ZiF Workshop
Quantum fields in the teraflop era
25 November, 2004

The future Japanese Physics Program on Teraflops Computers

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Center for Computational Sciences
University of Tsukuba

- *Introduction*
- *Looking back*
- *Looking forward*
- *International collaboration*
- *Summary*

30 years after the birth of lattice QCD

- Now is a special juncture of time
  - Realistic prospect toward Nf=2+1 dynamical simulations
    - MILC staggered project
    - CP-PACS/JLQCD Wilson-clover project
    - Domain-wall with QCDOC (RBC-UKQCD)
    - ……
- In this talk, from a Japanese (CP-PACS/JLQCD) perspective,
  - Look back on developments leading to this status
  - Look forward toward future in terms of
    - Machines
    - Physics targets and challenges

Lattice QCD in (Tsukuba) Japan

1980 1985 1990 1995 2000 2005

KEK

S810
315Mflops

S820
1Gflops

VPP500/80
128Gflops

SR8000F1/100
1.2Tflops

??
>20Tflops

JLQCD Collaboration

Supercomputer installation since 1985
Services Japanese LQCD community
Upgrade every 5-6 years

QCDPAX
14Gflops

CP-PACS
614Gflops

post
CP-PACS
10-20Tflops

Univ. of Tsukuba

CP-PACS Collaboration

Development of dedicated
computers
for scientific applications

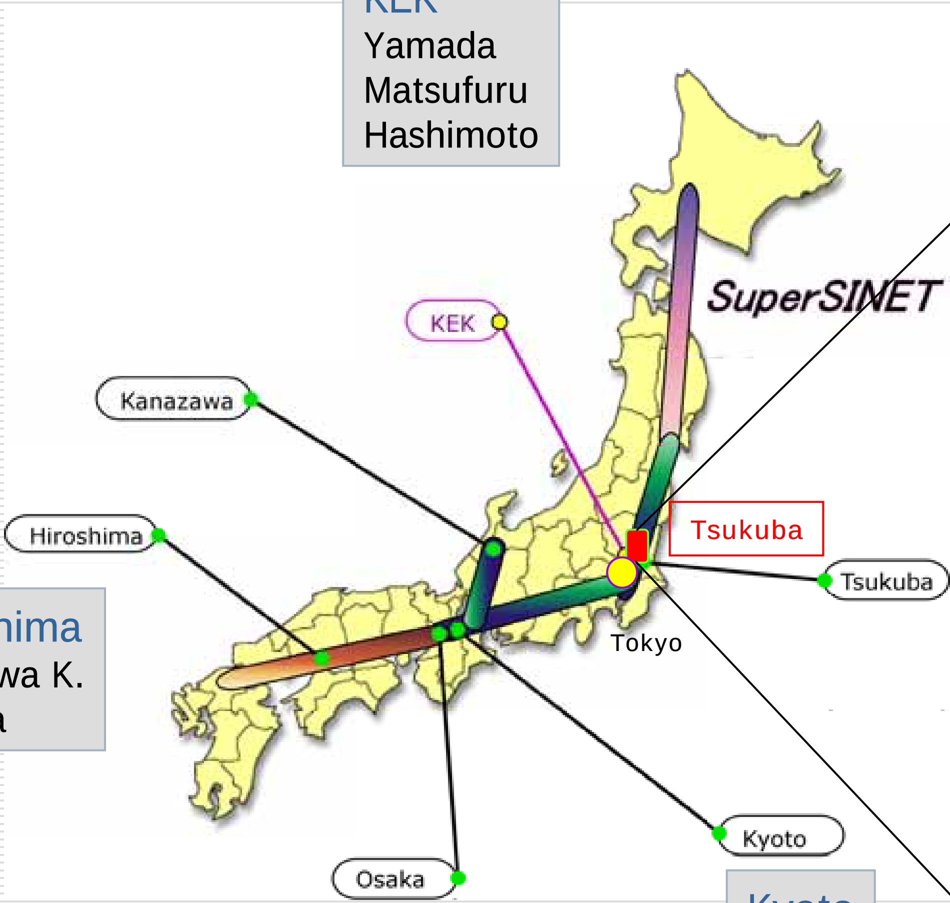
Center for
Computational Physics
1992

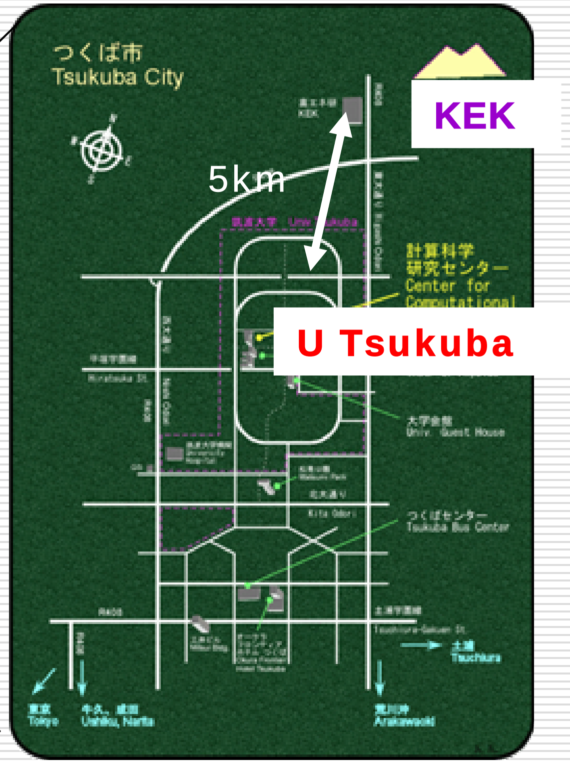
Center for
Computational Sciences
2004

Tsukuba
Ishikawa T.
Baer
Taniguchi
Kuramashi
Ishizuka
Aoki
Yoshie
Kanaya
Ukawa
Iwasaki

KEK
Yamada
Matsufuru
Hashimoto

Now elsewhere
Okamoto(FNAL)
Lesk(Imp. Coll.)
Noaki(Southampton)
Ejiri(Bielefeld)
Nagai(Zeuthen)
Aoki Y.(Wuppertal)
Izubuchi(Kanazawa)
Ali Khan(Berlin)
Manke
Shanahan(London)
Burkhalter(Zurich)





Hiroshima
Ishikawa K.
Okawa

Kyoto
Onogi

Highlights (I)

1980 1985 1990 1995 2000 2005

KEK

S810 315Mflops	S820 1Gflops	VPP500/80 128Gflops	SR8000F1/100 1.2Tflops	?? >20Tflops

First Nf=2 Wilson full QCD

Langevin algorithm

ILUCR for Wilson solver

5-10 acceleration over naïve CR or CG

9^3 x 18 lattice

Beta=5.7

20 configurations/kappa

1st order nature of pure SU(3) deconfinement transition

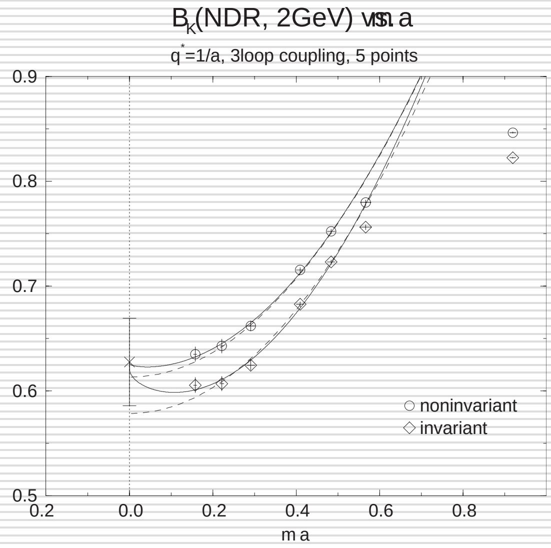
Finite size scaling analysis

8^3x4-32^3x4

High-precision calculation of BK with KS action

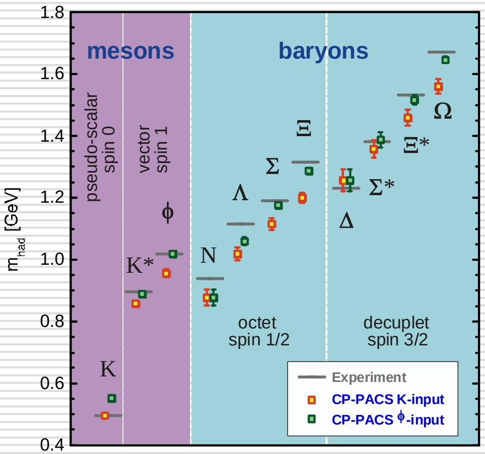
Systematic scaling analysis

JLQCD Collaboration



Highlights (II)

