Computing Challenges in Lattice QCD

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Introduction : Why & How

Computing Challenges

Current Scenario

Summary

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- Similar to structure in theory of electrons & photons (QED).
- *Unlike QED*, the coupling is usually very large and its eight "photons" interact amongst themselves.
- Very high interaction (binding) energies. E.g., $M_{Proton} \gg (2m_u + m_d)$, by a factor of 100 $\rightarrow$ Understanding it is knowing where the visible mass of Universe comes from.
- Much richer structure and phenomena : Quark Confinement, Dynamical Symmetry Breaking, Quark-Gluon Plasma, Colour Superconductivity..

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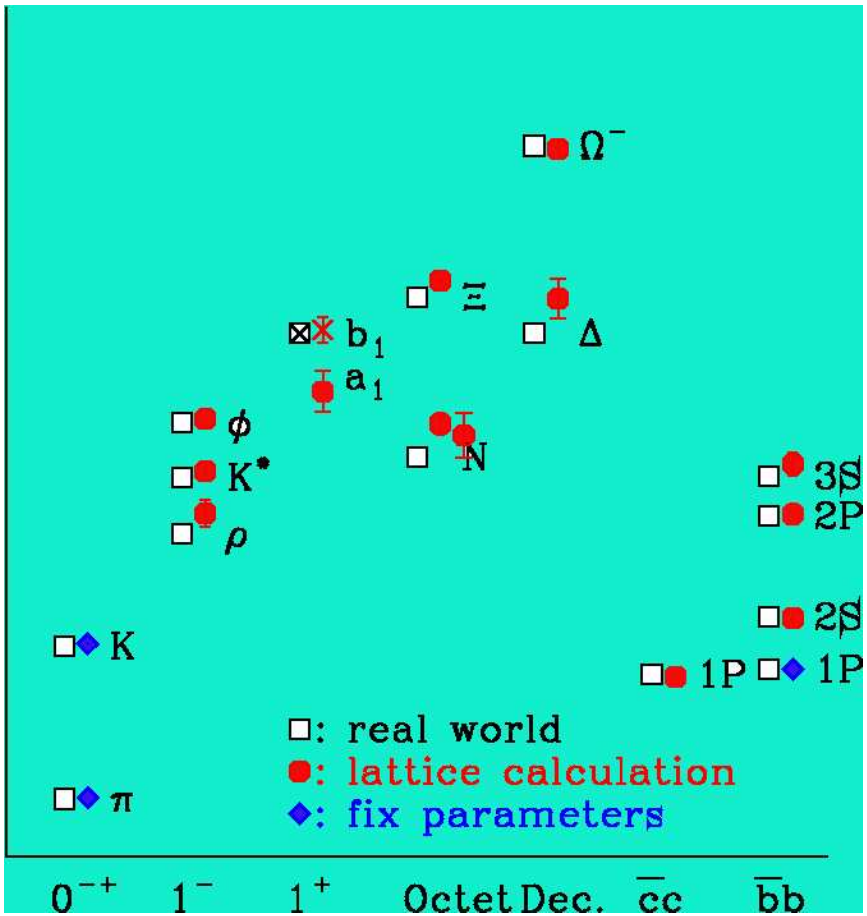

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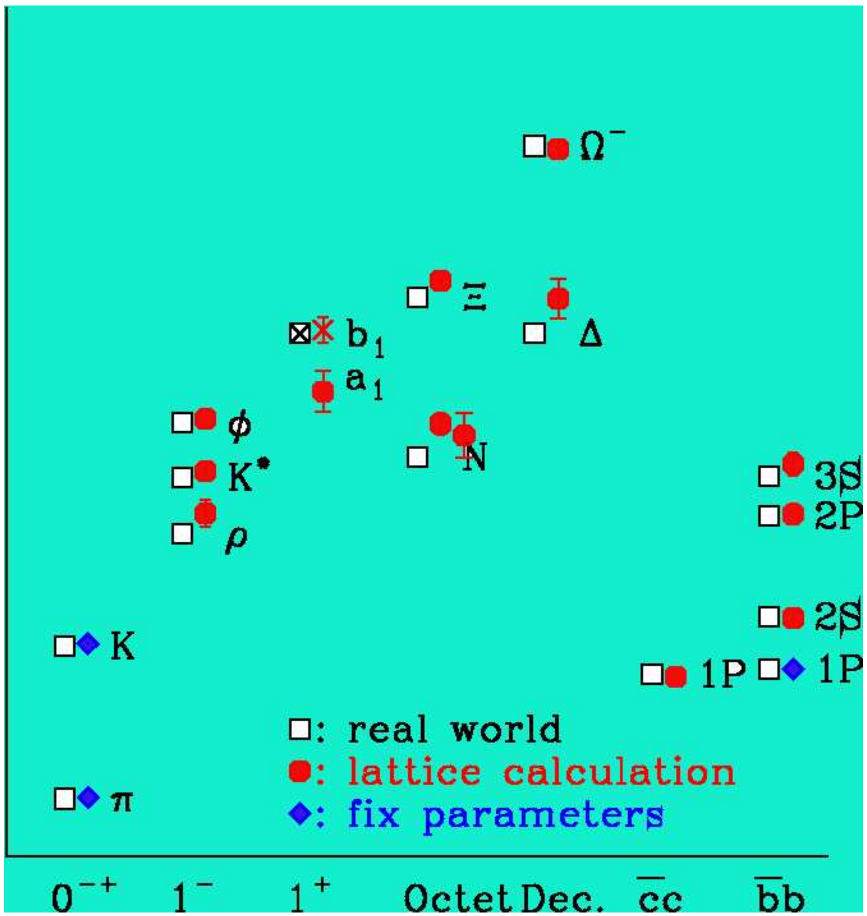

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♡ Strong Coupling Constant α_s computed from underlying theory.

♡ Heavy Meson properties predicted : m_{B_c}, f_B, f_D..

