

# QCD transition temperature: approaching the continuum

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new ('09) results of the Wuppertal-Budapest group  
(about scaling and lattice artefacts)

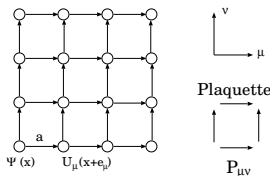
EMMI Workshop, September 1 2009, St. Goar



# Outline

- 1 Introduction
- 2 Discrepancy: 2006 literature
- 3  $a^2$  scaling
- 4 New results: Wuppertal-Budapest & 'hotQCD'
- 5 Summary

# Lattice QCD introduction



## Fundamental fields

Gauge fields:

$U_\mu(x) \in SU(3)$  live on the links ( $\mu$  index)

Quark fields:

$\Psi(x)$ ,  $\bar{\Psi}(x)$  anti-commuting Grassmann variables live on the sites

**Wilson fermions:** computationally expensive

**Staggered fermions:** faster, BUT taste symmetry violation

(only one pseudogoldstone pion instead of three)

fermion doubling is avoided by rooting: “good, bad or ugly?”

# Lattice formulation

$$Z = \int dU d\Psi d\bar{\Psi} e^{-S_E} \quad (1)$$

$S_E$  is the Euclidean action

Parameters:

gauge coupling  $g$

quark masses  $m_i$  ( $i = 1..N_f$ )

(Chemical potentials  $\mu_j$ )

Volume ( $V$ ) and temperature ( $T$ )

Finite  $T \leftrightarrow$  finite temporal lattice extension

$$T = \frac{1}{N_t a} \quad (2)$$

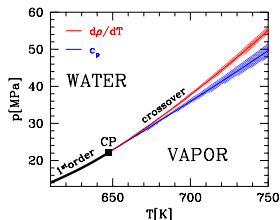
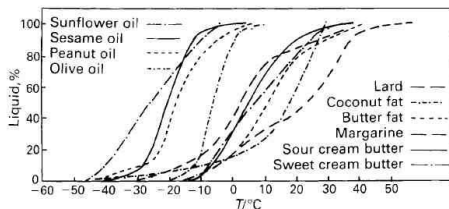
Continuum limit:  $a \rightarrow 0 \iff N_t \rightarrow \infty$

# The nature of the QCD transition

Y.Aoki, G.Endrodi, Z.Fodor, S.D.Katz, K.K.Szabo, Nature, 443 (2006) 675

**analytic transition (cross-over)**  $\Rightarrow$  it has no unique  $T_C$ :

examples: melting of butter (not ice) & water-steam transition



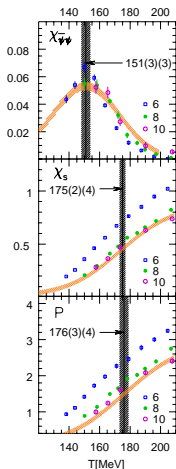
above the critical point  $c_p$  and  $d\rho/dT$  give different  $T_C$ s.

**QCD: chiral & quark number susceptibilities or Polyakov loop**

they result in different  $T_C$  values  $\Rightarrow$  physical difference

# The transition temperature: results and scaling

Y. Aoki, Z. Fodor, S.D. Katz, K.K. Szabo, Phys. Lett. B. 643 (2006) 46



Chiral susceptibility

$$T_C = 151(3)(3) \text{ MeV}$$

$$\Delta T_C = 28(5)(1) \text{ MeV}$$

Quark number susceptibility

$$T_C = 175(2)(4) \text{ MeV}$$

$$\Delta T_C = 42(4)(1) \text{ MeV}$$

Polyakov loop

$$T_C = 176(2)(4) \text{ MeV}$$

$$\Delta T_C = 38(5)(1) \text{ MeV}$$

# Literature: discrepancies between $T_c$

Bielefeld-Brookhaven-Riken-Columbia Coll. (+MILC='hotQCD'):

M. Cheng et.al, Phys. Rev. D74 (2006) 054507

$T_c$  from  $\chi_{\bar{\psi}\psi}$  and Polyakov loop, from both quantities:

$$T_c = 192(7)(4) \text{ MeV}$$

Wuppertal-Budapest group (WB):