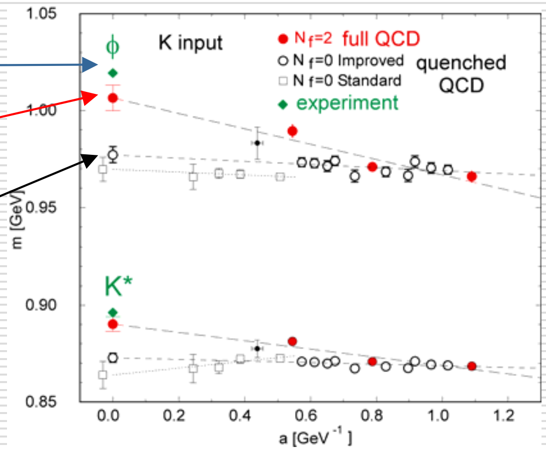
1980 1985 1990 1995 2000 2005



experiment

Nf=2

quenched



Wilson finite-temperature study with Iwasaki RG action

High precision hadron spectrum calculation

Quenched hadron spectrum in the continuum limit

Systematic Nf=2 full QCD
Continuum extrapolation
Small light quark masses

Univ. of Tsukuba

QCDPAX
14Gflops

CP-PACS
614Gflops

CP-PACS Collaboration

CP-PACS/JLQCD joint effort toward Nf=2+1

A three-year project 2003-2005

1980 1985 1990 1995 2000 2005

KEK

S810 315Mflops	S820 1Gflops	VPP500/80 128Gflops	SR8000F1/100 1.2Tflops	?? >20Tflops

JLQCD Collaboration

strategy

- Iwasaki RG gauge action
- Wilson-clover quark action — JLQCD/CP-PACS K. Ishikawa et al Lattice'03
  - *Fully O(a) improved* via Shcroedinger functional determination of c_sw
  - NP Z factors for operators via Schroedinger functional determination
- Algorithm
  - *Polynomial HMC for strange quark* — JLQCD K. Ishikawa et al PRD
  - Standard HMC for up and down quarks

Univ. of Tsukuba

QCDPAX 14Gflops	CP-PACS 614Gflops	post CP-PACS 10-20Tflops

CP-PACS Collaboration

Machines and run parameters

in progress

β =2.05
a ~ 0.07fm
28^3 x 56
2000 trajectory

β =1.83
a ~ 0.12fm
16^3 x 32
8000 trajectory

finished

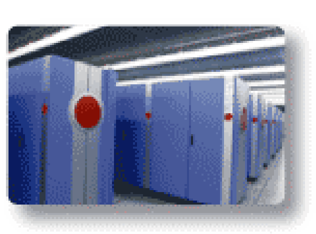
$\frac{1}{2}$ $\quad$ 1 $\quad$ $\frac{3}{2}$ $\quad$ a^2

Lattice spacing

Fixed physical volume
~ (2.0fm)^3

β =1.90
a ~ 0.10fm
20^3 x 40
8000 trajectory

already finished



Earth simulator
@ Jamstec

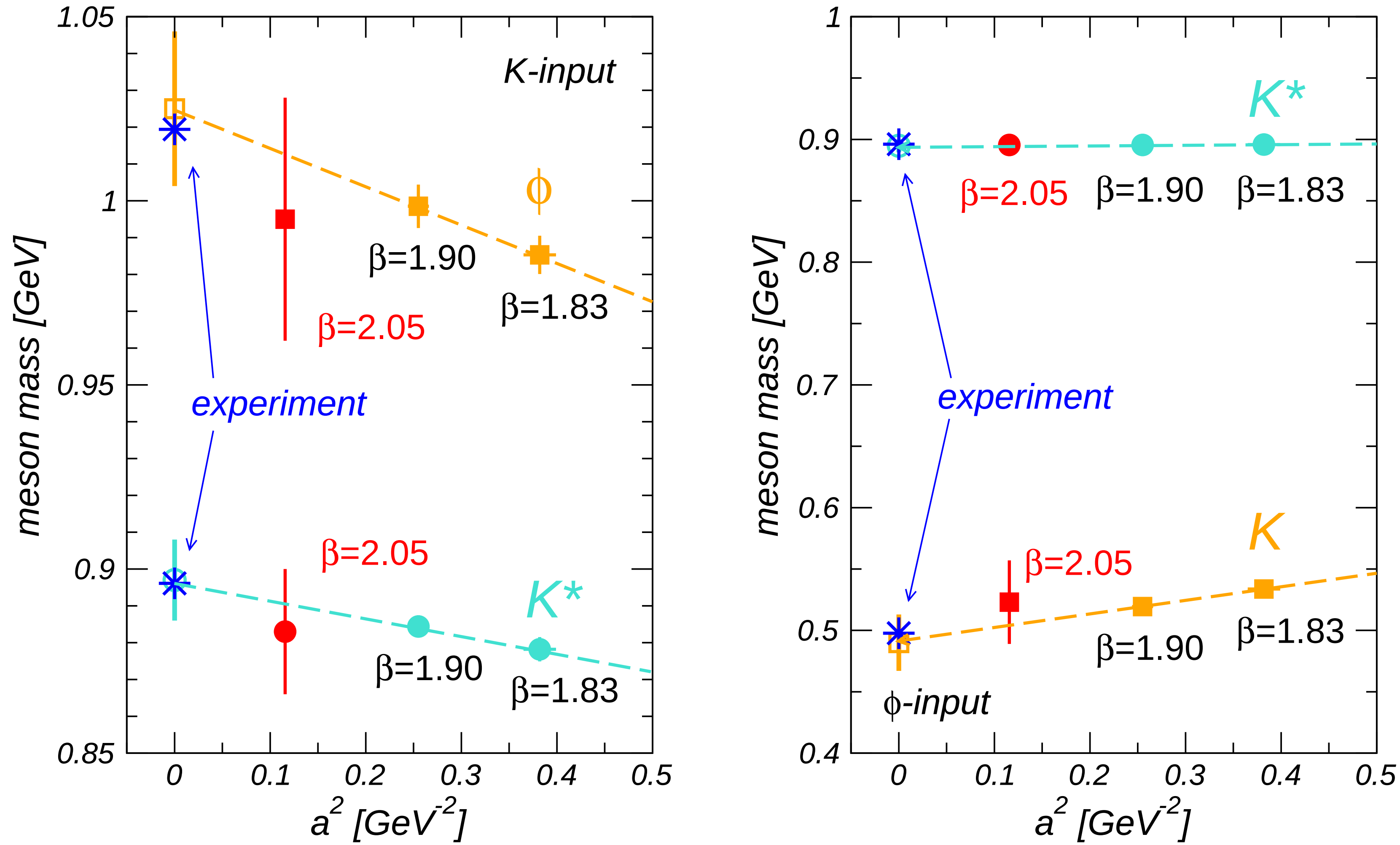
SR8000/F1
@KEK

CP-PACS
@Tsukuba

SR8000/G1
@Tsukuba

VPP5000
@Tsukuba

preliminary



Which direction do we wish to go?

