Numerical calculations and the evolution of the APE series

- Ape starts as a tool for numerical simulations of non perturbative phenomena in quantum chromodynamics
- People realised that a boost can be given to the field through the construction of optimized computers

The series

- 1984-1989: APE1
  - 16 nodes, 1 gigaflop
  - Primitive language

- 1990-1995: APE100
  - The first time custom
  - 2048 nodes
  - Speaks TAO
  - Integrated 300 Gigaflops

P. Bacilieri
INFN-CNAF, Bologna, Italy
S. Cabasino, A. Frighi, F. Marzano, N. Matone, P. S. Paolucci, S. Petrarca, G. Salina
INFN, Sezione di Roma, Italy
N. Cabibbo, E. Marinari, G. Parisi
Dipartimento di Fisica, II Univerita' di Roma "Tor Vergata"; INFN, Sezione di Roma, Italy
F. Costantini, G. Fiorentini, S. Galeotti, D. Passuello, R. Tripiccione
Dipartimento di Fisica, Univerita' di Pisa; INFN, Sezione di Pisa, Italy
A. Fucci, R. Petronzio, F. Rapuano
CERN, Geneva, Switzerland
D. Pascoli, P. Rossi
Dipartimento di Fisica, Univerita' di Padova; INFN, Sezione di Padova, Italy
E.Remiddi
Dipartimento di Fisica, Univerita' di Bologna; INFN-CNAF, Bologna, Italy; INFN, Sezione di Bologna, Italy
R.Rusack
Rockefeller University, New York, U.S.A.
B.Tirozzi
Dipartimento di Matematica - Universita' "La Sapienza" Roma, Italy

1984-1989

The series continued

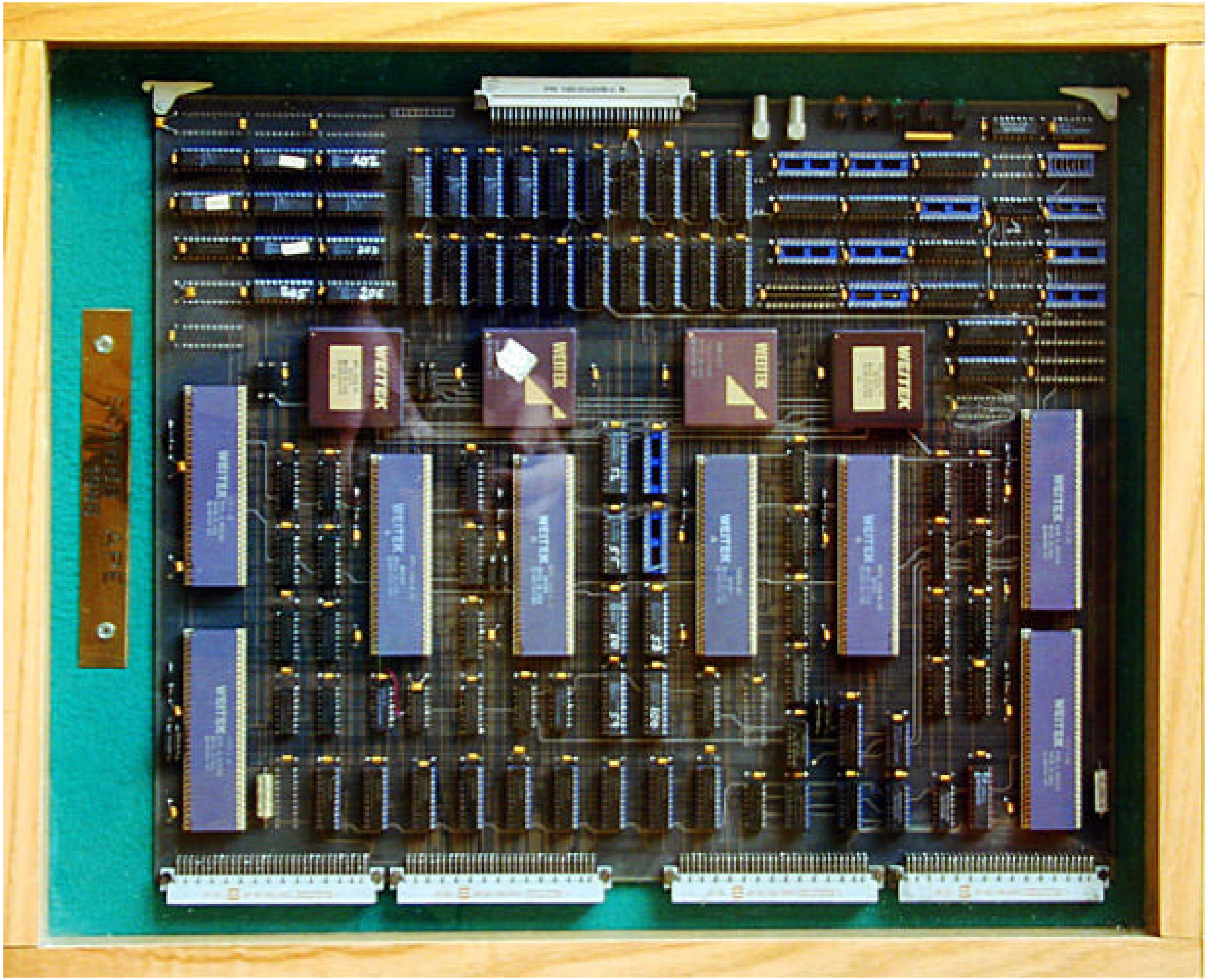
- 1995-2000: APE1000
  - A INFN-Desy effort
  - Nodes connected in a three dimensional mesh
  - Integrated 2 Teraflops deployed