Y. Aoki, Z. Fodor, S.D. Katz, K.K. Szabo, Phys. Lett. B. 643 (2006) 46

chiral susceptibility:  $T_c = 151(3)(3) \text{ MeV}$

Polyakov and strange susceptibility:  $T_c = 175(2)(4) \text{ MeV}$

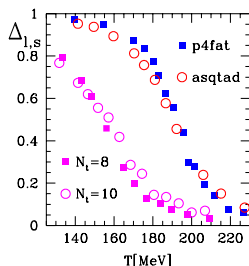
'chiral  $T_c$ ':  $\approx 40 \text{ MeV}$ ; 'confinement  $T_c$ ':  $\approx 15 \text{ MeV}$  difference

both groups give continuum extrapolated results with physical  $m_\pi$

# Literature: discrepancies between T dependences

Reason: shoulders, inflection points are difficult to define?

Answer: no, the whole temperature dependence is shifted



for chiral quantities  $\approx 35$  MeV; for confinement  $\approx 15$  MeV  
 this discrepancy would appear in all quantities (eos, fluctuations)

150 MeV transition temperature: isn't it a bit too small?

lattice works in  $V \rightarrow \infty$ , which gives much smaller  $T_c$

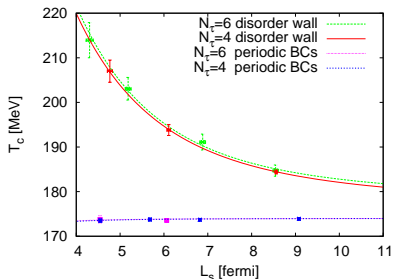


## $T_c$ strongly depends on the geometry

nanotube-water doesn't freeze, even at hundred degrees below  $0^\circ\text{C}$

exploratory study: [A. Bazavov and B. Berg, Phys.Rev. D76 \(2007\) 014502](#)

use 'confined' spatial boundary conditions: more like experiments



large deviation (upto 30 MeV) from the infinite volume limit  
if  $V \rightarrow \infty$  is 150 MeV a  $100 \text{ fm}^3$  system might have 170 MeV

# Possible reasons for the discrepancy

## “Non-lattice artefact/formulation” related reasons

- a. **bug** in the codes
- b. **systematic errors** are largely underestimated

## “Lattice artefact/formulation” related reasons

- a. the **pion mass** is not small enough:  
'hotQCD' 230MeV  $\Rightarrow$  shift of 5 MeV, WB: 135 MeV pseudogoldstone
- b. not small enough **lattice spacings**: new 'hotQCD'/WB upto  $N_t=8/12$
- c. actually it is **not QCD**, what we are studying  
(most large scale thermodynamics studies use staggered fermions)

## Discretization errors in the transition region

we always have discretization errors: nothing wrong with it as long as

- result: close enough to the continuum value (error subdominant)
- we are in the scaling regime ( $a^2$  in staggered)

various types of discretization errors  $\Rightarrow$  we improve on them (costs)

we are speaking about the **transition temperature region**  
**interplay** between hadronic and quark-gluon plasma physics  
 smooth cross-over: one of them takes over the other around  $T_c$

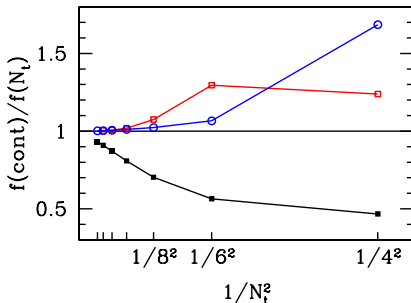
both regimes (low T and high T) are equally important  
**improving for one:  $T \gg T_c$ , doesn't mean improving for the other:  $T < T_c$**

example: 'expansion' around a Stefan-Boltzman gas (van der Waals)  
 for water: it is a fairly good description for  $T \gtrsim 300^\circ$

calculate the boiling point: more accuracy needed for the liquid phase

# Examples for improvements, consequences

how fast can we reach the continuum pressure at  $T=\infty$ ?