- Machines
- Physics

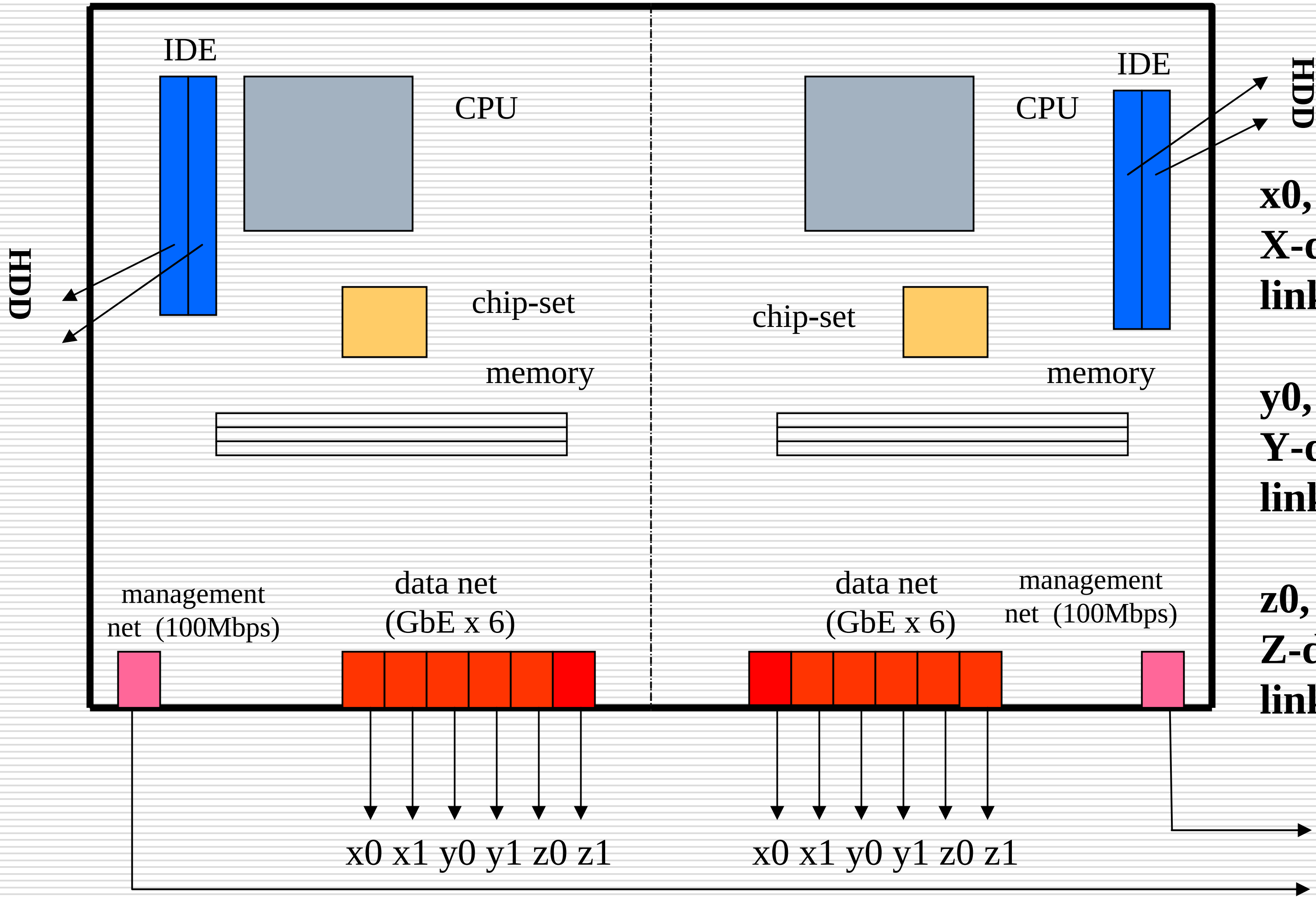
Machine perspective in Japan

- KEK
  - Upgrade of SR8000F1 in March 2006
  - Government supercomputer procurement in progress
  - >20Tflops/10TB peak performance targetted
- Center for Computational Sciences, U. of Tsukuba
  - Successor to CP-PACS planned
  - Funding requested for JFY2005-2007
  - MPP in terms of commodity components
  - At least 12Tflops/4TB system by March 2006; further installation in later years

CP-PACS successor outline

- Strategy:MPP in terms of commodity components
  - Node
    - Single CPU (Xeon 3GHz)
    - 2GB PC3200 memory with FSB800
    - 200GB disk (Raid0 mirror)
  - Network
    - 3-dimensional hypercrossbar, i.e., crossbar switch in each direction
    - Dual GbEthernet for each direction, i.e., 025GB/s/link and an agregate 0.75GB/s/node
  - System size
    - At least 2048 CPU (16x16x8, 12Tflops/4TB) and hopefuly more

