s/20$**,** ϵ **and** $3p$

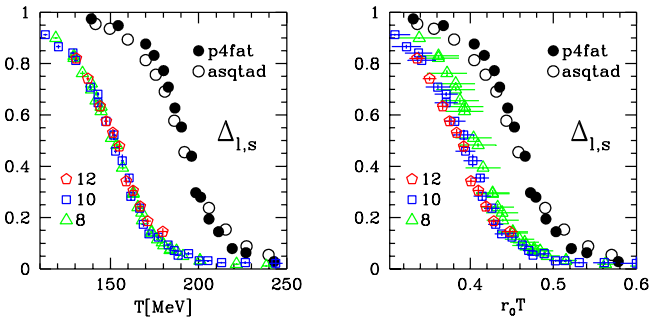
$N_t = 8 \Rightarrow \; a = 1/(TN_t) \sim 0.15$ **fm at the transition**

Continuum/chiral limit under control. Quark fluctuations saturate Stefan Boltzmann at $\sim 1.5T_c$

ϵ **and** $3p$ **do not saturate till** $3T_c$**: QGP interactions still important, but interesting physics is likely in the gluon sector (OK with large** N_c **limit ideas, contribution from topological defects? magnetic monopoles?)**

Systematic uncertainties comes back when comparing results from different collaborations about the location of the deconfinement transition and of chiral symmetry restoration:

- **RBC-Bielefeld collaboration reports coinciding deconfining and chiral restoring pseudo-critical temperatures around 190 MeV**
- **Budapest-Marseille-Wuppertal collaboration reports deconfinement at ~ 170 MeV and chiral restoration at ~ 150 MeV. Uncertainties 5-10 MeV for both collaborations**



The discrepancy is likely due residual lattice artifacts (the two collaborations use different actions) or different scale settings.

Future determinations, also using different fermion discretizations (Wilson, Ginsparg-Wilson) are mostly welcome to solve this problem

Transport coefficients: bulk and shear viscosity

Euclidean temporal correlators of the energy-momentum tensor $T_{\mu\nu}$ are related via an integral equation to its spectral density, whose low energy behaviour gives information about shear and bulk viscosities. e.g.

$$C(x_0) = \frac{1}{T^5}\int d^3\mathbf{x}\langle T_{12}(0)T_{12}(x_0,\mathbf{x})\rangle = \frac{1}{T^5}\int_0^\infty \rho_{12}(\omega)\frac{\cosh\omega(\frac{1}{2}L_0 - x_0)}{\sinh\frac{\omega L_0}{2}}d\omega \qquad \eta(T) = \pi\left.\frac{d\rho_{12}}{d\omega}\right|_{\omega=0}$$

main computational difficulties:

- **large statistics needed for measurements precise enough to solve the integral equation; limited number of points in the temporal direction anyway**
- **Some arbitrariness in the choice of the functional form of ρ and of its low energy behaviour**

Present computations still limited to pure gauge theory (Meyer, 2007, 2010; Huebner, Karsch and Pica, 2008). Shear viscosity $\eta \sim 0.2$ up to $T \sim T_c$. More problems with the bulk viscosity ζ.

6 – The sign problem at finite baryon density

A finite baryon density can be introduced by adding a finite chemical potential

$$Z(\mu) = \mathrm{Tr}\left(e^{-\frac{H_{\mathrm{QCD}}-\mu N}{T}}\right)$$

where $N = \int d^3x \psi^\dagger \psi = \int d^3x \bar{\psi}\gamma_0\psi$ **is the quark (baryonic) number operator.**

$\det M[\mu]$ **becomes complex** $\Longrightarrow$ **the path integral measure** $\mathcal{D}U e^{-S_G} \det M[U]$ **becomes complex and Monte Carlo simulations are not feasibile.**

This is usually known as the sign problem.

It is an unavoidable problem strictly related to the fact that we want to create a net unbalance between particles and antiparticles:

the Polyakov line $\mathrm{Tr}P$ **and its conjugate** $\mathrm{Tr}P^\dagger$ **describe static quark or antiquark propagation, both have real expectation values, but** $\langle \mathrm{Tr}P \rangle \neq \langle \mathrm{Tr}P^\dagger \rangle$**.**

Similar problems are met even in the path integral of two non-relativistic free fermions: solution is a clever rewriting of the partition function (restricted path integral): analogous solutions in QCD??