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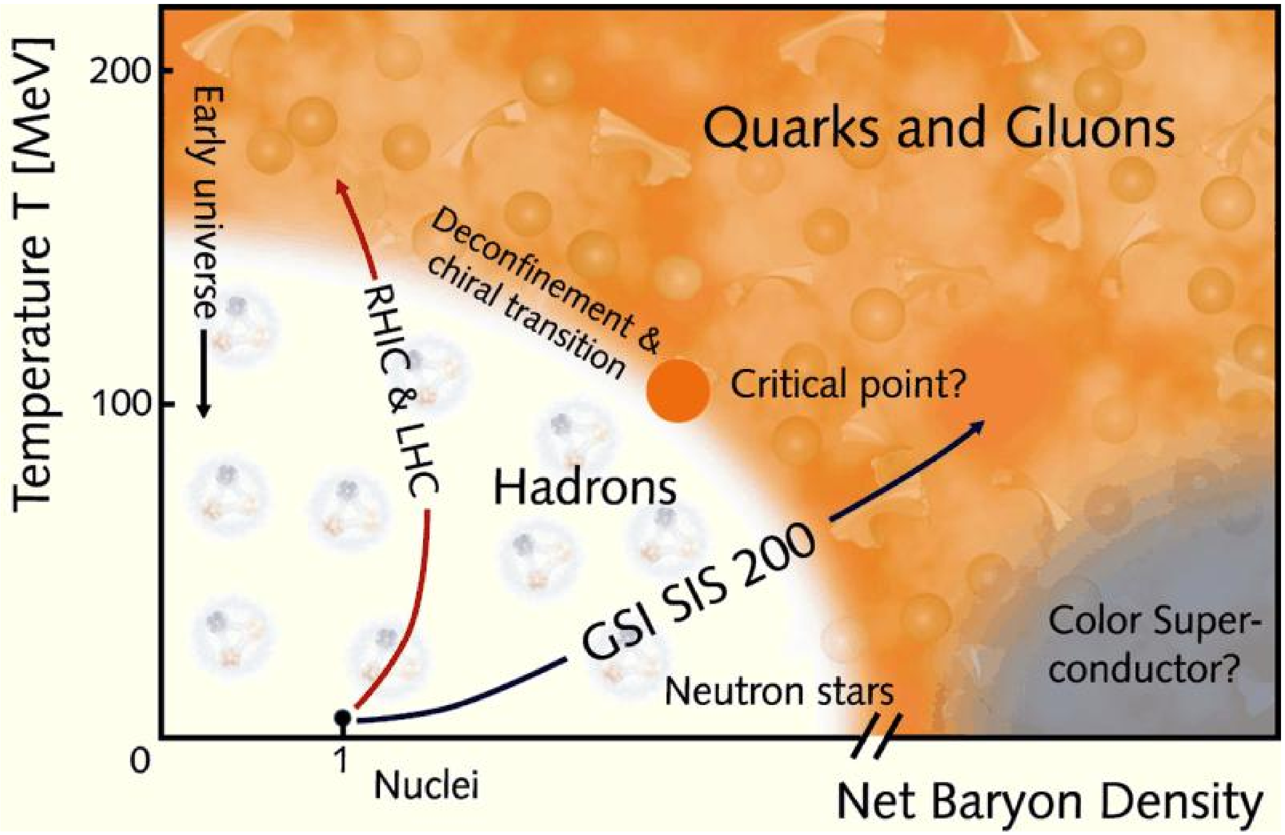

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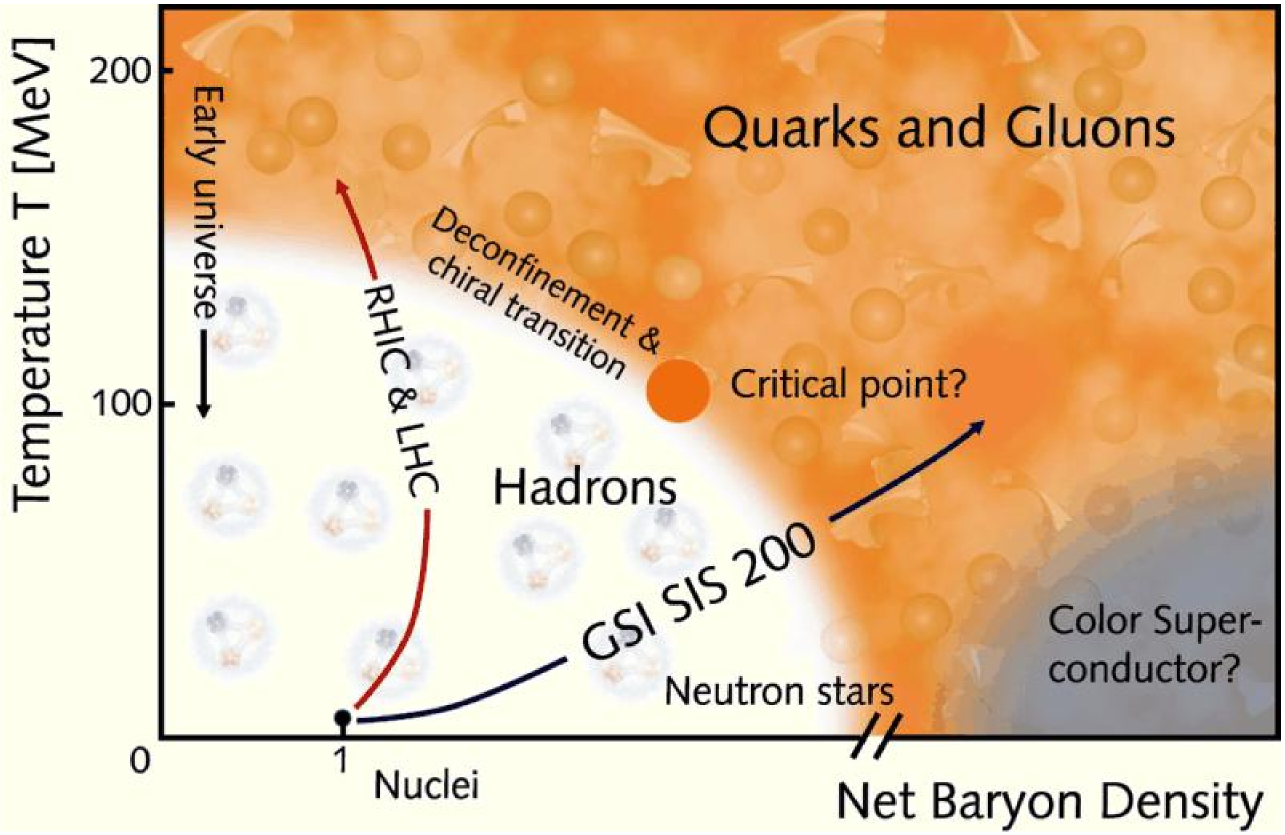

- New States at High Density & Temperatures, expected on basis of models. (Figure from H. Stöcker)