Board layout



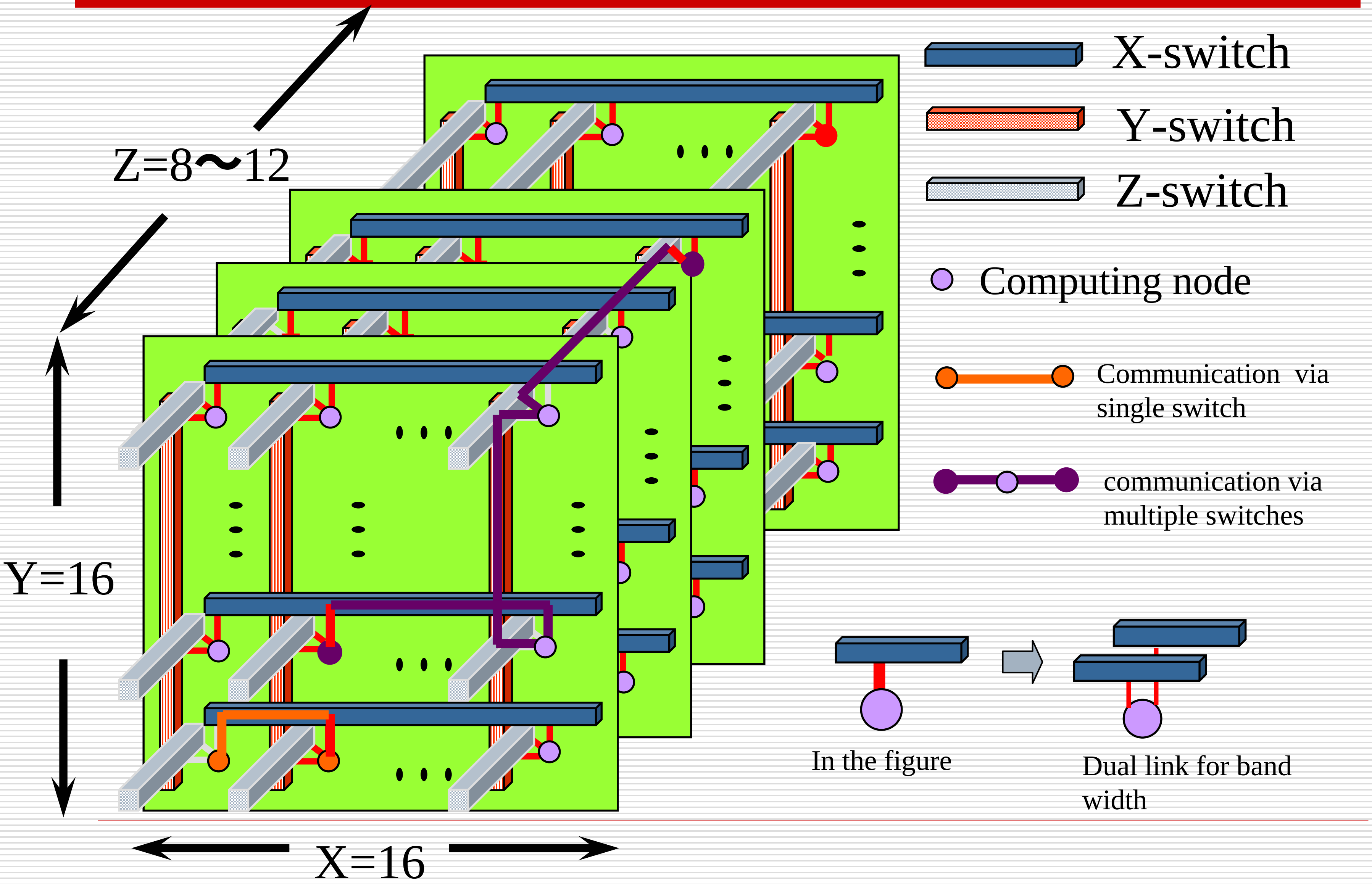
x0, x1:
X-direction dual link

y0, y1:
Y-direction dual link

z0, z1:
Z-direction dual link

management network switch

3-dimensional hypercrossbar network



Rack layout and network connections

Connections for CPU([0-F],[0-F],[0-1]) (1/6th =512 CPU) are shown

Y1-Y2,Z CPU rack(x=0〜F,y=Y1〜Y2,z=Z)

X-connection (1 line =128cables)

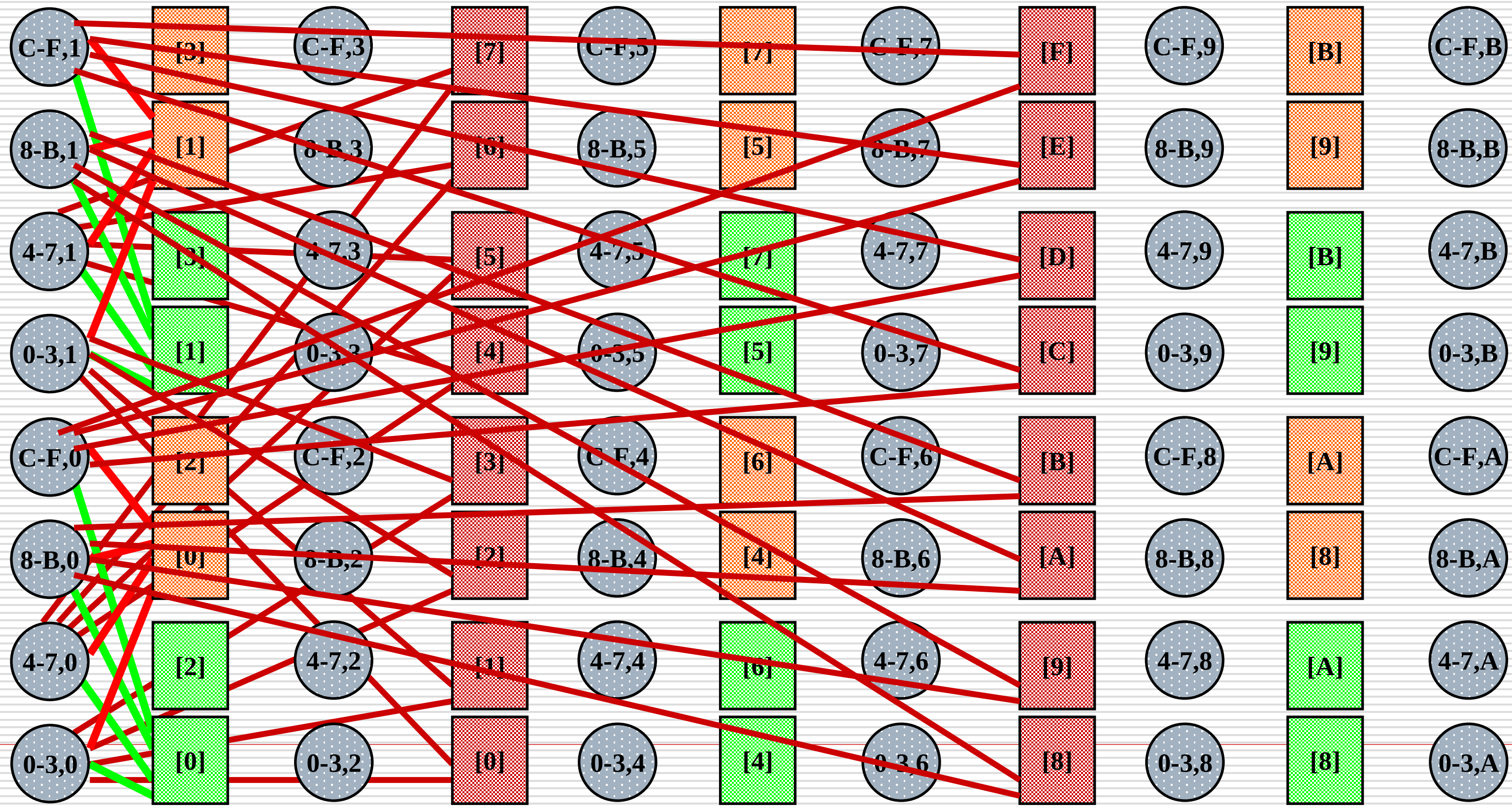
Y-connection (1 line = 128cables)

Z-connection (1 line = 32 cables)

[Z] X-switch rack(y=0〜15, z=Z)

[Z] Y-switch rack(x=0〜15, z=Z)

[Y] Z-switch rack(x=0〜15, y=Y)



Physics possibilities on the new machines

- Wilson-clover Nf=2+1 simulation
  - Runs with old machines
    - Three lattice spacings $a \approx \sqrt{\frac{3}{2}} \times 0.1\, fm\, ,\, 0.1\, fm\, ,\, \sqrt{\frac{1}{2}} \times 0.1\, fm$
    - But only down to $\frac{m_\pi}{m_\rho} \approx 0.6 \quad i.e., \quad \frac{m_{ud}}{m_s} \approx 0.5$
  - *Wish to go down to* $\frac{m_\pi}{m_\rho} \approx 0.4 \quad i.e., \quad \frac{m_{ud}}{m_s} \approx 0.2$ *or less...*
- Domain wall/overlap
  - Under discussion
- Staggered
  - ....

Performance Benchmark estimate (I)

- Wilson-clover Nf=2+1 PHMC code
- Parameters

pi/rho	mq(GeV)
0.7	0.079
0.6	0.044
0.5	0.0255
0.4	0.0145
0.3	0.0075
0.2	0.0025

*

$$\textit{lattice size} \quad N_s^3 \times N_t$$

$$\textit{BiCGStab inversions} \quad N_{inv} = 31 + \frac{10.7}{m_q a} \quad *$$

$$\textit{polynomial order} \quad N_{poly}$$

$$\textit{HMC step size} \quad d\tau = \left(0.223 m_q(GeV) - 0.620 m_q(GeV)^2\right) \times \frac{24}{N_s} \quad *$$

$$\textit{node array} \quad n_x \times n_y \times n_z$$

*Nf=2 empirical fit ; need revision for Nf=2+1

- Flop/node/trajectory

$$\#\, flops = \left(130938 + 8808 N_{inv} + 3666 N_{poly}\right) \times \frac{N_s^3 \times N_t}{n_x n_y n_z} \frac{1}{d\tau}$$

- Data sent/node/trajectory

$$\#\, data\ sent = \left(10 + 8N_{inv} + \frac{7}{2} N_{poly}\right) \times 192 \times \left(\frac{N_t}{2} + 1\right) \times 2 \times \left(\frac{N_s}{n_x}\frac{N_s}{n_y} + perm\right) \frac{1}{d\tau} \quad Byte$$

Performance Benchmark estimate (II)

- Target runs

lattice size	$24^3 \times 48$ at $a \approx 0.1\,fm$, $32^3 \times 64$ at $a \approx \sqrt{\frac{1}{2}}0.1\,fm$
#trajectories	10000
polynomial order	300