Possible partial solutions (short list ...)

Reweighting: Sampling is done with a different (positive) weight, the complex phase is then included in the averages. Importance sampling may fail, especially on large volumes: sampled configurations may be not relevant to finite μ physics.

Barbour et al. 1998; Z. Fodor and S, Katz, 2002

Taylor Expansion: Compute derivatives in μ of thermal quantities at $\mu = 0$. Computationally very expensive for high orders, restricted to small μ

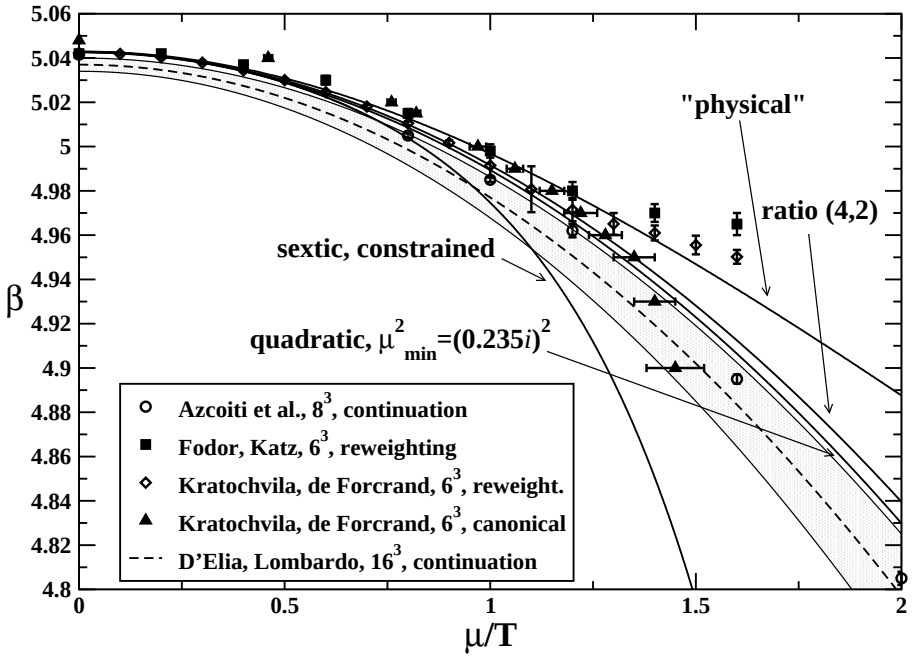
Bielefeld-Swansea collaboration 2002; R. Gavai, S. Gupta 2003

Analytic Continuation: numerical simulations are feasible for imaginary chemical potentials ($\mu^2 < 0$). A given ansatz for the dependence of physics on μ^2 can be continued to $\mu^2 < 0$ and fitted against numerical data at imaginary μ.

Predictivity restricted by domains of analyticity. Systematics affected by the choice of the ansatz.

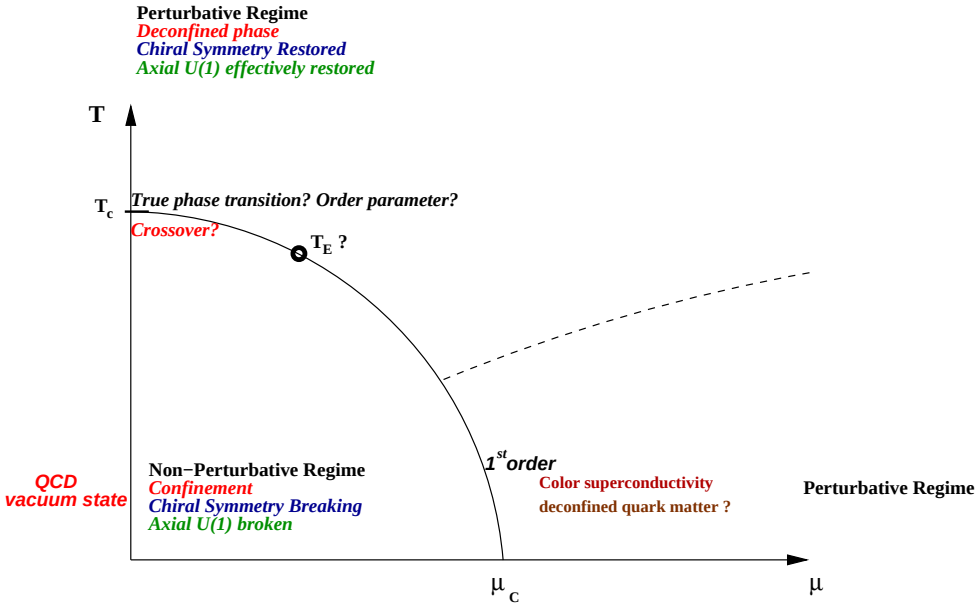
Alford, Kapustin, Wilczek, 1999; A. Hart et al. 2000; P. de Forcrand and O. Philipsen, 2002; M.D'E. and M.P. Lombardo 2003.