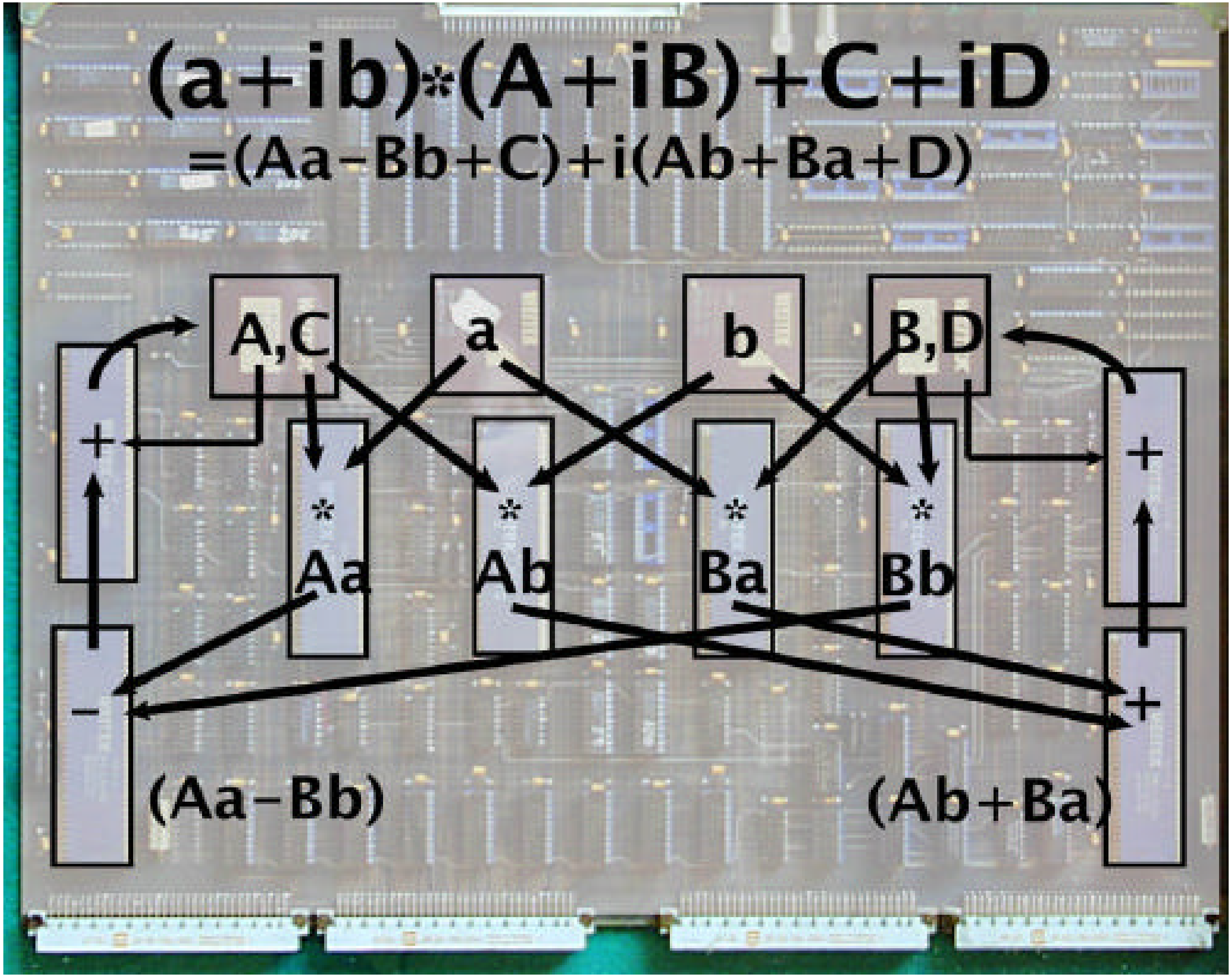
- 2001-2005: apeNEXT
  - INFN-Desy-Orsay collaboration
  - 64 bit arithmetics
  - 10 teraflops installation