- Machine assumptions

system size	$2048\,CPU$
job partition	$8^3 = 512\,CPU \times 4$
CPU performance	$2\,Gflops$
network performance	$0.2\,GB/s/link$ (3 *directions overlapped*)
network latency	$20\,\mu s$

Performance Benchmark estimate (III)

				Standard HMC					
1/a	lattice size		pi/rho	Ninv	1/dt	time/ traj (hr)			10000traj
(GeV)	Ns	Nt				calc	comm	total	(days)
2	24x48		**0.6**	517	116	0.12	0.13	0.25	**26**
			0.5	870	189	0.30	0.32	0.62	**65**
			0.4	1507	322	0.84	0.89	1.73	**180**
			0.3	2884	611	2.93	3.11	6.03	**629**
			0.2	8591	1806	25.00	26.57	51.57	**5372**
2.83	32x64		**0.6**	719	155	0.67	0.46	1.13	**118**
			0.5	1218	252	1.72	1.19	2.91	**303**
			0.4	2118	430	4.86	3.39	8.25	**860**
			0.3	4066	814	17.16	11.99	29.14	**3036**
			0.2	12143	2408	148.23	103.66	251.89	**26238**

Rather dismal number of days .....

Acceleration possibilities (I)

- Hasenbusch acceleration M. Hasenbusch Hep-lat/0107019

$$\det M^{+}M = \int d\phi_1^{+} d\phi_1 \exp\left(-\phi_1^{+}\frac{1}{W^{+}W}\phi_1\right)\cdot\int d\phi_2^{+} d\phi_2 \exp\left(-\phi_2^{+}\frac{1}{\tilde{M}^{+}\tilde{M}}\phi_1\right)$$

$$M = 1-\kappa^2 M_{oe}M_{eo}$$

$$W = M+\rho$$

$$\tilde{M} = W^{-1}M$$

  - Factor 2 larger step size without fine tuning of ρ
  - Implementation in progress

- Domain-decomposition techniques M. Luescher Hep-lat/0409106

Acceleration possibilities (II)

- Domain decomposition acceleration

$$\det D^{+}D = \int d\phi_{\Omega}^{+} d\phi_{\Omega} \exp\left(-\phi_{\Omega}^{+} \frac{1}{D_{\Omega}{}^{+} D_{\Omega}} \phi_{\Omega} \right) \cdot \int d\phi_{\Omega^*}^{+} d\phi_{\Omega^*} \exp\left(-\phi_{\Omega^*}^{+} \frac{1}{D_{\Omega^*}{}^{+} D_{\Omega^*}} \phi_{\Omega^*} \right) \cdot \int d\phi_{R}^{+} d\phi_{R} \exp\left(-\phi_{R}^{+} \frac{1}{R^{+} R} \phi_{R} \right)$$

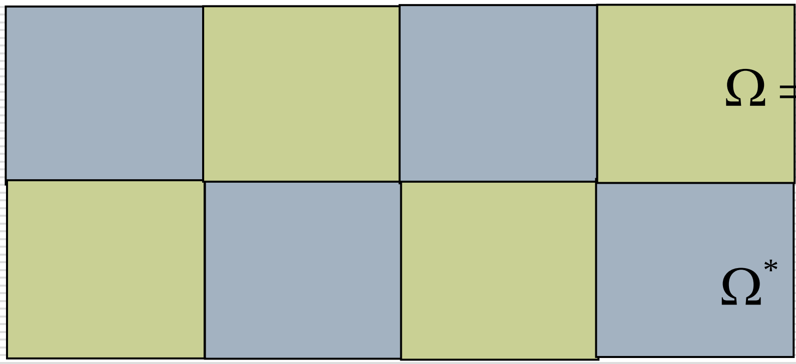
$$D_{\Omega} = \sum_{n} D_{\Lambda_n} \quad , \quad D_{\Omega^*} = \sum_{n} D_{\Lambda_n^*}$$

Dirichlet b.c. on $\partial\Omega = \sum_{n} \partial\Lambda_n \, , \partial\Omega^* = \sum_{n} \partial\Lambda_n^*$

$$R = 1 - \theta_{\partial\Omega^*} D_{\Omega}^{-1} D_{\partial\Omega} D_{\Omega^*}^{-1} D_{\partial\Omega^*}$$

Values only on the boundary of domains

$$R^{-1} = 1 - \theta_{\partial\Omega^*} D^{-1} D_{\partial\Omega^*}$$



$$\Omega = \prod_{n} \Lambda_n$$

$$\Omega^* = \prod_{n} \Lambda_n^*$$

Acceleration possibilities (III)

- Crucial observation(Luescher)

F_0 force due to gauge action

F_1 force due to D_Ω and D_{Ω^*}

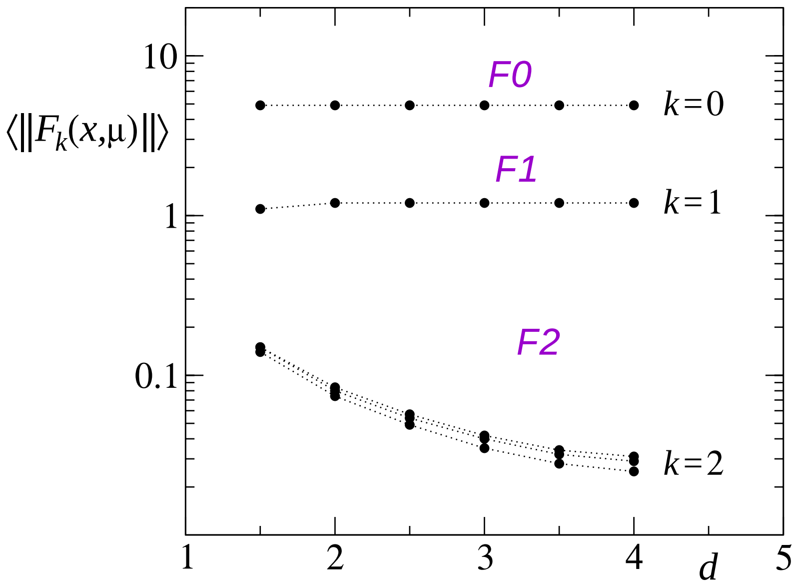
F_2 force due to R

Numerically at $\frac{m_\pi}{m_\rho} \approx 0.7 - 0.4$ and $a^{-1} \approx 2.4\text{GeV}$

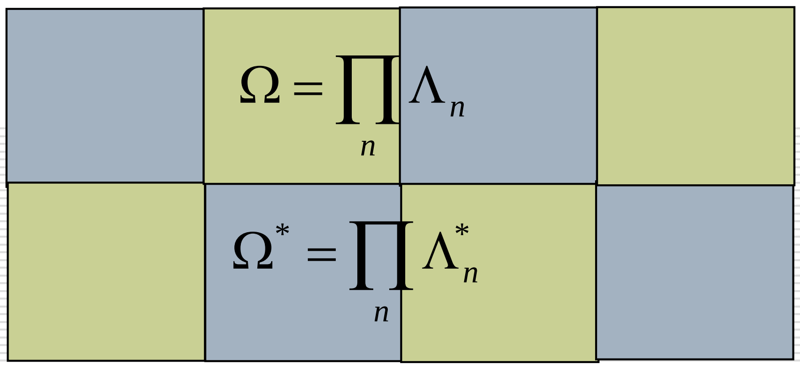
$$F_0 : F_1 : F_2 \approx 5:1:0.2 = 25:5:1$$

Use larger step sizes for quarks

$$d\tau_0 : d\tau_1 : d\tau_2 \approx 1:5:25$$



From M. Luescher Hep-lat/0409106



Acceleration possibilities (IV)