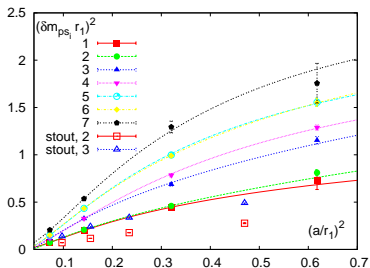
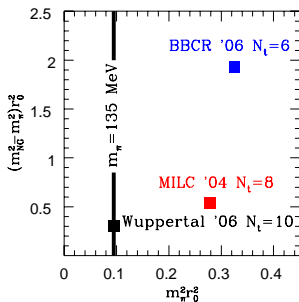
p4 action is essentially designed for this quantity  $T \gg T_c$

asqtad designed mostly for  $T=0$  physics (but good at high  $T$ , too)

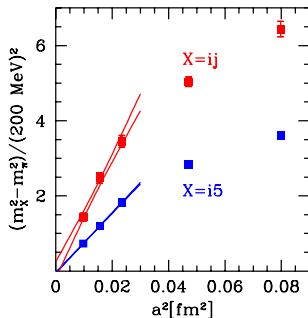
stout-smearred one-link converges slower but in the  $a^2$  scaling regime (e.g. extrapolation from  $N_t=8,10$  provides a result within about 1%)

# Chiral symmetry breaking and pions

transition temperature for remnant of the chiral transition:  
 balance between the chirally broken and chirally symmetric sectors  
 chiral symmetry breaking: 3 pions are the pseudo-Goldstone bosons  
 staggered QCD: 1 pseudo-Goldstone instead of 3 (taste violation)  
 staggered lattice artefact  $\Rightarrow$  disappears in the continuum limit  
 WB: stout-smearing improvement is designed to reduce this artefact



# Scaling for the pion splitting



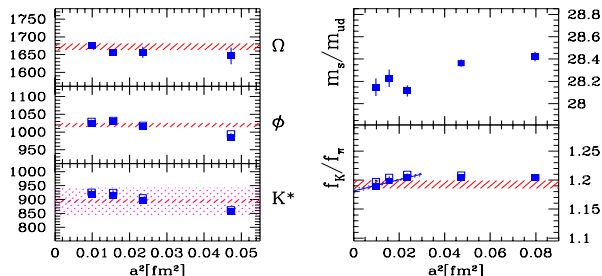
scaling regime is reached if  $a^2$  scaling is observed  
 asymptotic scaling starts only for  $N_t > 8$  ( $a \lesssim 0.15$  fm): two messages

- $N_t = 8, 10$  extrapolation gives 'p' on the  $\approx 1\%$  level: good balance
- stout-smear improvement is designed to reduce this artefact  
 most other actions need even smaller 'a' to reach scaling

# Setting the scale in lattice QCD

in meteorology, aircraft industry etc. grid spacing is set by hand  
 in lattice QCD we use  $g, m_{ud}$  and  $m_s$  in the Lagrangian ('a' not)  
 measure e.g. the vacuum mass of a hadron in lattice units:  $M_\Omega a$   
 since we know that  $M_\Omega = 1672$  MeV we obtain 'a' and  $T = 1/N_t a$

Y.Aoki et al. [Wuppertal-Budapest Collaboration] arXiv:0903.4155



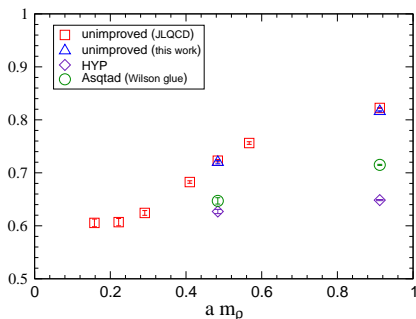
independently which quantity is taken (we used physical masses)

⇒ one obtains the same 'a' and T, result is safe

# Scaling of $B_K$ in quenched simulations

HPQCD and UKQCD Collaborations, Phys. Rev. D73 (2006) 114502

$B_K^{\text{NDR}}$  (2 GeV) in the quenched approximation



unimproved action has large scaling violations

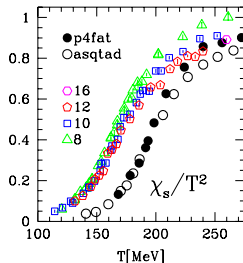
asqtad action is somewhat better

HYP smeared improvement  $\Rightarrow$  almost perfect scaling



# T>0 results: strange susceptibility

Y.Aoki et al. [Wuppertal-Budapest Collaboration] arXiv:0903.4155



'hotQCD' results are on  $N_t=8$ , WB results are on  $N_t=8,10,12,(16)$

'hotQCD': results with two different actions are almost the same

WB: for large T one extrapolates according to the known  $a^2$  behaviour

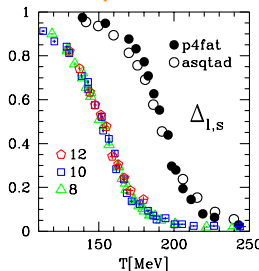
WB: no change in the lattice results compared to our 2006 paper