100T
10T
1T
100G
10G
1G
100M
10M
1970
1975
1980
1985
1990
1995
2000
2005
Earth Simulator
ASCI Q
ASCI white
ApeNext
ASCI BP
Ape1000
T3E
SX-4
VPP500
SR2201
Ape100
T3D
SX-3
S-3800
C90
YMP
VP2600
XMP
Ape
Cray-1
Illiac-IV

The APE innovations

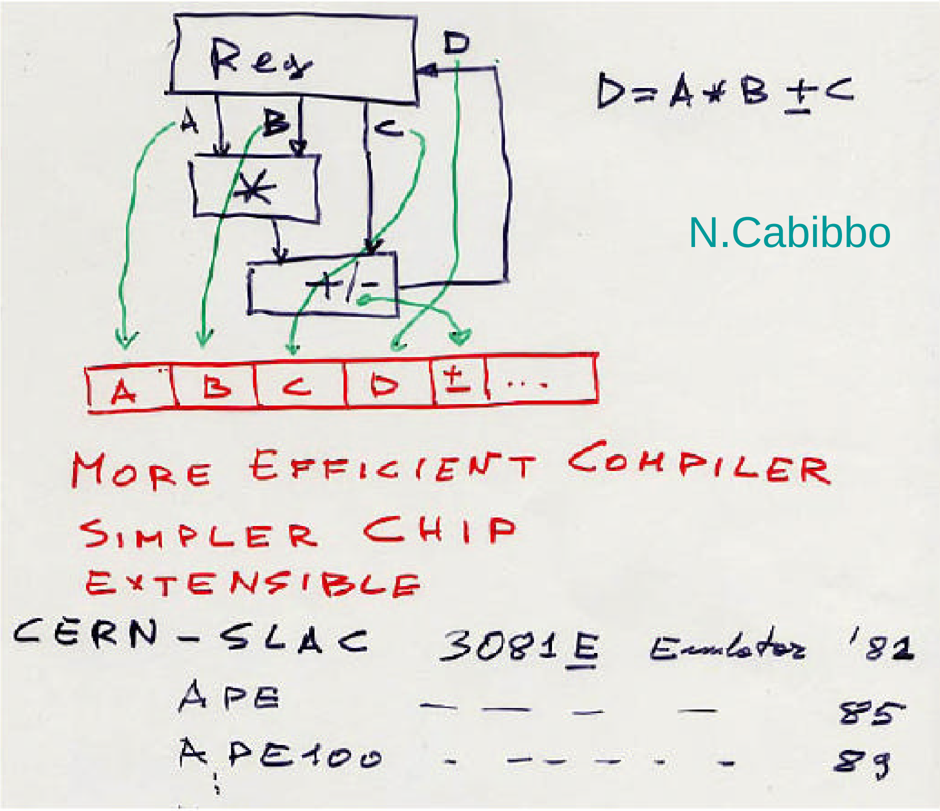
- The “core” $(a+ib)*(A+iB) + C + iD$ operation built in




(a+ib)*(A+iB)+C+iD
=(Aa-Bb+C)+i(Ab+Ba+D)
A,C
a
b
B,D
+
*
Aa
*
Ab
*
Ba
*
Bb
+
-
+
(Aa-Bb)
(Ab+Ba)