1/a	lattice size		pi/rho	standard HMC 10000traj	domain-decomposed HMC #steps			time/traj(hr)			10000traj	acceleration
(GeV)	Ns	Nt		(days)	N0	N1	N2	calc	comm	total	(days)	
2	24x48		**0.6**	**26**	4	5	5	0.031	0.005	0.037	**4**	7
			0.5	**65**	4	5	6	0.058	0.010	0.068	**7**	9
			0.4	**180**	4	5	7	0.110	0.019	0.129	**13**	13
			0.3	**629**	4	5	8	0.230	0.041	0.271	**28**	22
			0.2	**5372**	4	5	9	0.747	0.13[illegible]	0.880	**92**	59
2.83	32x64		**0.6**	**118**	5	6	6	0.181	0.018	0.199	**21**	6
			0.5	**303**	5	6	7	0.333	0.033	0.366	**38**	8
			0.4	**860**	5	6	9	0.713	0.071	0.784	**82**	11
			0.3	**3036**	5	6	10	1.475	0.147	1.622	**169**	18
			0.2	**26238**	5	6	11	4.739	0.473	5.213	**543**	48

- Only a paper estimate, but more than encouraging .....
- Implementation in progress

Physics issues – standard targets (I)

- Light hadron spectrum within a few % accuracy
  - Nucleon mass
  - rho meson as a resonance
    - Finite-size techniques
    - Wilson chiral perturbation theory

- Light quark masses and strong coupling constant
  - Non-perturbative RG running and Z factors
    - Schroedinger functional methods
- Hadron physics
  - eta' meson and topology
  - exotics (glueballs, multi-quark states)

Physics issues – standard targets (II)

Interface with the electro-weak sector

- K meson system
  - BK
    - Non-perturbative Z factor
  - Kl3 form factor

German-Japan Workshop
S. Hashimoto

- Charm and bottom quark systems
  - Onium and heavy-light spectra
  - Decay constants and B parameters
  - weak form factors
    - Relativistic heavy quark action (Aoki-Kuramashi-Tominaga)

German-Japan Workshop
Y. Kuramashi

Physics issues – standard targets (III)

- Finite-temperature behavior
  - Physical Nf=2+1 Phase diagram
  - Critical temperature
  - Equation of state
  - Finite-temperature effects in the hadron spectra
    - Issue of parity-broken phase
- Finite-density behavior
  - Small chemical potential
  - Large chemical potential?

Physics issues – some challenges

- K->pipi decays and CP violation
  - Calcuation with two pions in the final state
    - Already some success in the I=2 channel
    - Much advance in the related pipi 2-body calculations
    - Finite-size theoretical setup by Lellouch-Luescher

- Hadron scattering and nulcear binding
  - Nucleon-nucleon potential
    - Dependence on quark mass is a very interesting issue
      e.g., deuteron may not bound if quarks are heavier….(?)
  - Kaon-nucleon potential
    - Relevant for penta-quark

- ……

However, before we begin,...

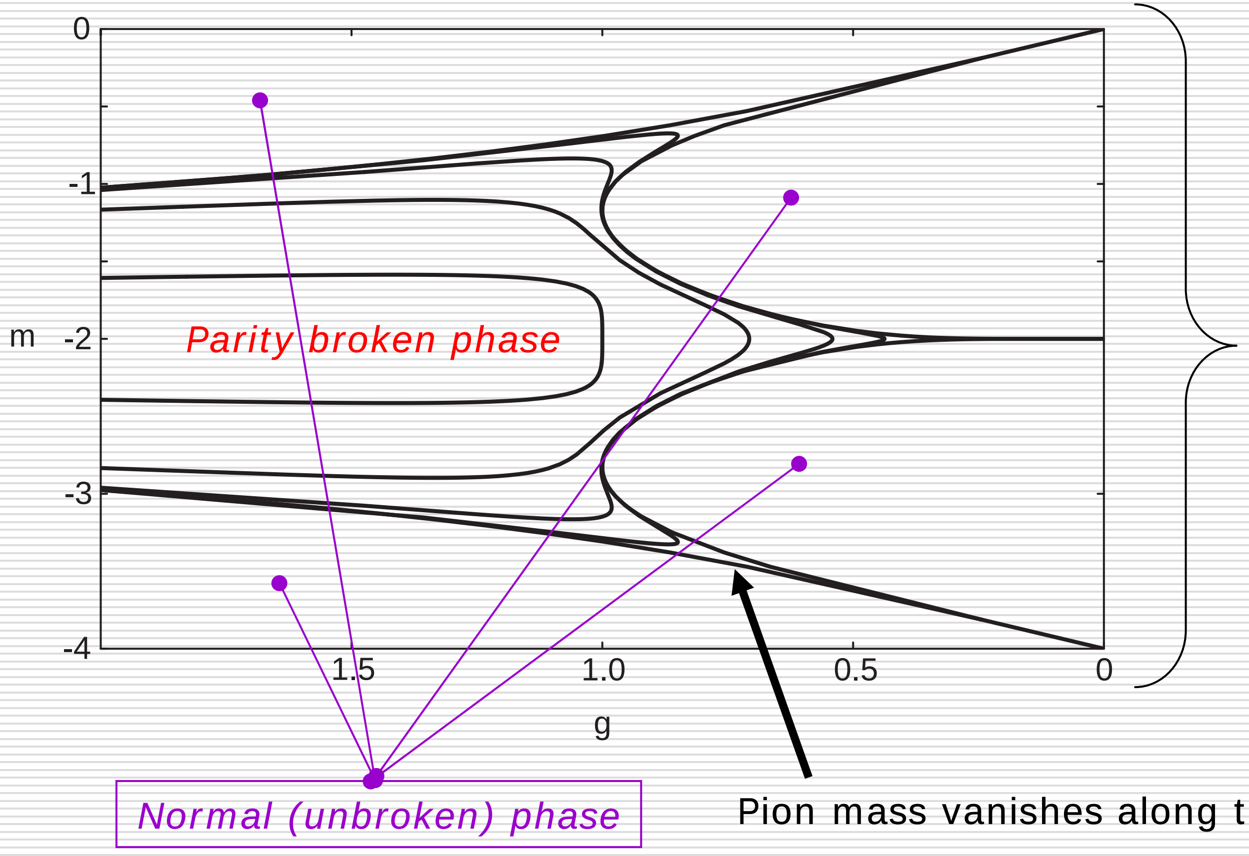
we have to clarify the phase diagram of Wilson-clover lattice QCD……

- S. Aoki (1984) massless pion ←→parity-broken phase
  - Long-discussed issue with many subsequent sudies
    - Studies by Aoki-Goksch
    - Finite-tempereture studies by MILC, QCDPAX, my own work with Aoki,...
    - "tmQCD" studies by Bitar, by Ilgenfritz et al,...

- *Personally, I was convinced that the parity-broken phase provided a satisfactory picture at both zero and finite temperature.*

- *However…..*

Parity-broken phase in 2d Gross-Neveu model



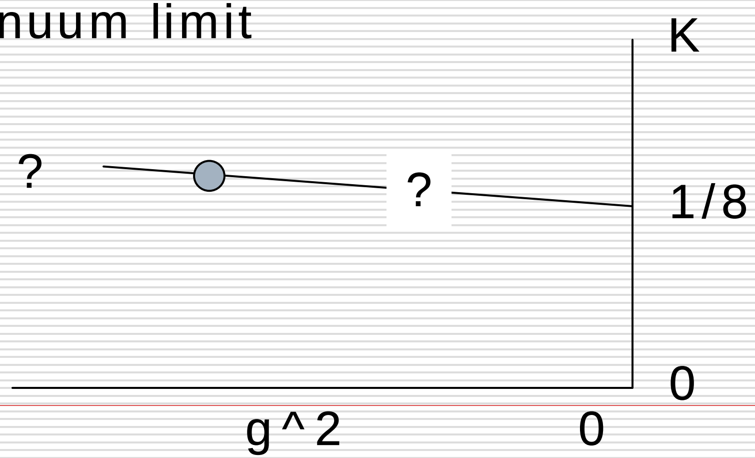
Expect five such fingers of parity broken phase in the case of QCD