note, that the experimental value of  $f_K$  decreased by 3% since 2006

about 20 MeV difference between the results

# $T > 0$ results: chiral condensate

Y.Aoki et al. [Budapest-Wuppertal Collaboration] arXiv:0903.4155



'hotQCD' results are on  $N_t=8$ , WB results are on  $N_t=8, 10, 12$

'hotQCD': results with two different actions are almost the same

WB: no lattice spacing dependence observed for  $N_t=8, 10, 12$

WB: no change in the lattice results compared to our 2006 paper

about 35 MeV difference between the results

# transition temperatures for various observables

	$\chi_{\bar{\psi}\psi}/T^4$	$\chi_{\bar{\psi}\psi}/T^2$	$\chi_{\bar{\psi}\psi}$	$\Delta_{l,s}$	L	$\chi_s$
WB'09	146(2)(3)	152(3)(3)	157(3)(3)	155(2)(3)	170(4)(3)	169(3)(3)
WB'06	151(3)(3)	-	-	-	176(3)(4)	175(2)(4)
BBCR	-	192(4)(7)	-	-	192(4)(7)	-

renormalized chiral susceptibility, renormalized chiral condensate  
Polyakov loop and strange quark number susceptibility

no change compare to our 2006 data (errors are reduced)

note, that the experimental value of  $f_K$  decreased by 3% since 2006

Particle Data Group now gives  $f_K=155.5(2)(8)(2)$  MeV (error 0.5%)

$r_0$  is not directly measurable:

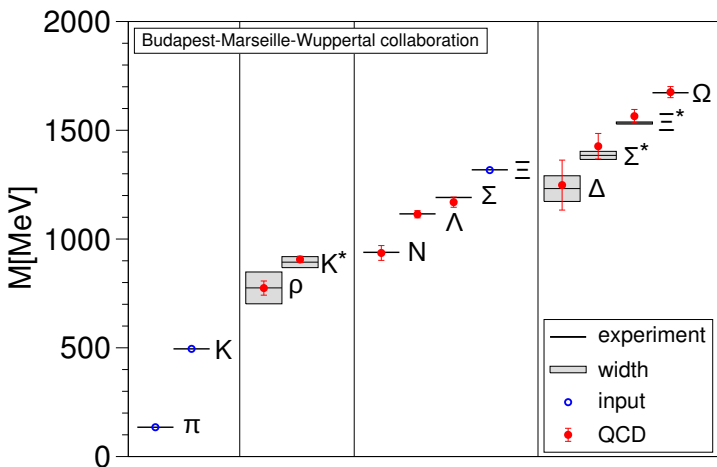
ETM:0.444(4) fm, QCDSF:0.467(6) fm,

HPQCD&UKQCD:0.469(7) fm, PACS-CS:0.492(6)(+7) fm

# Summary

- new (2009) results for the transition temperature
- three major improvements since 2006
  - a. at  $T=0$  all simulations are done with physical quark masses
  - b. to verify that the results are independent of the scale setting we use 5 experimentally well-known quantities:  $f_K, f_\pi, m_{K^*}, m_\Omega, m_\Phi$
  - c. even smaller lattice spacings:  $N_t=12$  (in one case  $N_t=16$ )
- all findings are in complete agreement with our 2006 results
- Particle Data Group reduced the experimental value of  $f_K$ : 3%
- discrepancy between Wuppertal-Budapest & 'hotQCD' results
  - a. for the remnant of the deconfinement transition: about 20 MeV
  - b. for the remnant of the chiral transition: about 35 MeV $\Rightarrow$  finding the reason: task for the future
- Wilson fermions: theoretically cleaner option

# Final result for the hadron spectrum



# CP violation, $K^0-\bar{K}^0$ mixing and $B_K$

$K_L \rightarrow e_R^+ \nu_L \pi^-$ : 20.2% and  $K_L \rightarrow e_R^- \bar{\nu}_L \pi^+$ : 0%

the reason is the maximal C-violation

do we know the absolute definition of left and right?