The APE innovations

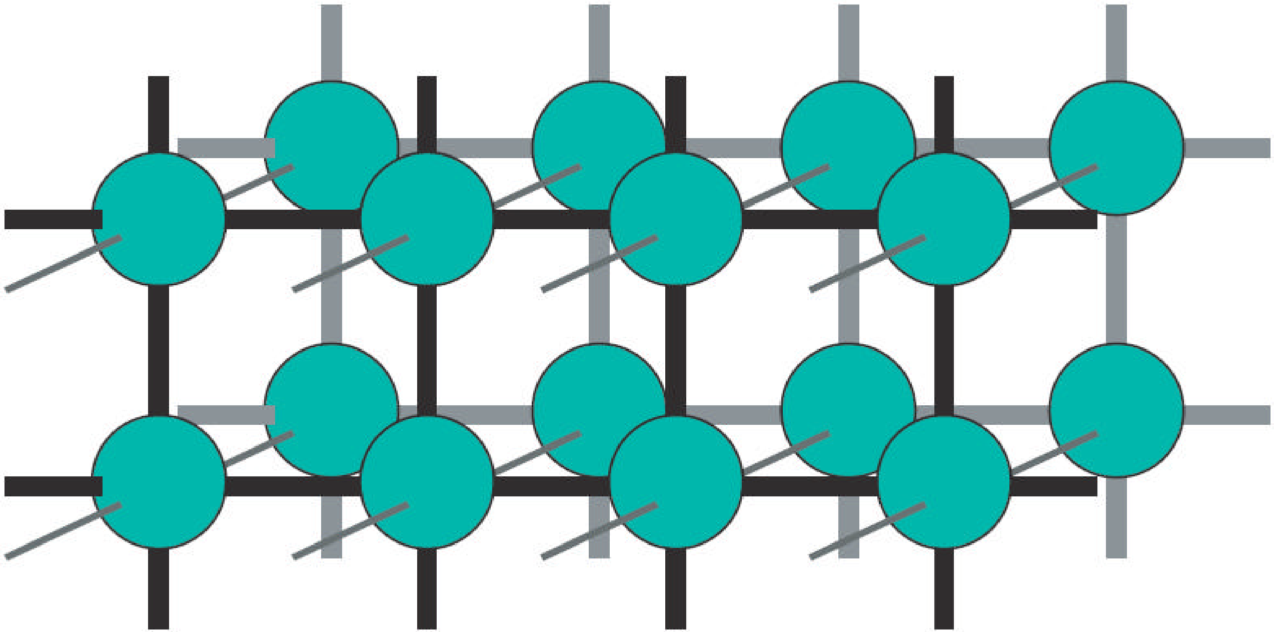
- VLIW: very long instruction word
  - Simplifies the decoding effort

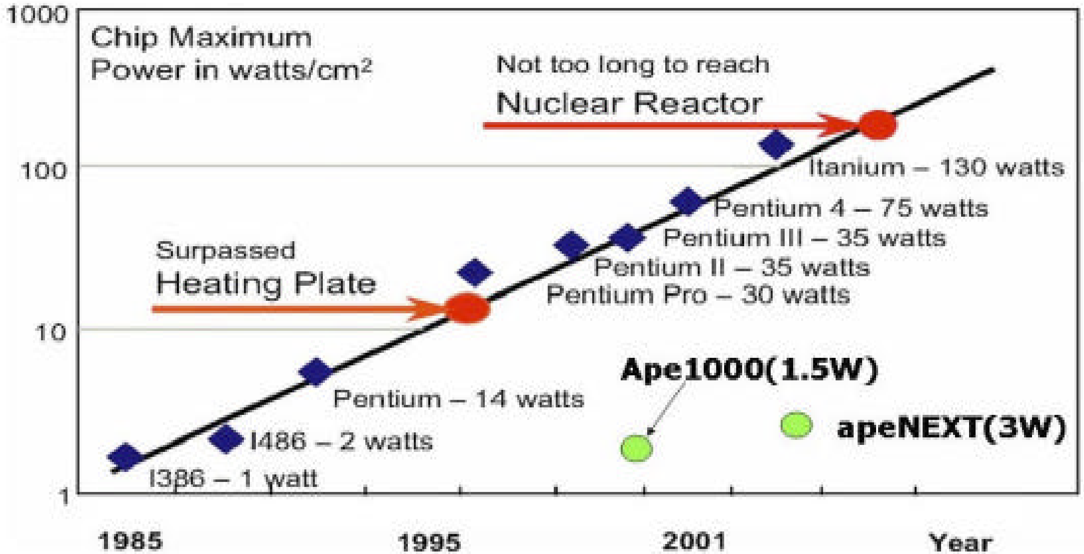


N.Cabibbo

The APE innovations

- SIMD architecture and strong 3-d connectivity





Machine	RLX TM5600	RLX TM5800	Avalon	ASCI Red	ASCI White	apeNEXT
Performance (Gflops)	21.4	3.3	17.6	600	2500	3670
Power (kilowatts)	5.2	0.52	18.0	1200	2000	80
Perf/Power (Mflops/watt)	4.12	6.35	0.978	0.5	1.25	46