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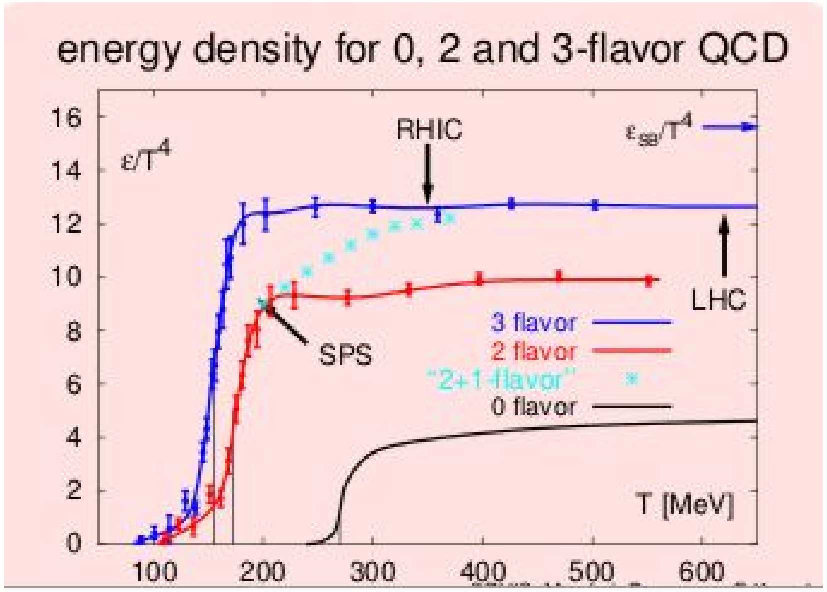

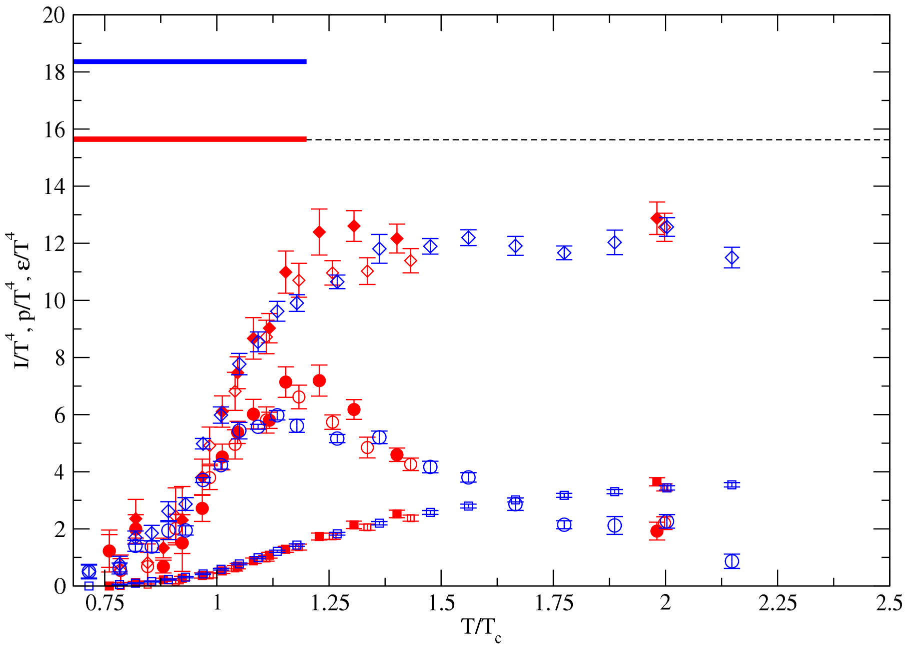

$N_t = 4$ Lattices

Bielefeld 2001 (Karsch hep-ph/0103314)

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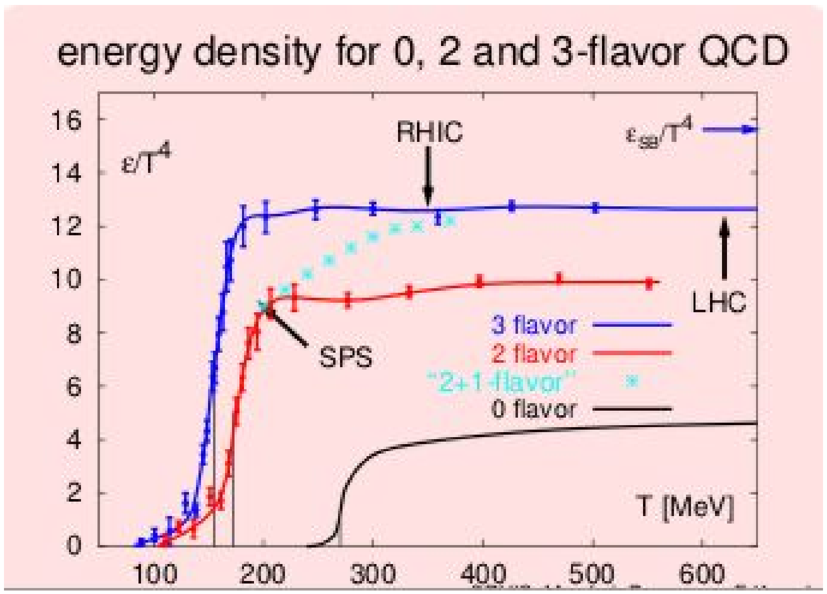

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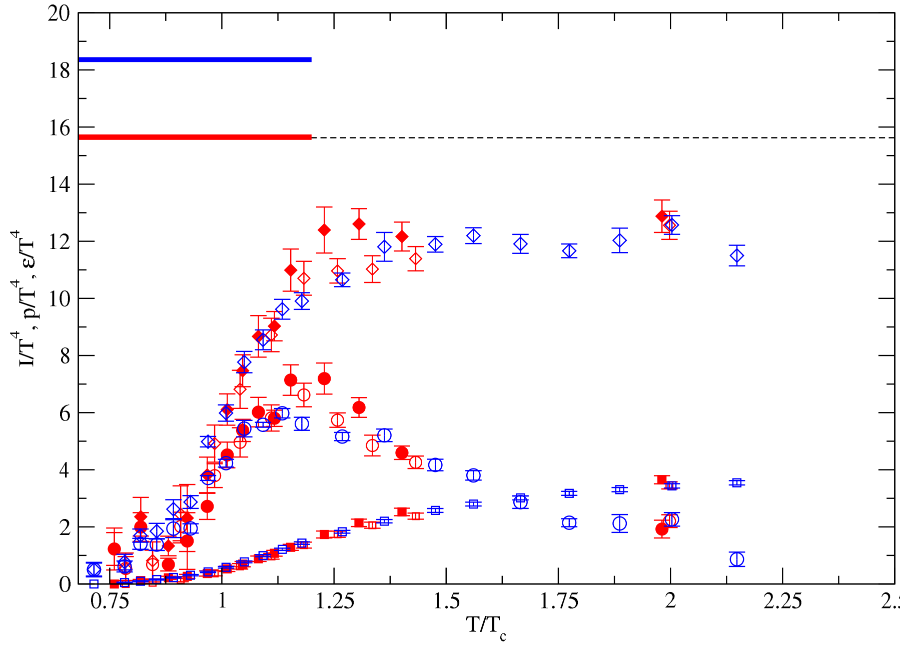

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- Other quantities for Heavy Ion Physics: the Wróblewski Parameter λ_s, J/ψ-dissolution, dileptons, speed of sound, transport coefficients... etc.