As a matter of fact, fully reliable results can be obtained only in a restricted region $\mu/T \lesssim 1$, where different methods and extrapolations do agree

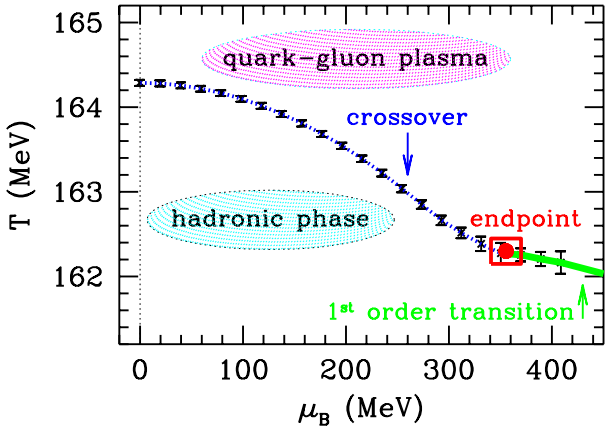


Different determinations and extrapolations of the critical line for $N_f = 4$ QCD (P. Cea, L. Cosmai, M.D., A. Papa, arXiv:1004.0184).

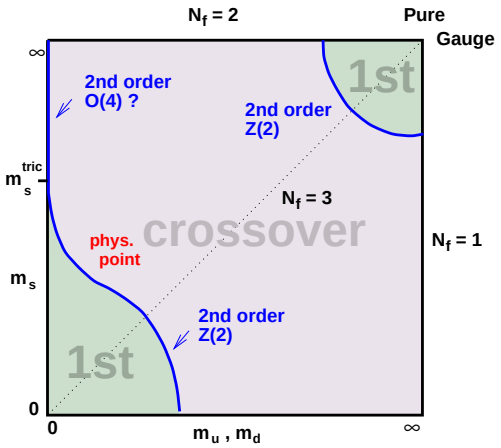
Fully reliable quantities obtainable nowadays for finite density QCD only in the region of high T and low μ.



What about the largely searched QCD critical endpoint?



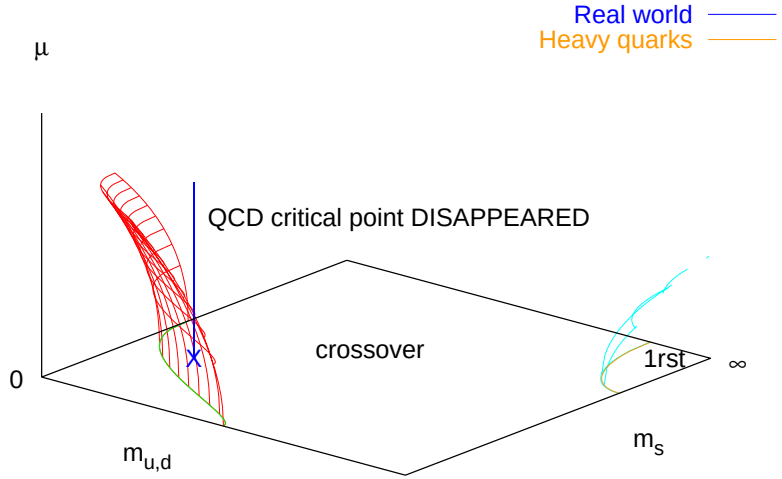
There are well known predictions (e.g. Fodor & Katz, see figure) which are however still affected by unpredictable systematic uncertainties (small volume, severe sign problem, ...)