Table 4. Performance-Power Ratio for Five Parallel-Computing Systems

Machine	RLX TM5600	RLX TM5800	Avalon	ASCI Red	ASCI White	apeNEXT
Performance (Gflops)	21.4	3.3	17.6	600	2500	3670
Area (feet^2)	6	6	120	1600	9920	72
Perf/Power (Mflops/feet^2)	3500	550	150	375	252	50972

Table 5. Performance-Space Ratio for Five Parallel-Computing Systems

The physics

- The accuracy of lattice calculations goes with the reduction of the discretisation effects
  - The lattice resolution
  - The finite volume

Number of points

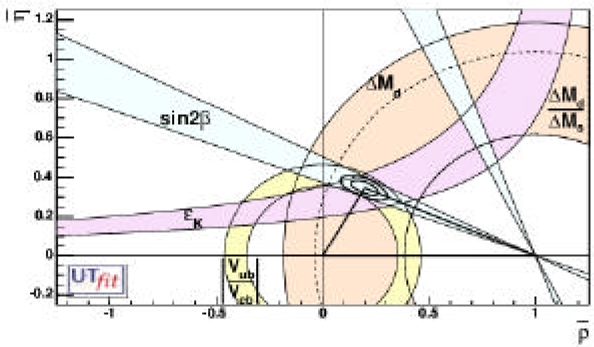
CPU and memory

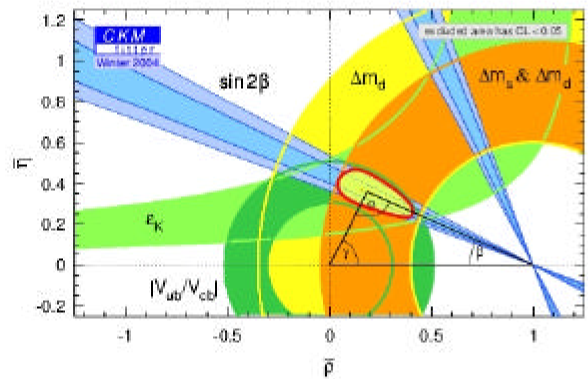
The physics

- Chirality on the lattice
  - Recovered in the “continuum limit”
  - Obtained at finite lattice spacing at the expenses of introducing a fifth dimension

CPU and memory

CKM Lattice QCD queries





	$\lvert\epsilon_K\rvert$	ΔM_{B_s}	$\dfrac{\Delta M_{B_s}}{\Delta M_{B_d}}$	$B \to \begin{pmatrix}\pi \\ \rho\end{pmatrix} l\nu$	$B \to \begin{pmatrix}D \\ D^*\end{pmatrix} l\nu$
CKM	$\mathrm{Im}[V_{td}]$	$\lvert V_{ts}\rvert^2$	$\lvert V_{ts}\rvert^2/\lvert V_{td}\rvert^2$	$\lvert V_{ub}\rvert^2$	$\lvert V_{cb}\rvert^2$
Matrix Elements	$\hat{B}_K$	$f_{B_s}^2 \hat{B}_{B_s}$	$\dfrac{f_{B_s}^2 \hat{B}_{B_s}}{f_{B_d}^2 \hat{B}_{B_d}}$	$\lvert\langle {}^{\pi}_{\rho} \lvert J_L^{ub} \rvert B\rangle\rvert^2$	$\lvert\langle {}^{D}_{D^*} \lvert J_L^{cb} \rvert B\rangle\rvert^2$