- λ_s — Measure of Production of strange quark-antiquark pairs; Expts agree with estimates from the new state Quark-Gluon Plasma.
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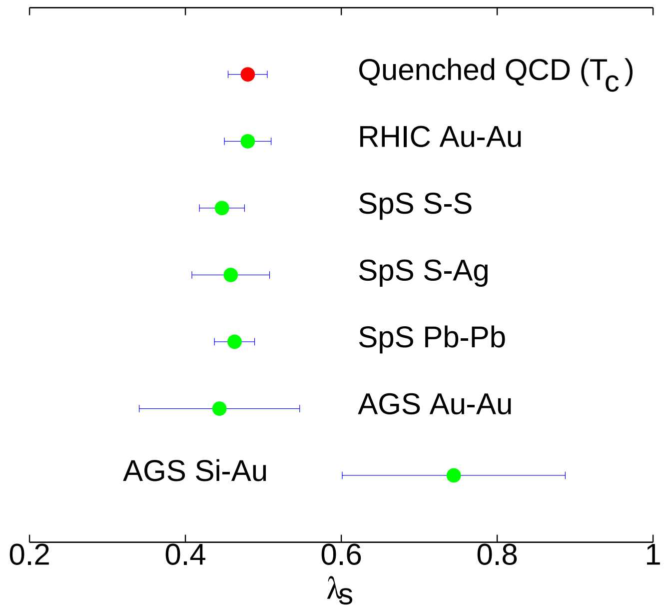
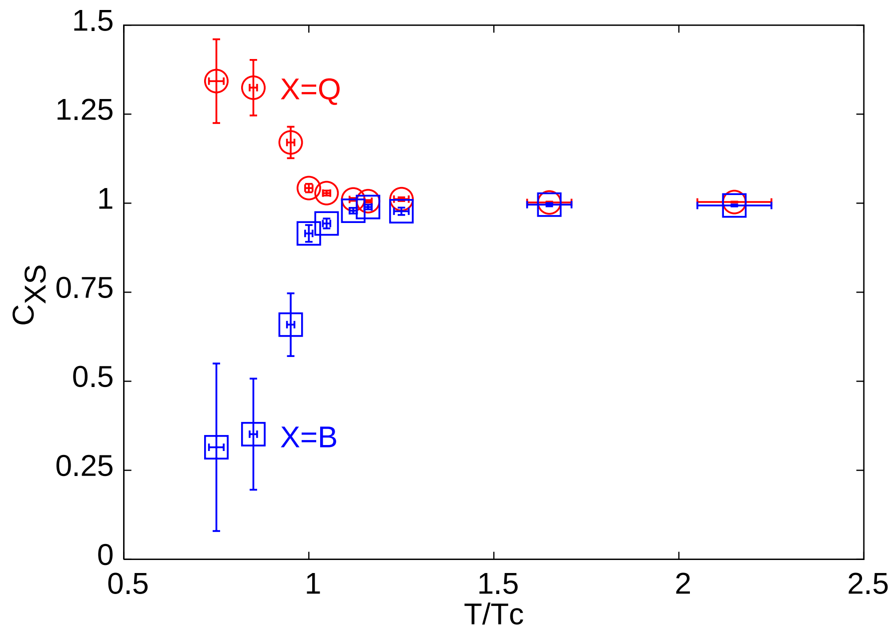
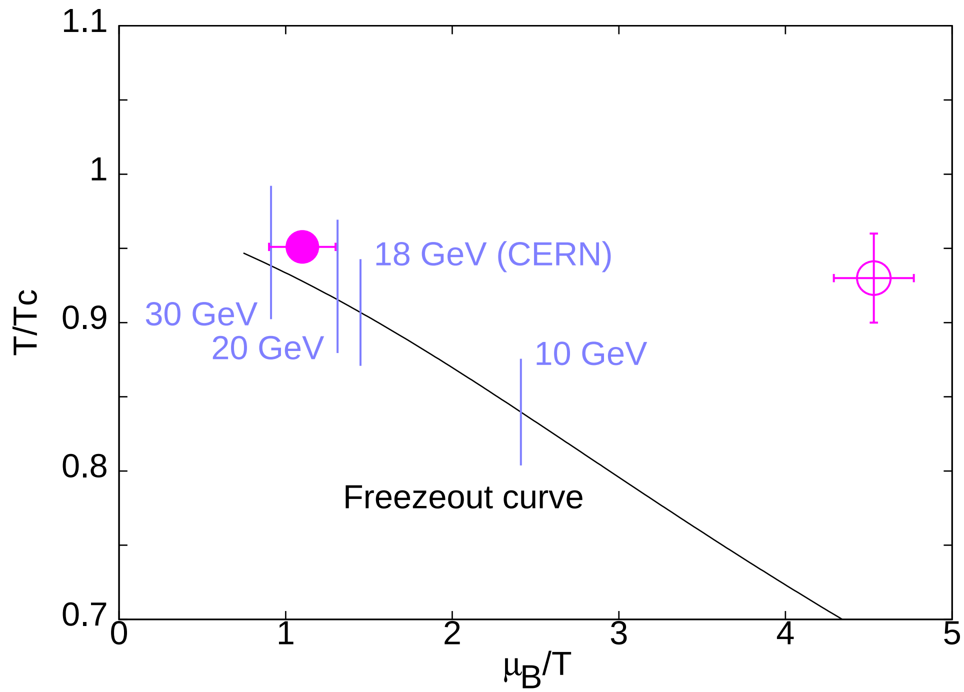