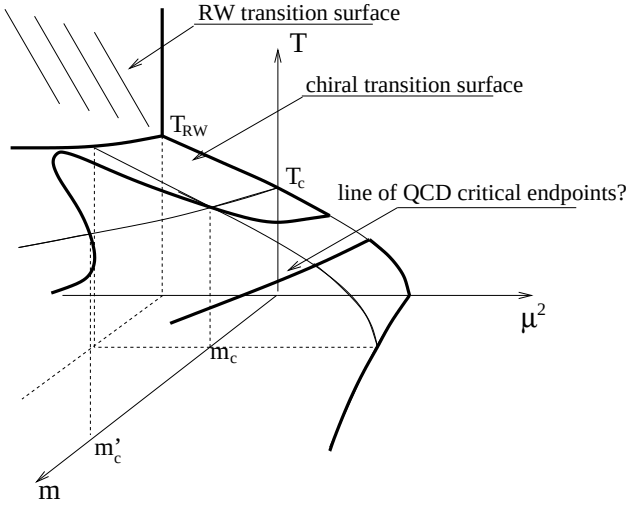
There is something that we are understanding, however: is the critical endpoint connected to the border of the chiral first order region present at $\mu = 0$? **Likely not ...**

1) The transition weakens as μ is increased from zero (de Forcrand and Philipsen)

2) The chiral first order region at $\mu = 0$ could be related to the phase structure in the $T - \mathrm{Im}(\mu)$ plane (M.D., Sanfilippo)



P. de Forcrand and O. Philipsen, arXiv:0808.1096



M.D. and F. Sanfilippo, arXiv:0909.0254

7 – The Problem of Computational Power

Largest facilities available to the lattice community around the world (partial list ...)

- **QPACE 3 dedicated installations (4608 Cell cores each) in Germany (Jülich, Regensburg, Wuppertal) for a total of ~ 150 Tflops**
- **QCDDOC (UKQCD, Columbia University, BNL) 3 dedicated installations, ~ 30 Tflops**
- **New York Blue (Stony Brook/ BNL, non dedicated), Blue Gene architeture. ~ 100 Tflops**
- **Juropa (Jülich, Sun Blade architecture), non dedicated, ~ 300 Tflops**
- **Jugene (Jülich, non dedicated): based on Bluegene, expected 1 Pflop next June, third in the TOP500 list (after Jaguar, US, 2 Pflops and Roadrunner, US)**
- **In Italy instead: CINECA 61th in TOP500 with ~ 100 Tflops. And the italian lattice community? ~ 10 Tflops on the whole (apeNEXT + minor resources)**

In some way we are still well alive (the italian miracle ...)

But what do we need to stay alive also tomorrow?

- **Computation of matrix elements and SM parameters with experiment-matching precision:** 60 Tflops in 2010 and 1-10 Pflops starting 2012 (quoting V. Lubicz, com. IV 2009)
- **QCD thermodynamics and phase diagram:** competing groups have already O(100) Tflops available, that should be matched in one year at most.

We have a renowned tradition of machine building:

1988 APE

1993 APE100

1999 APEmille

2005 APEnext

How do we proceed next?

Mid-long term possible solutions

- **AURORASCIENCE PROJECT: (Provincia di Trento, INFN (Pr, Fe, Mi): 3D APE-like network of intel processors. Expected: 20 Tflops by end 2010, 100 Tflops in 2011.**
- **apeNET+ (PC cluster with fast APE-like link) and long term PetApe project (RM1, RM2): expected O(100) Tflops in 2011.**

Pflop possible by 2012-2013 in both cases

Short term solutions: some of us (Pisa, Genova) are starting simulations on GPUs. 1Tflop (peak) for 2Keuros with a sustained efficiency of O(10%)

Possible hybrid solutions explorable: GPU network connected via apeNET+ fast link?

8 – Conclusions

- **There are problems that can be sistematically solved within the next few years with > 100 Tflops machines: SM parameters, transition temperature and nature, QGP equilibrium properties**

- **Other issues (like the determination of transport coefficients) are at a preliminary stage (pure gauge till now) and more demanding**

- **Finally, there are problems, like QCD at finite density, which are not completely solvable within the next few years without algorithmic breakthroughs**