APE1

Beginning of weak interactions on the lattice

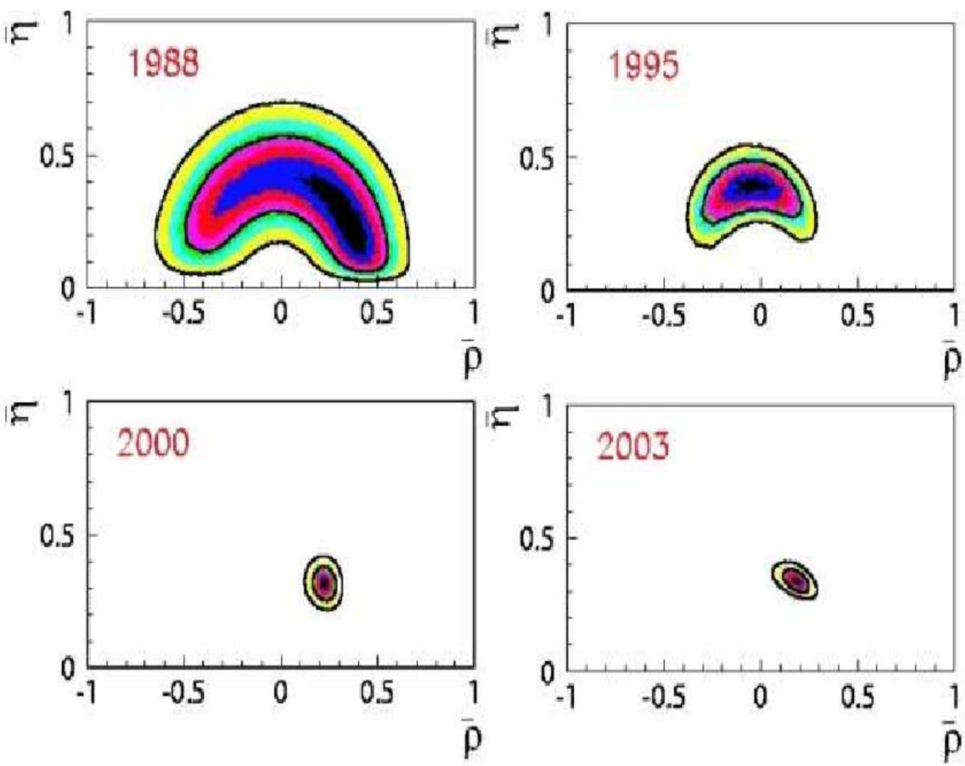
10^3*20 lattice

APE1000

Lattice spacing 0.05 Fermi

Volume 2 Fermi

M. Bona et al. [UTfit] 04



APE100

Improvements to ameliorate the continuum limit

24^3*48 lattice

Still APE1000

CP-PACS

Continuum limits

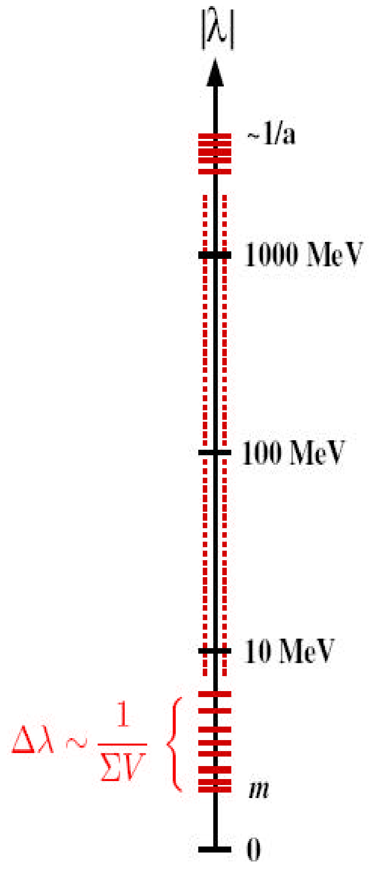
The NEXT physics

- Accounting q–qbar pair creation (unquenching)
  - A non local effective gauge interaction
  - Monte Carlo scale badly with the volume and with the quark mass

CPU and memory.. may not be enough

Unquenching, a multiscale problem

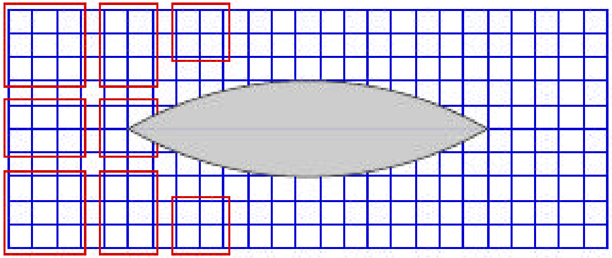
The inclusion of sea quark loops needs the calculation of the determinant of an operator with a LARGE hyerarchy of scales, from the quark mass to the chiral cutoff

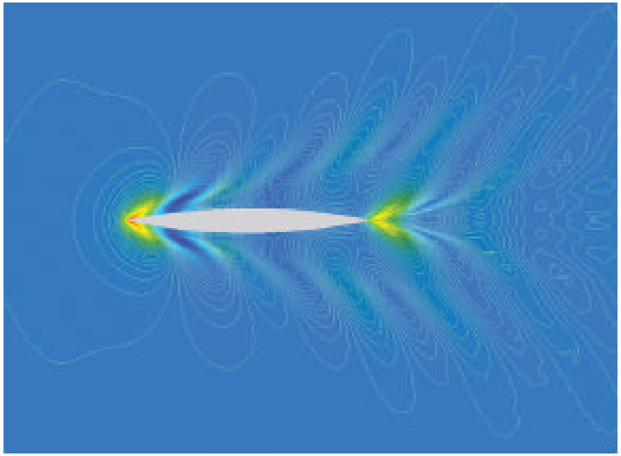


$$\mathrm{C_{ost}} \propto \mathrm{N_{conf}}\, m_q^{-3}\, L^5\, a^{-8}$$

Water flow and wave calculation

* Solve Reynolds-Averaged Navier-Stokes equations
* Mesh discretization
* Domain decomposition and multigrid methods