R. V. Gavai and Sourendu Gupta, Phys Rev D65, 2002 and hep-lat/0510044.

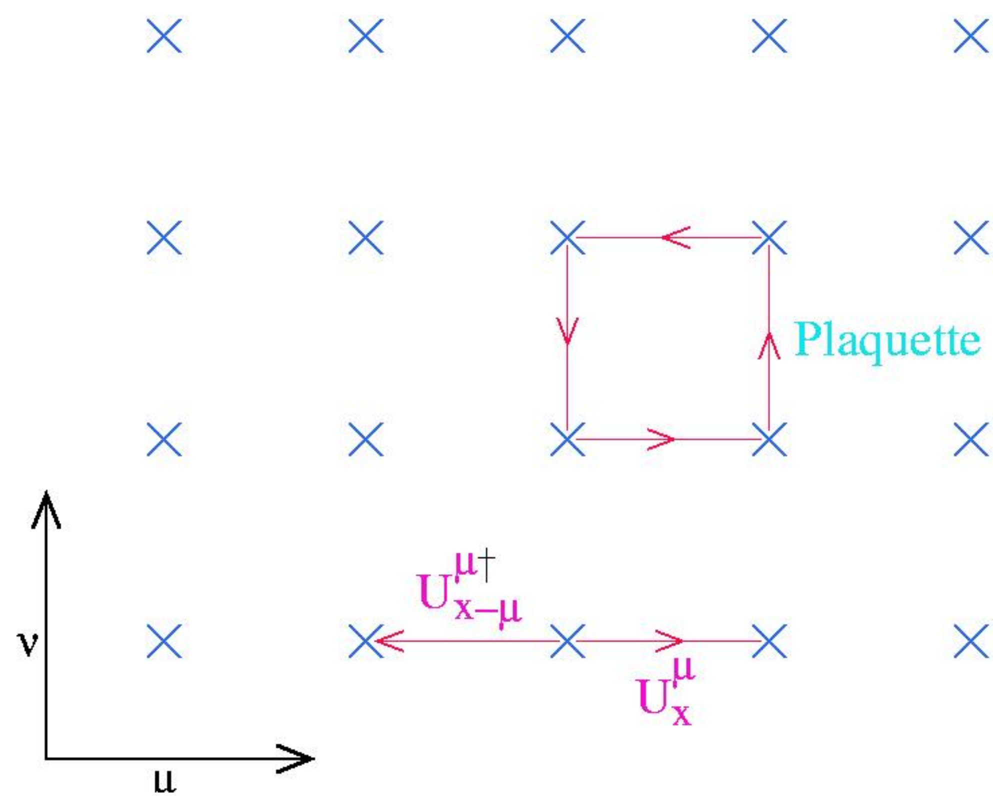


R. V. Gavai and Sourendu Gupta, PRD 2005.

♠ Lattice QCD has yielded information on the critical point of QCD, which may be discovered in energy scans at RHIC (Open circle from Fodor-Katz JHEP 2002).

Basic Lattice QCD

- Discrete space-time : Lattice spacing a UV Cut-off.



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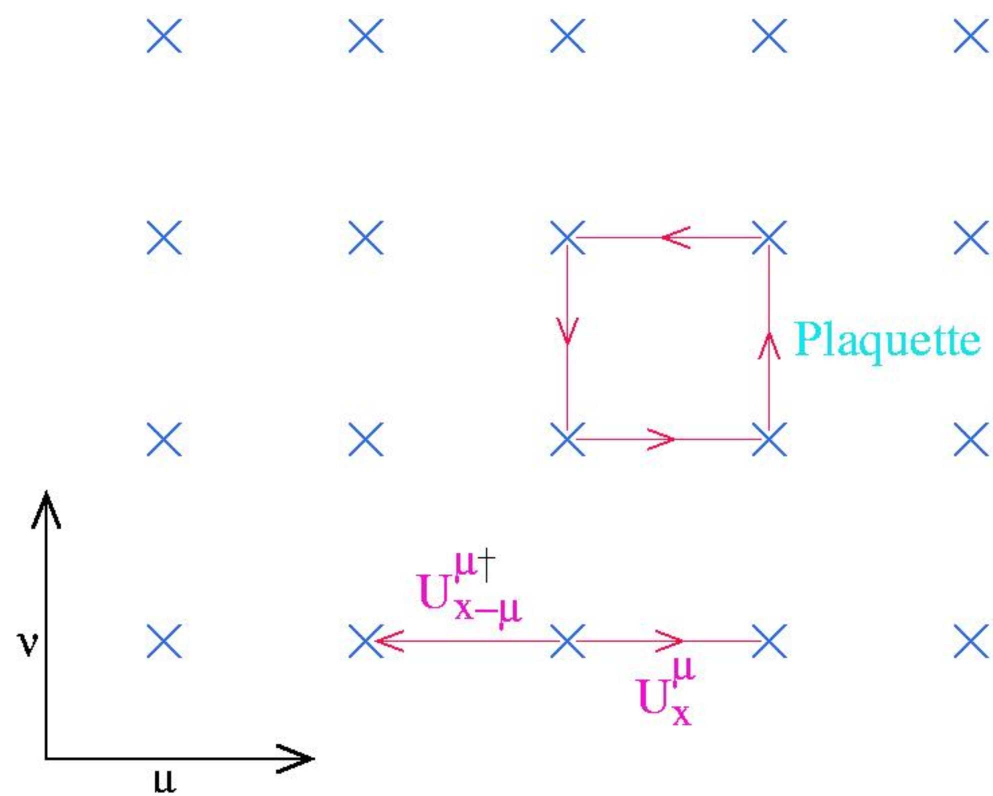