exchange also left and right  $K_L \rightarrow e_L^- \bar{\nu}_R \pi^+$ : 20.2%

do it more precisely:

$K_L$  slightly prefers to decay into  $e^+ \nu \pi^-$  than  $e^- \bar{\nu} \pi^+$

$$\frac{\Gamma(K_L \rightarrow e^+ \nu \pi^-)}{\Gamma(K_L \rightarrow e^- \bar{\nu} \pi^+)} = 1.007 = 1 + f(\bar{\eta}, \bar{\rho} \dots) \quad \langle \bar{K}^0 | \mathcal{H} | K^0 \rangle = 1 + f(\bar{\eta}, \bar{\rho} \dots) \frac{8}{3} m_K^2 f_K^2 B_K$$

CKMfitter Group, UTfit Collab. still use quenched  $B_K$  from 1997

# Importance sampling

$$Z = \int \prod_{n,\mu} [dU_\mu(n)] e^{-S_g} \det(M[U])$$

we do not take into account all possible gauge configuration

each of them is generated with a probability  $\propto$  its weight

importance sampling, Metropolis algorithm:

(all other algorithms are based on importance sampling)

$$P(U \rightarrow U') = \min [1, \exp(-\Delta S_g) \det(M[U']) / \det(M[U])]$$

gauge part: trace of  $3 \times 3$  matrices (easy, **without M: quenched**)

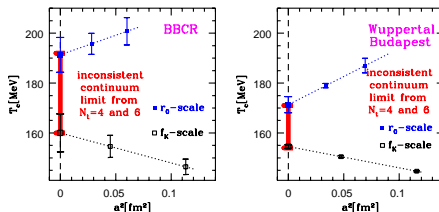
fermionic part: determinant of  $10^6 \times 10^6$  sparse matrices (hard)

more efficient ways than direct evaluation ( $Mx=a$ ), but still hard

# Consequences of the non-scaling behaviour

for large 'a' no proper  $a^2$  scaling (e.g. due to large  $m_\pi$  splitting)  
 how do we monitor it, how to be sure being in the scaling regime?  
 dimensionless combinations in the  $a \rightarrow 0$  limit:

$T_c r_0$  or  $T_c/f_K$  for the remnant of the chiral transition



$N_t=4,6$ : inconsistent continuum limit

$N_t=6,8,10$ : consistent continuum limit (stout-link improvement)

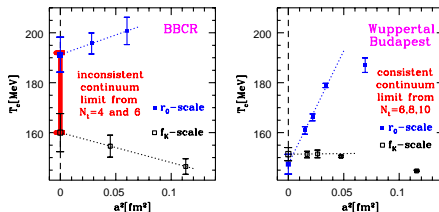
independently which quantity is taken one obtains the same  $T_c$   
 signal: **extrapolation is safe**, we are in the  $a^2$  scaling regime



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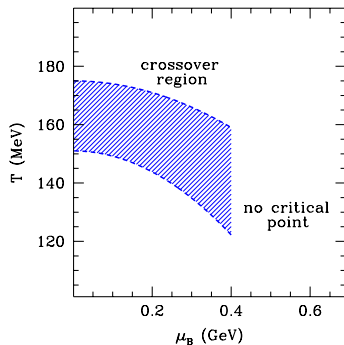
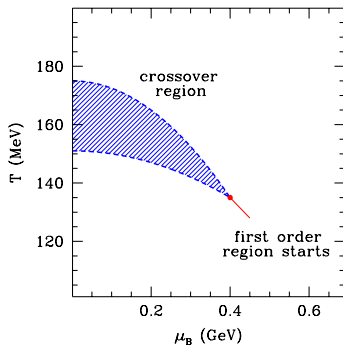


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# Scenarios for $\mu > 0$

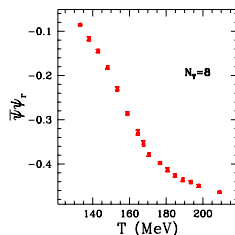
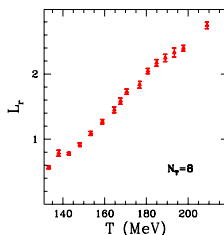
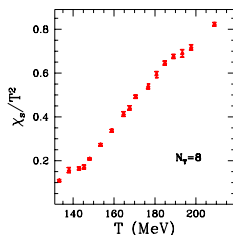


Does the crossover region shrink or expand?