$\infty \times N\_t$ lattice , N_t=2,4, 8,16, ∞ from inside to outside

F. Farchioni et al, hep-lat/0406039, 0410031

- 1^{st} order transition in Nf=2 QCD
  - First observed for Plaquette + naïve Wilson quark
    Beta=5.2, K=0.17150 on 12^3x24 (for mu=0)
  - m_pi is non-zero at the transition
  - Weakens but stays for DWB2 improved gauge action
    Beta=0.67, K=0.167-0.168 on 12^3x24 (for mu=0)
    Mpi～300-400MeV at the transition

- Their interpretation and suggestion
  - c_2<0 in the language of Sharpe-Singleton analysis of the Aoki phase
  - Will continue to the continuum limit



Sharpe-Singleton analysis of Aoki Phase

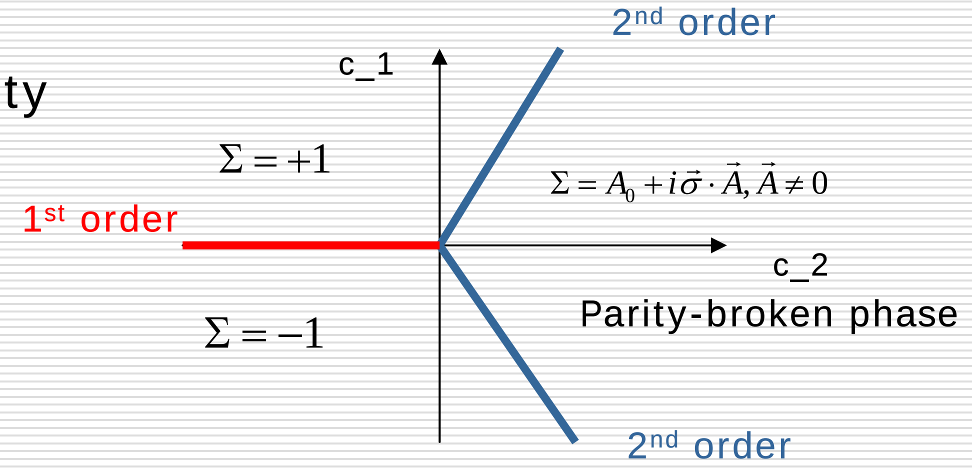
Nf=2

Sharpe and Singleton, Hep-lat/9804028 PRD 58,074501('98)

- Chiral lagrangian for Wilson quark action for Nf=2 flavors

$$L = \frac{f^2}{4} Tr\left(\partial_\mu \Sigma \partial_\mu \Sigma^+\right) - \frac{c_1}{4} Tr\left(\Sigma + \Sigma^+\right) + \frac{c_2}{16}\left(Tr\left(\Sigma + \Sigma^+\right)\right)^2$$

- If c_2>0, there is a region of parity-broken phase sandwiched by symmetric phase
- If c_2<0, there is no parity broken phase, but a 1st order transition



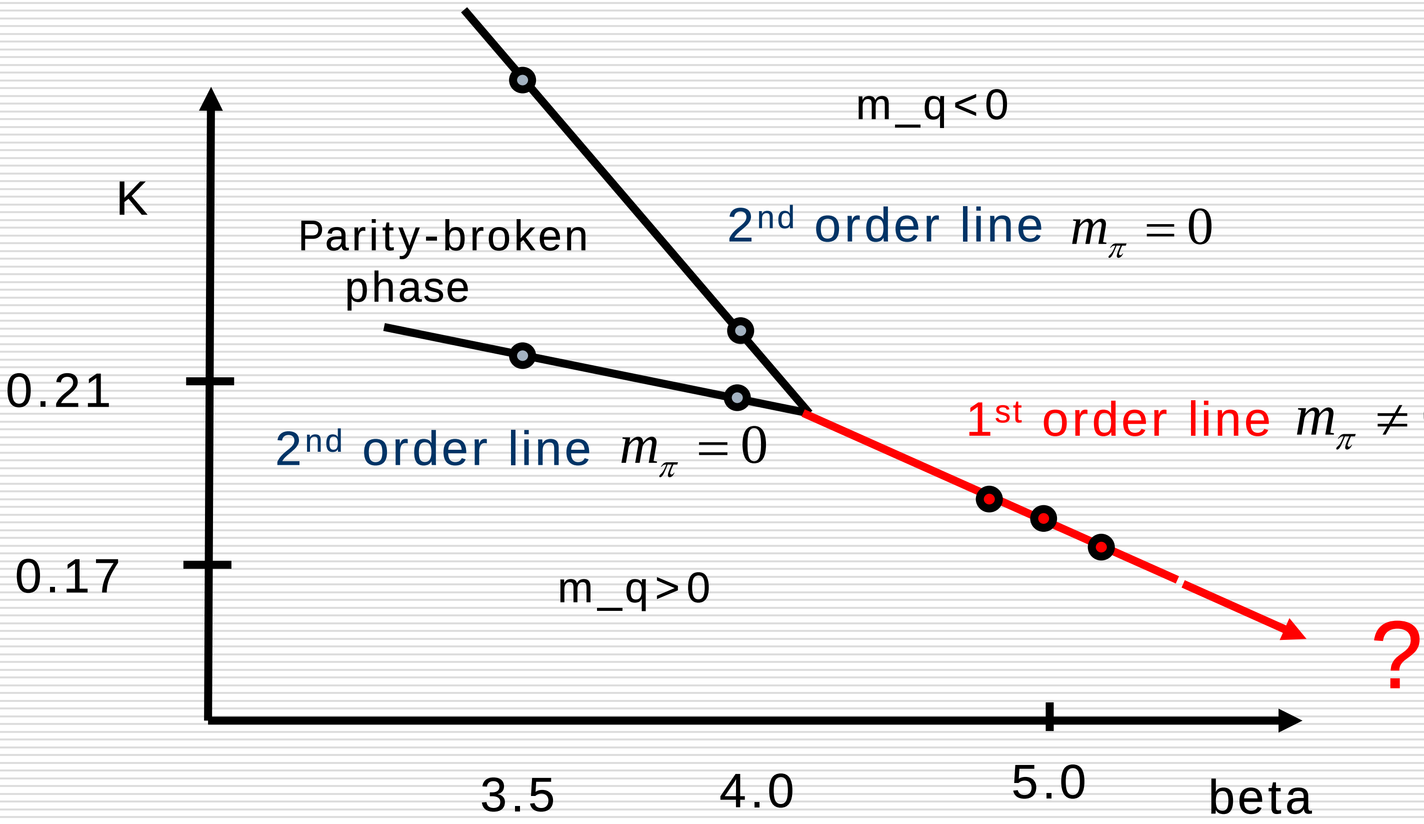
$$L = \frac{f^2}{4} Tr\left(\partial_\mu \Sigma \partial_\mu \Sigma^+\right) - \frac{c_1}{4} Tr\left(\Sigma + \Sigma^+\right) + \frac{c_2}{16}\left(Tr\left(\Sigma + \Sigma^+\right)\right)^2$$

$$+ \frac{c_3}{16}\left(Tr\left(\Sigma - \Sigma^+\right)\right)^2 + \frac{c_4}{16} Tr\left(\left(\Sigma + \Sigma^+\right)^2\right)$$

Extension to Nf=3 straightforward,
but conclusions far less definite
because 4 couplings are allowed

Putting old and new work together……

Perhaps, the tip simply stops moving and turns into a line of 1st order transition at some vakue of beta near 4.0…..



Cf M. Creutz, hep-lat/9608024

If the 1st order transition continues to the continuum limit ...