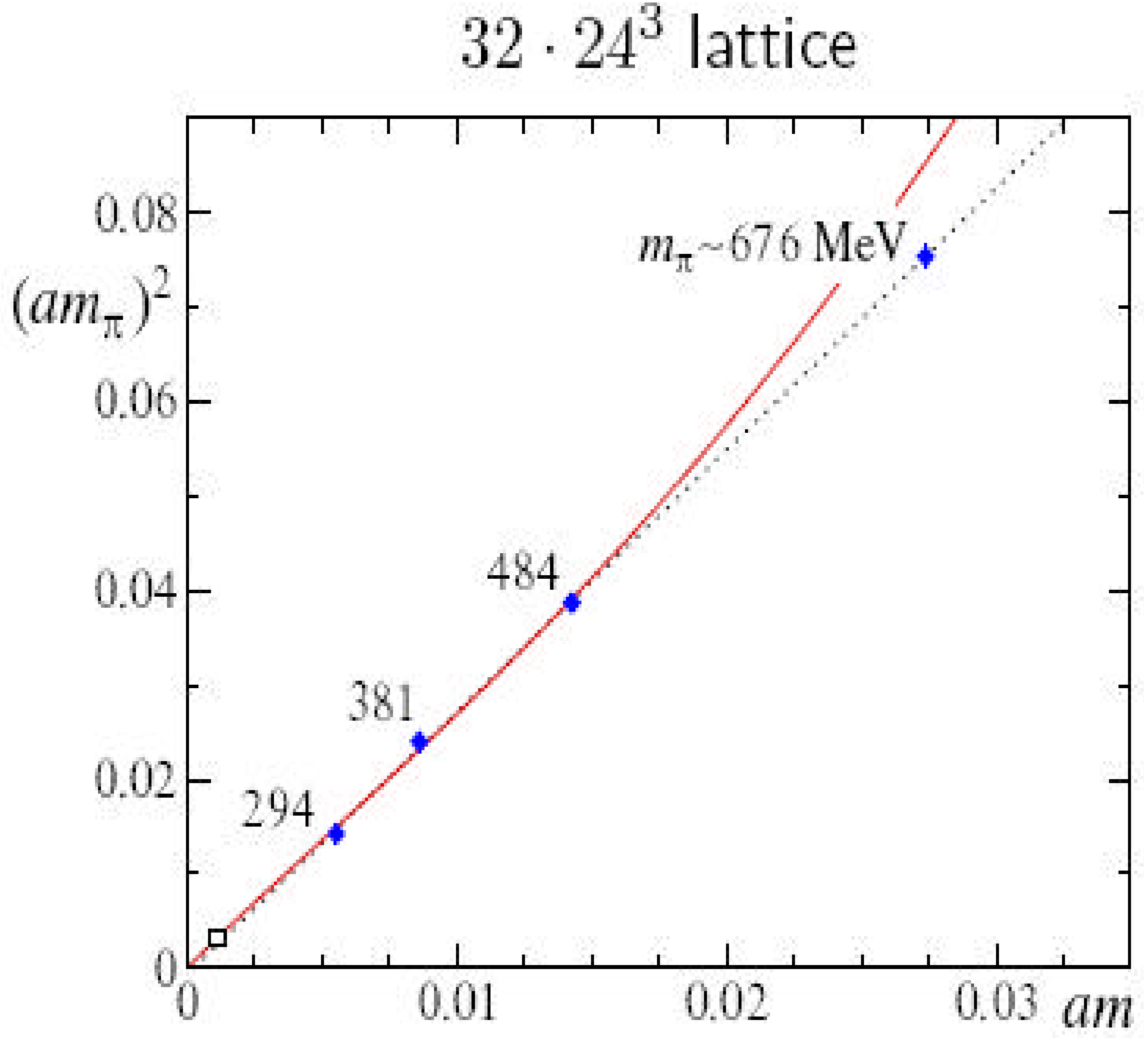




Luescher et al.

$$\mathrm{Cost} \propto \mathrm{N_{conf}}\, m_q^{-1}\, L^5\, a^{-6}$$

EPFL, J. Wynne '03



32 · 24³ lattice
(amπ)²
0.08
0.06
0.04
0.02
0
0
0.01
0.02
0.03
am
mπ~676 MeV
484
381
294