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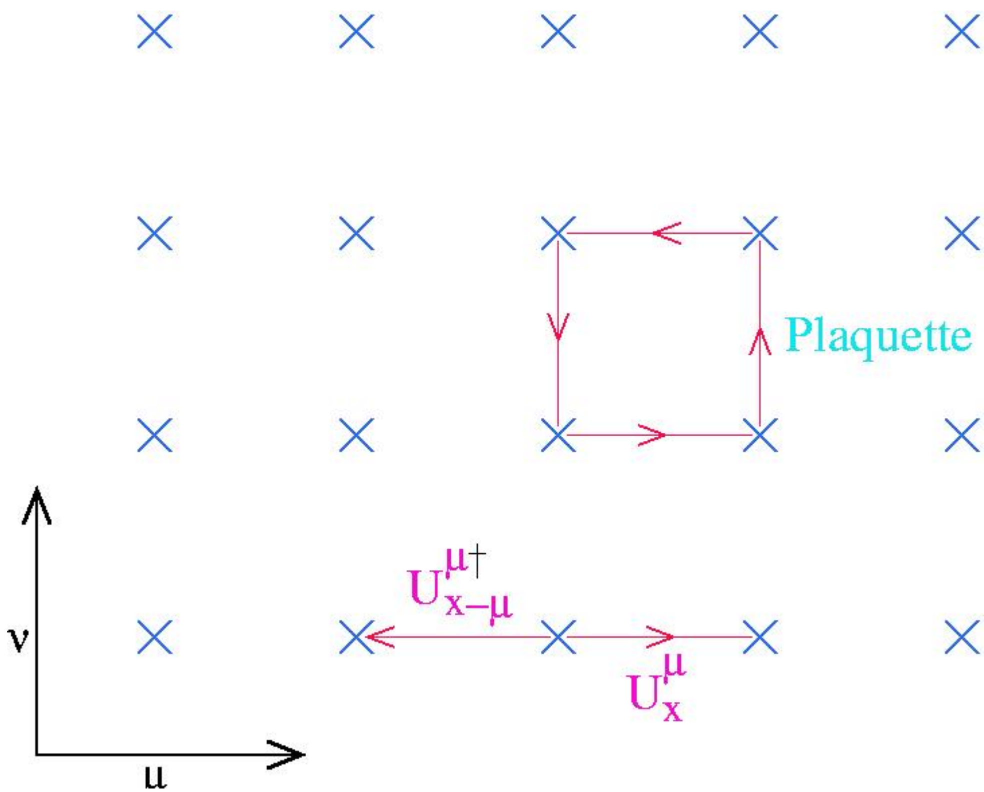
- Gauge invariance : Actions from Closed Wilson loops, e.g., plaquette.



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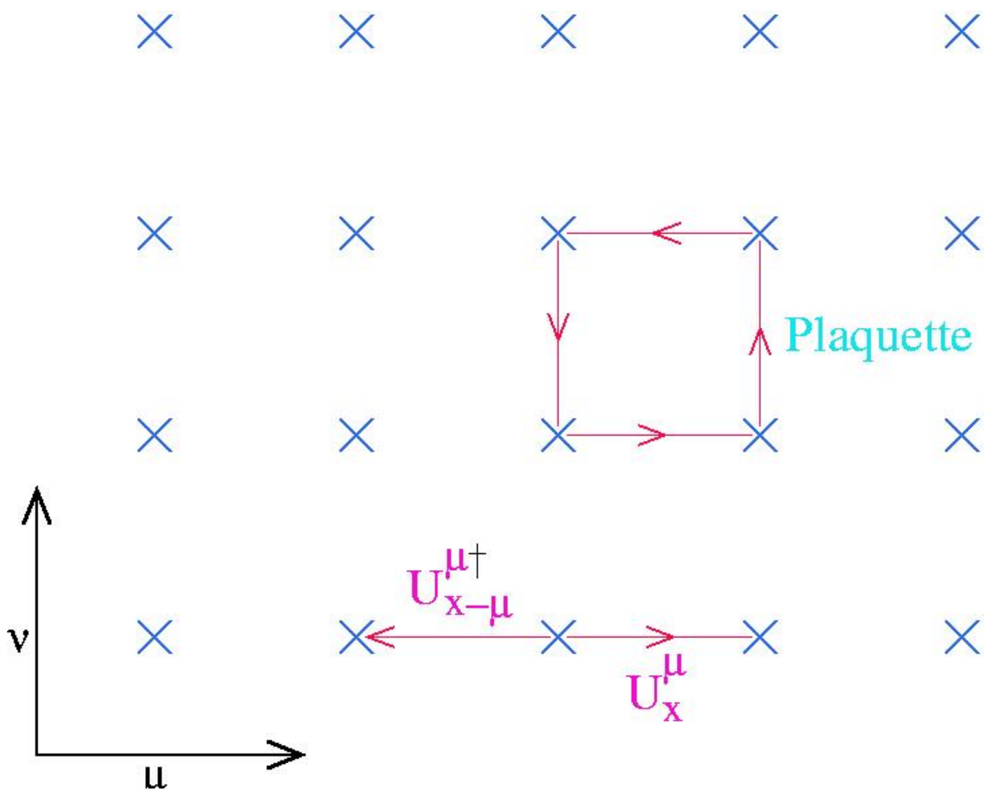
- Fermion Actions : Staggered, Wilson, Overlap..



Typically, we need to evaluate

$$\langle \Theta(m_v) \rangle = \frac{\int DU \exp(-S_G)\Theta(m_v) \ \mathrm{Det} \ M(m_s)}{\int DU \exp(-S_G) \ \mathrm{Det} \ M(m_s)} \quad , \tag{1}$$

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Lattice scaffolding must be removed : Continuum limit $a \to 0$.
$\rightsquigarrow$ Computer Simulations, $\langle \Theta \rangle$ is computed by averaging over a set of configurations $\{U_\mu(x)\}$ which occur with probability $\propto \exp(-S_G) \cdot \mathrm{Det}\ M$.

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Complexity of evaluation of Det $M \Longrightarrow$ approximations : Quenched ($m_s = \infty$ limit) and Full (low $m_s = m_u = m_d$) $\rightsquigarrow$ Computer time $\uparrow$ and Precision $\downarrow$.

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- Large-scale– such as QCD spectrum or thermodynamics for realistic light quark (physical pion) masses. Need large lattices to have reasonable box size in units of m_π^{-1}, i.e., more computational power.

- Most CPU time in full QCD simulations goes in obtaining the quark propagator M^{-1} by using Conjugate Gradient, i.e., in solving $M \cdot X = r$, for a given source vector r.

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- Suitable for both parallelization and vectorization. Both aspects have been exploited efficiently in Lattice QCD computations.

- Lattice QCD experts are actively involved in design and development of new parallel technology in hardware and software.

Current Scenario

- Factors governing choice of machines :
  - Processor – high sustained performance for QCD code, large cache, fast interface to memory/network.
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  - Ease of Programming – Standard Languages (C/C++, Fortran), Efficient compilers and system libraries.
  - Costs – Machine (Hardware/Software) and Operational costs like Power and Cooling.
  - Space Requirement.