The curvature can affect the existence of the **critical endpoint**

Estimate: if  $\mu_{crit} = 360$  MeV  $\rightarrow \Delta\kappa \approx 0.02$

# Observables

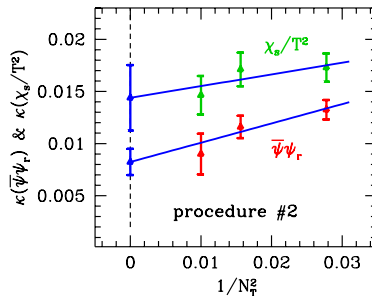
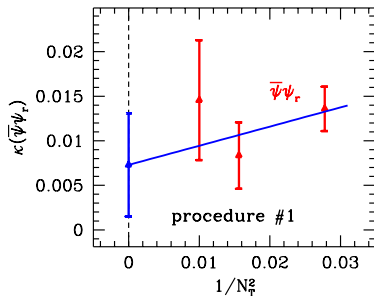


$T_C$  is defined as inflection point or given value ( $\frac{\mathcal{O}(T=0)+\mathcal{O}(T=\infty)}{2}$ )  
 $\mu$  dependence by Taylor expansion  $\rightarrow$  curvature

Two procedures:

1. determine inflection point as a function of  $\mu$
2. average shifts for different  $T$ -s

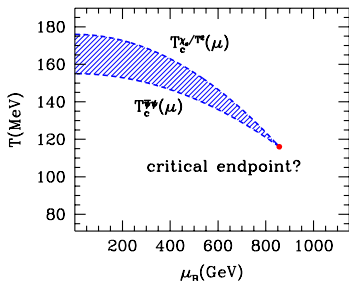
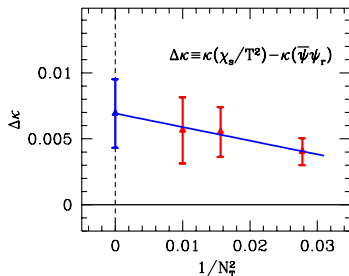
# Preliminary results



Continuum extrapolated results from  $N_t = 6, 8$  and  $10$ ;  
both procedures

Polyakov loop result consistent with  $\chi_s/T^2$

# Preliminary results



Difference  $\Delta\kappa \equiv \kappa(\chi_s/T^2) - \kappa(\bar{\psi}\psi_r)$  not consistent with zero  
 Necessary condition for the critical point

**But not sufficient**

Strength of the transition from individual quantities  $\rightarrow$   
 more statistics needed

## more statistics in the Taylor method

determining the inflection point needs 10-times more statistics  
to that end the whole T dependence should be determined  
this gives more than just the inflection point  
a clear signal for broadening or shrinking will be seen  
 **$a \rightarrow 0$  can be done with present resources**

the Taylor procedure gives only the leading order term(s) in  $\mu$   
 $N_t=4$  unimproved staggered experience [Fodor-Katz'01, Fodor-Katz'04]  
the leading order terms are insensitive to the critical point  $\Rightarrow$   
evaluation of the whole determinant, **we need all the terms in  $\mu$**

**our action** (smeared improved): better at  $T=0$  & **evaluation possible**  
for p4, asqtad or hisq no such eigenvalue structure (det) is known

(it gives certainly more information than just the leading order terms)

## memory/CPU requirements for full determinants

$N_t=4$  &  $N_s=8,10,12$  needed 1 GB memory & 25 CPU years (in '04)  
 memory requirements grow as  $N_t^6$ , CPU requirements as  $N_t^9$

accumulate the same statistics (shown by the first CPU row)  
 to reach the same  $\mu a$ : **exponentially more configs are needed**

'05 observation: applicability range  $\propto V^{-0.35}$  and  $\mu a \propto V^{-0.25}$

$\Rightarrow$  additional increase of the statistics (second CPU<sup>+</sup> row)

$N_t$	4	6	8	10
memory [GB]	1	11	64	244
'04 CPU [kyears]	0.025	1	13	95
'04 CPU <sup>+</sup> [kyears]	0.025	1	18	150
machine [year]	cluster	cluster	2 BG/P	15 BG/P

$\Rightarrow N_t=6,8,10$ : our present resources are not enough for that