Computing Challenges in Lattice QCD

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Introduction: Why & How
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Summary
Introduction : Why Lattice QCD

• QCD — A (Gauge) Theory of interactions of quarks-gluons.

• Similar to structure in theory of electrons & photons (QED).
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- Unlike QED, the coupling is usually very large and its eight “photons” interact amongst themselves.
Introduction: Why Lattice QCD

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- 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 → 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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♥ Strong Coupling Constant $\alpha_s$ computed from underlying theory.

♥ Heavy Meson properties predicted: $m_{B_c}$, $f_B$, $f_D$.
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- New States at High Density & Temperatures, expected on basis of models.  
  (Figure from H. Stöcker)
• The Transition Temperature $T_c$ ($\sim 170$ MeV) and Equation of State (EOS) have been predicted by lattice QCD.
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- Other quantities for Heavy Ion Physics: the Wróblewski Parameter $\lambda_s$, $J/\psi$-dissolution, dileptons, speed of sound, transport coefficients... etc.
• $\lambda_s$ — Measure of Production of strange quark-antiquark pairs; Expts agree with estimates from the new state Quark-Gluon Plasma.
  — Lattice QCD suggests that strangeness carried by quark-like objects
  — Robust correlations like BQ are better observables.
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— Robust correlations like BQ are better observables.

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
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  • Gauge transform $V_x \in SU(3)$  
    $\Rightarrow \psi'(x) = V_x \psi(x)$,  
    $U'_\mu(x) = V_x U_\mu(x)V^{-1}_{x+\hat{\mu}}$.

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• Fermion Actions: Staggered, Wilson, Overlap..
Typically, we need to evaluate

\[
\langle \Theta(m_v) \rangle = \frac{\int DU \exp(-S_G) \Theta(m_v) \ Det \ M(m_s)}{\int DU \exp(-S_G) \ Det \ M(m_s)} ,
\]

where \( M \) is the Dirac matrix in \( x, \) colour, spin, flavour space for fermions of mass \( m_s, \) \( S_G \) is the gluonic action, and the observable \( \Theta \) may contain fermion propagators of mass \( m_v. \)
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Lattice scaffolding must be removed: Continuum limit \( a \to 0 \).

\( \leadsto \) Computer Simulations, \( \langle \Theta \rangle \) is computed by averaging over a set of configurations \( \{U_\mu(x)\} \) which occur with probability \( \propto \exp(-S_G) \cdot \det M \).
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Monte Carlo integrations of a few million dimensional integrals.
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Monte Carlo integrations of a few million dimensional integrals.

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

• Variety of interesting problems and corresponding challenges. Broadly two classes — A) Algorithmic and B) Large-scale or precision dominated.
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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 $m_{\pi}^{-1}$, i.e., more computational power.
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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.
  - Memory & Network – Sufficient external memory with low latency and high bandwidth access. Network topology important.
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  - Processor – high sustained performance for QCD code, large cache, fast interface to memory/network.
  - Memory & Network – Sufficient external memory with low latency and high bandwidth access. Network topology important.
  - 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),
  * Ape/Apemille/Apenext(Italy/Europe)
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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

![Graph showing speed vs. number of processors for IBM p690 @ 1.7 GHz & Cray]

- IBM
- Cray
- HP
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

From D. J. Holmgren.
Scaling: BlueGene/L
Wilson Fermion Conjugate Gradient

Future Prospects

• PC Clusters will continue to play a major role.
  – Jlab and Fermilab – 1000 node Infiniband
  – PACS-CP (Tsukuba) – 2560 node Xeon
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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.