- Lattice results have been (will be) obtained with
  - Custom-Design machines, e.g.,
    - CP-PACS(Tsukuba)
    - QCDSP/QCDOC (Columbia),
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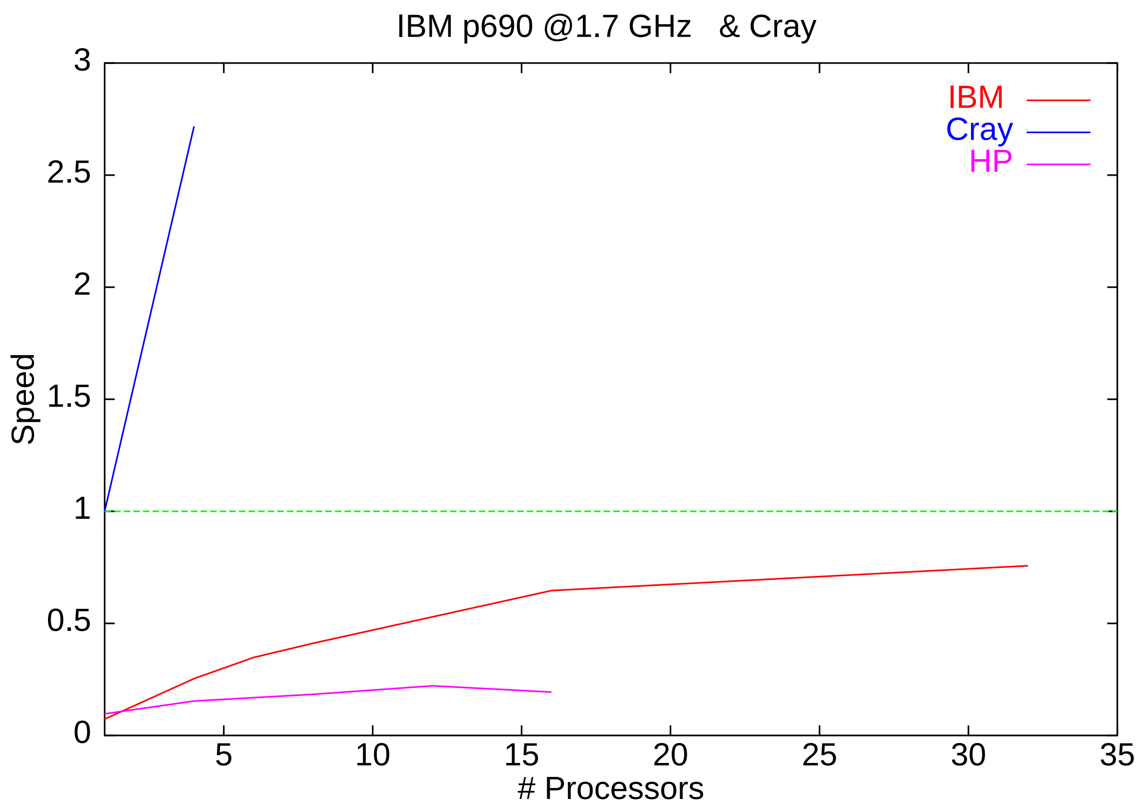
  - PC Clusters, e.g., Wuppertal, JLAB, Fermilab