- NOT a problem of principle in constructing a chirally symmetric continuum QCD

  Cf. 2-dim Gross-Neveu model

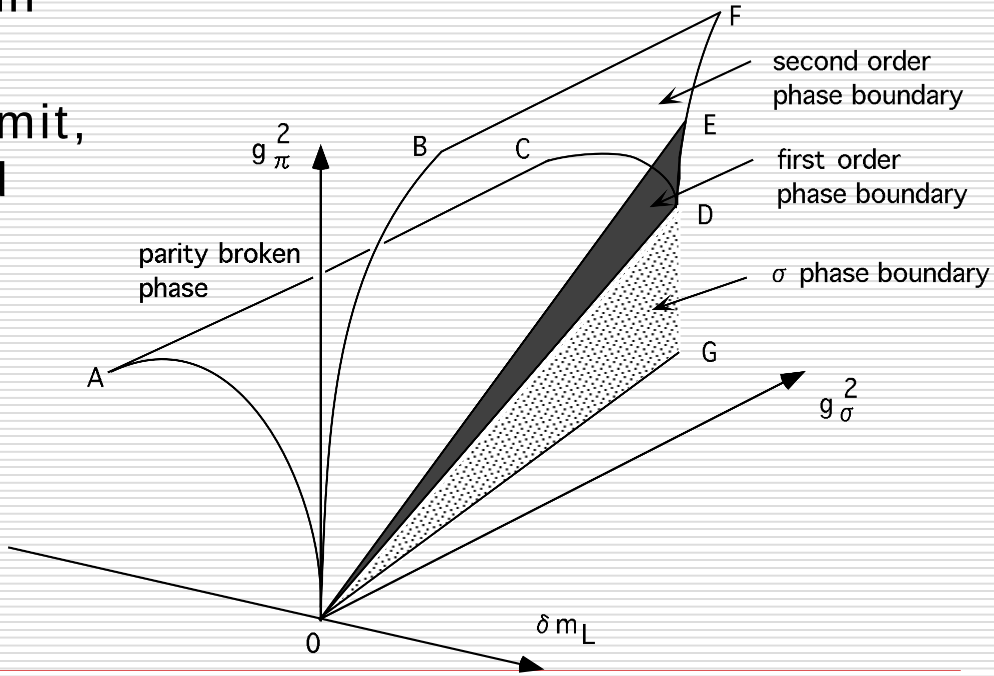
- However, less than welcome in terms of phenomenology
  - If m_pi∼O(100)MeV at 1/a∼2GeV, meaningful phenomenology is impossible at lattice spacings accessible today; would need m_pi∼O(10)MeV or less.
  - Otherwise, have to take the continuum limit first, and then fix the dimensionful parameters, quark masses and the QCD lambda parameter, a difficult procedure.....
  - And heavy quark physics will be in jeopardy......

2D Gross-Neveu model in the large N limit

Noaki-Izubuchi-Ukawa, PRD

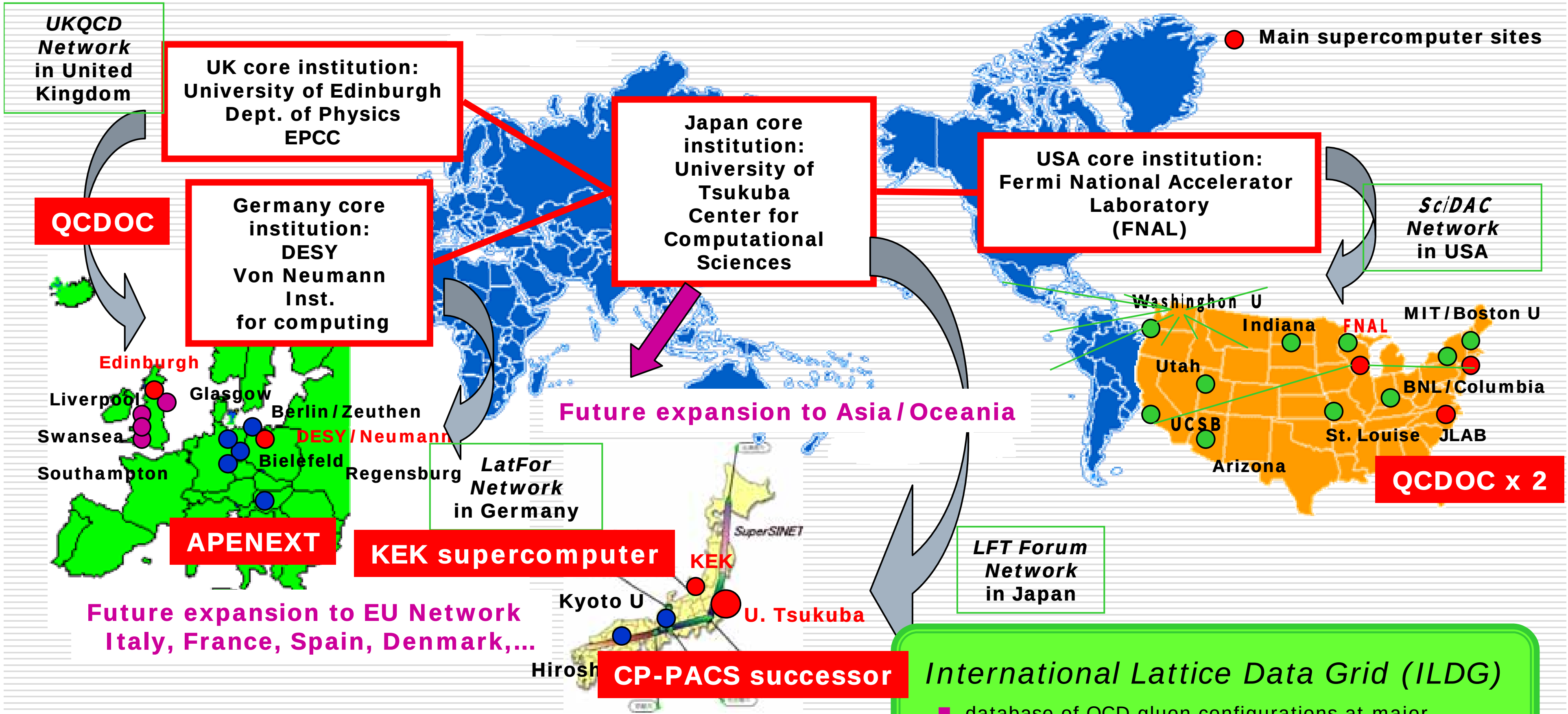
$$L = \bar{\psi}\gamma_\mu \cdot \left(\nabla_\mu + \nabla_{-\mu} - \frac{1}{2}\nabla_\mu \nabla_{-\mu} \right)\psi + \frac{g_\sigma}{N}(\bar{\psi}\psi)^2 + \frac{g_\pi}{N}(\bar{\psi}i\gamma_5\psi)^2$$

- Need two couplings to restore chiral symmetry in the continuum limit
- Solvable in the large N limit, but a rather complicated phase diagram



International Research Network for Computational Particle Physics

JSPS core-to-core program



International Lattice Data Grid (ILDG)

- database of QCD gluon configurations at major supercomputer facilities
- acceleration of research via mutual usage of QCD gluon configurations via fast internet
- future international sharing of supercomputing and data storage resources

Summary

- *Welcome prospect toward precision QCD predictions with realistic quark spectrum in sight*
  - *Firm numbers to our phenomenology/experiment colleagues*
  - *Quantitative understanding of the full range of strong interactions*
    - 1935 meson theory (Yukawa)
    - 1951 strangeness (Gell-Mann-Nishijima)
    - 1961 chiral symmetry and pion(Nambu-Jona-Lasinio)
    - 1973 QCD and asymptotic freedom(Gross-Wilczek-Politzer)
    - 1974 Lattice QCD(Wilson)
    - 1981 Monte Carlo simulation of QCD(Creutz-Jacobs-Rebbi)
- *Enhanced research effort with international collaboration and coordination all the more important and effective in our field in the years to come*