B physics, another multiscale problem

- High resolution to properly account for bottom quark dynamics
- Large volume to include a heavy-light system

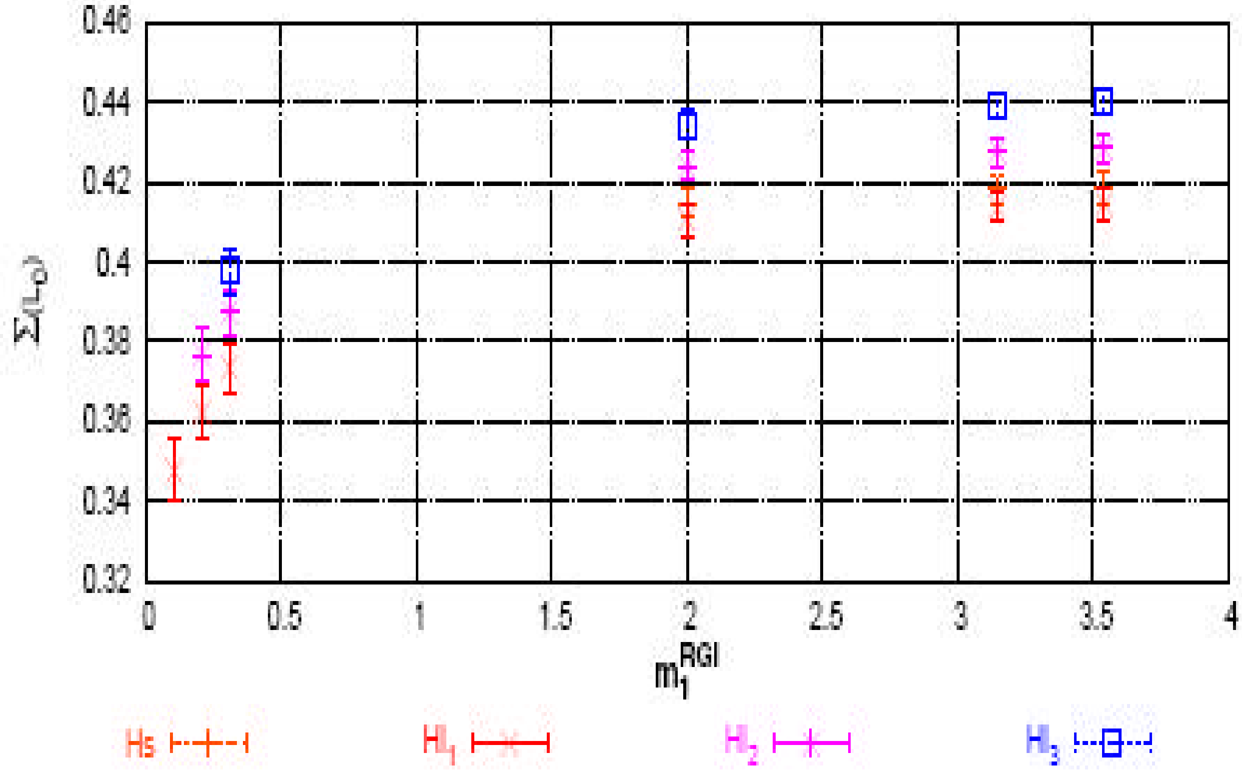
100^3*200 lattice

The step scaling method

- Finite volume effects should manly depend upon the light quark and be rather insensitive to the heavy quark mass

$$f_{h\ell}(L_\infty) = f_{h\ell}(L_0)\,\frac{f_{h\ell}(L_1)}{f_{h\ell}(L_0)}\,\frac{f_{h\ell}(L_2)}{f_{h\ell}(L_1)}\cdots, \qquad L_0 < L_1 < L_2 \ldots$$

$$\frac{f_{h\ell}(L_1)}{f_{h\ell}(L_0)} = \Sigma(L_1)$$


0.46
0.44
0.42
0.4
0.38
0.36
0.34
0.32
0
0.5
1
1.5
2
2.5
3
3.5
4
$\Sigma(L_0)$
m_1^{RGI}
Hs
HI_1
HI_2
HI_3

The NEXT generation

- “definite” calculations of spectra and kaon physics
- B physics with sea quarks without brute force

perspectives

- New ideas for a PETAflop generation
- Distributed computing for parallel simulations (GRID)
- Computer architecture optimization for a large class of scientific problems
  - Standard language support
  - Modularity in communication
- Closing chapters in lattice QCD