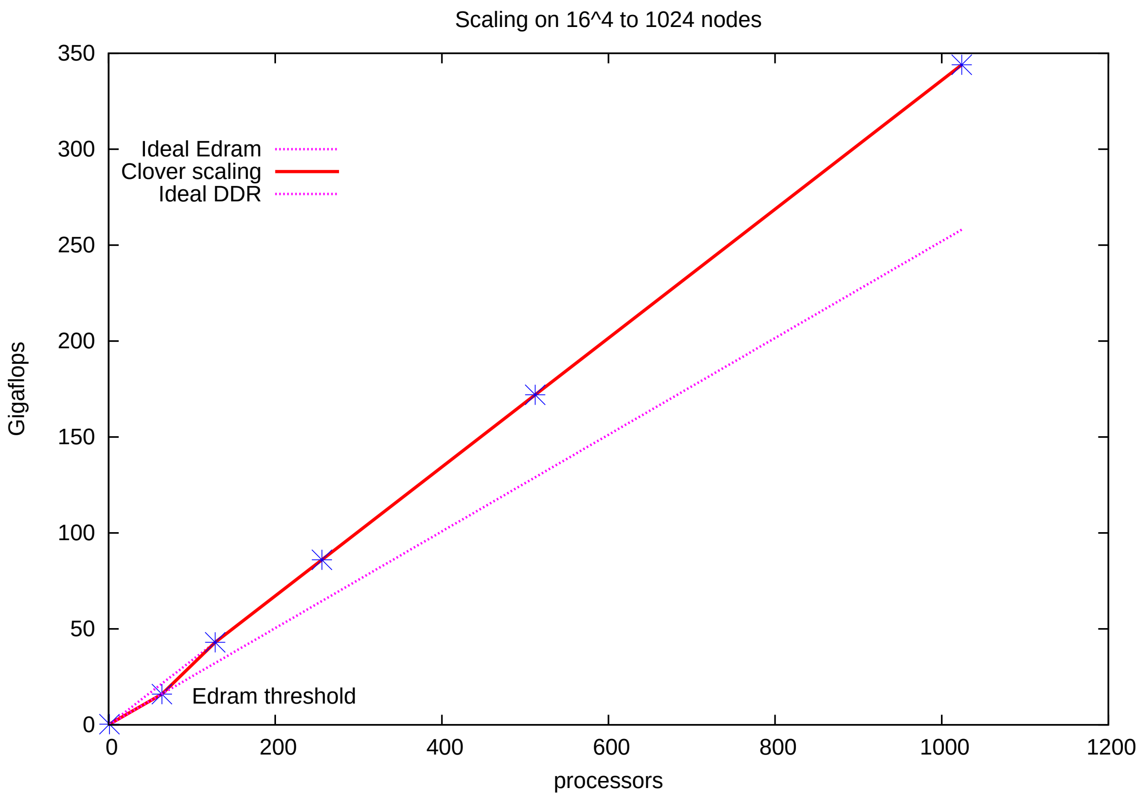
Our Main Workhorse

CRAY X1 of I L G T I , T I F R, Mumbai

Strong Scaling : Problem size fixed
Hybrid Monte Carlo – Full QCD

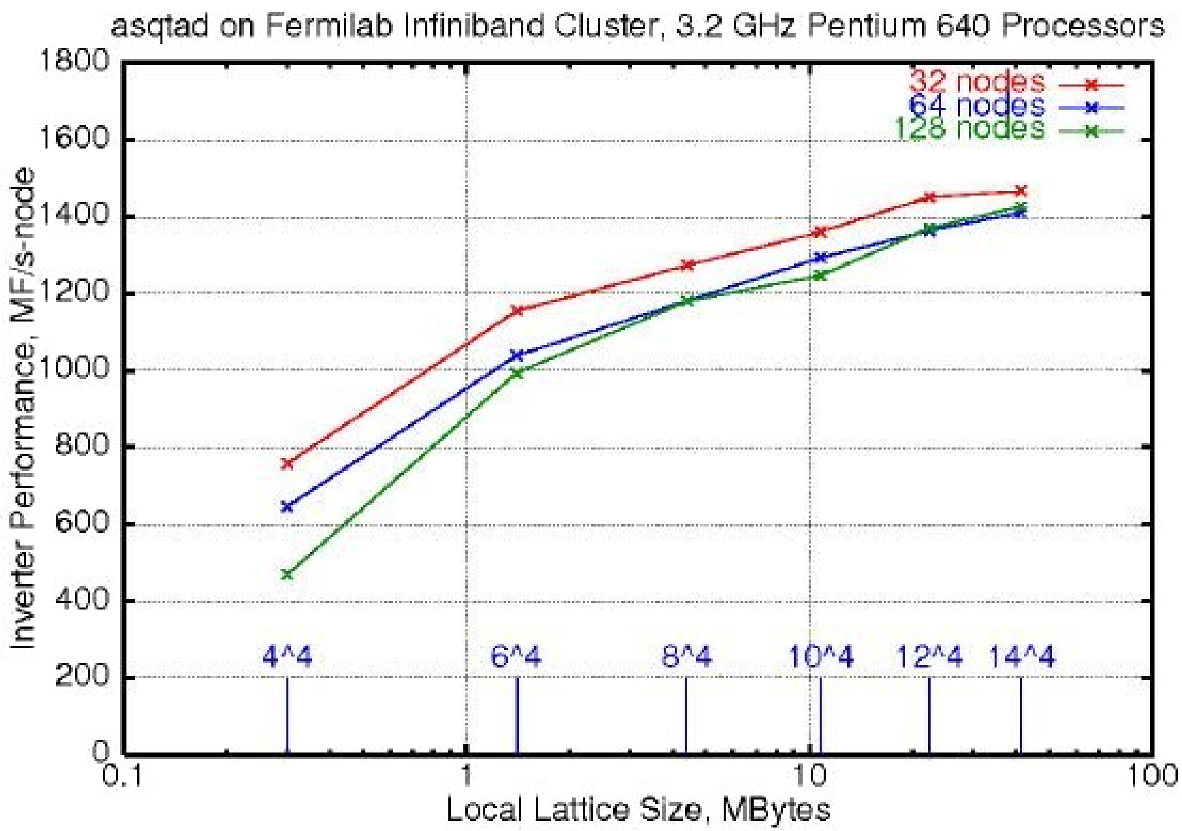


Strong Scaling : Problem size fixed
QCDOC - Clover Conjugate Gradient



P. A. Boyle et al., NP B(PS) 140 (2005) 169.

Weak Scaling : Local volume fixed
Staggered Fermion Conjugate Gradient

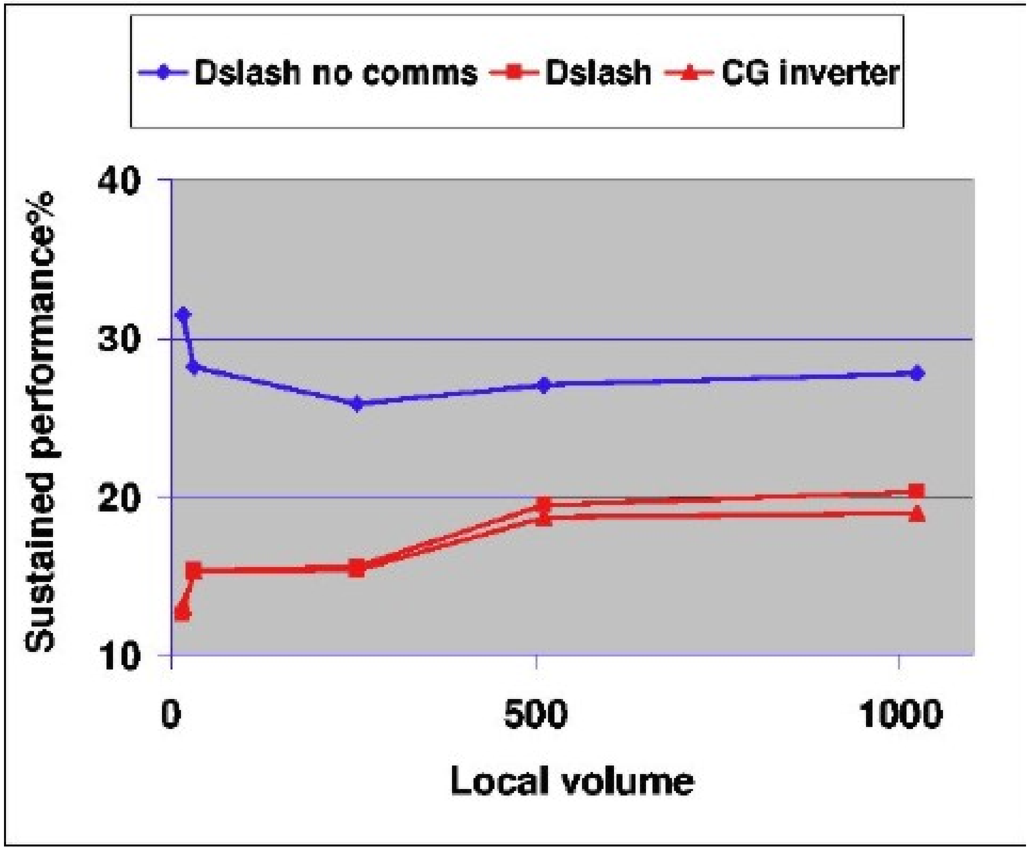


Weak scaling curves on new cluster

From D. J. Holmgren.

Scaling : BlueGene/L

Wilson Fermion Conjugate Gradient



G. Bhanot, D. Chen, A. Gara and P. Vranas, NP B(PS) 140 (2005) 823.

Future Prospects

- PC Clusters will continue to play a major role.
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- So will commercial supercomputers, e.g.,
  - IBM BlueGene/P, successor to BlueGene/L
  - CRAY Black Widow successor to X1, Strider 3
  - Fujitsu has plans for 3 PFlops by 2010

- Custom-Design machines ?

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All three avenues, i.e., custom-designed machines, commercial supercomputers and PC clusters, likely to continue playing important role in future.