

# Quantum Chromodynamics

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# Scientific Objectives

- The goals of high energy and nuclear physicists are to identify the fundamental building blocks of matter, and to determine the interactions among them.
- The Standard Model is a major step towards these goals
  - Unified theory of weak and electromagnetic interactions
  - Quantum Chromodynamics (QCD), the theory of the strong interactions
- The study of QCD requires large scale numerical simulations within the framework of lattice gauge theory

# Relationship to Experimental Programs

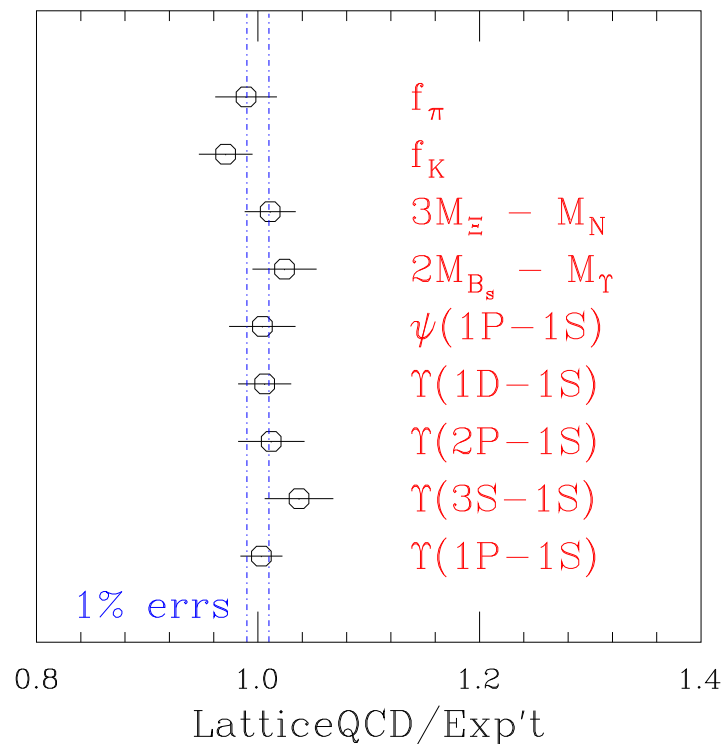
- Major goals of the experimental programs in high energy and nuclear physics are to:
  - Verify the Standard Model, or discover its limits
  - Understand the properties of strongly interacting matter under extreme conditions
  - Determine the masses and internal structure of strongly interacting particles
- Lattice QCD calculations are essential to research in all of these areas

# Characteristics of the Simulations

- Uniform, four–dimensional grids
- Regular, predictable communications
- Low memory requirements
- Modest I/O requirements
- Challenges
  - Extrapolation to the continuum limit
  - Control of finite size effects
  - Extrapolation in the light quark mass

# Current Status of Simulations

- The U.S. Lattice QCD Community presently sustains 0.5–1.0 Tflop/s
- These resources have allowed the determination of several key quantities to an accuracy of a few percent



# Example of a Near Term Objective

- An accurate determination of the decay constants of B and D mesons, coupled with results from ongoing experiments, would provide an important test of the Standard Model
- Current resources enable a determination to an accuracy of 5%
- An accuracy of 1% is required to have a major impact on our knowledge of the Standard Model

# Resources for 1% Calculation of Decay Constants

$m_l$	$a(\text{fm})$	Lattice	PF-Hrs	Mem(GB)
$0.20 m_s$	0.09	$28^3 \times 96$	1	2.4
$0.10 m_s$	0.09	$32^3 \times 96$	7	3.4
$0.05 m_s$	0.09	$36^3 \times 96$	54	5.0
$0.20 m_s$	0.045	$56^3 \times 192$	100	37.7
$0.10 m_s$	0.045	$64^3 \times 192$	900	54.2
$0.05 m_s$	0.045	$72^3 \times 192$	6900	80.0

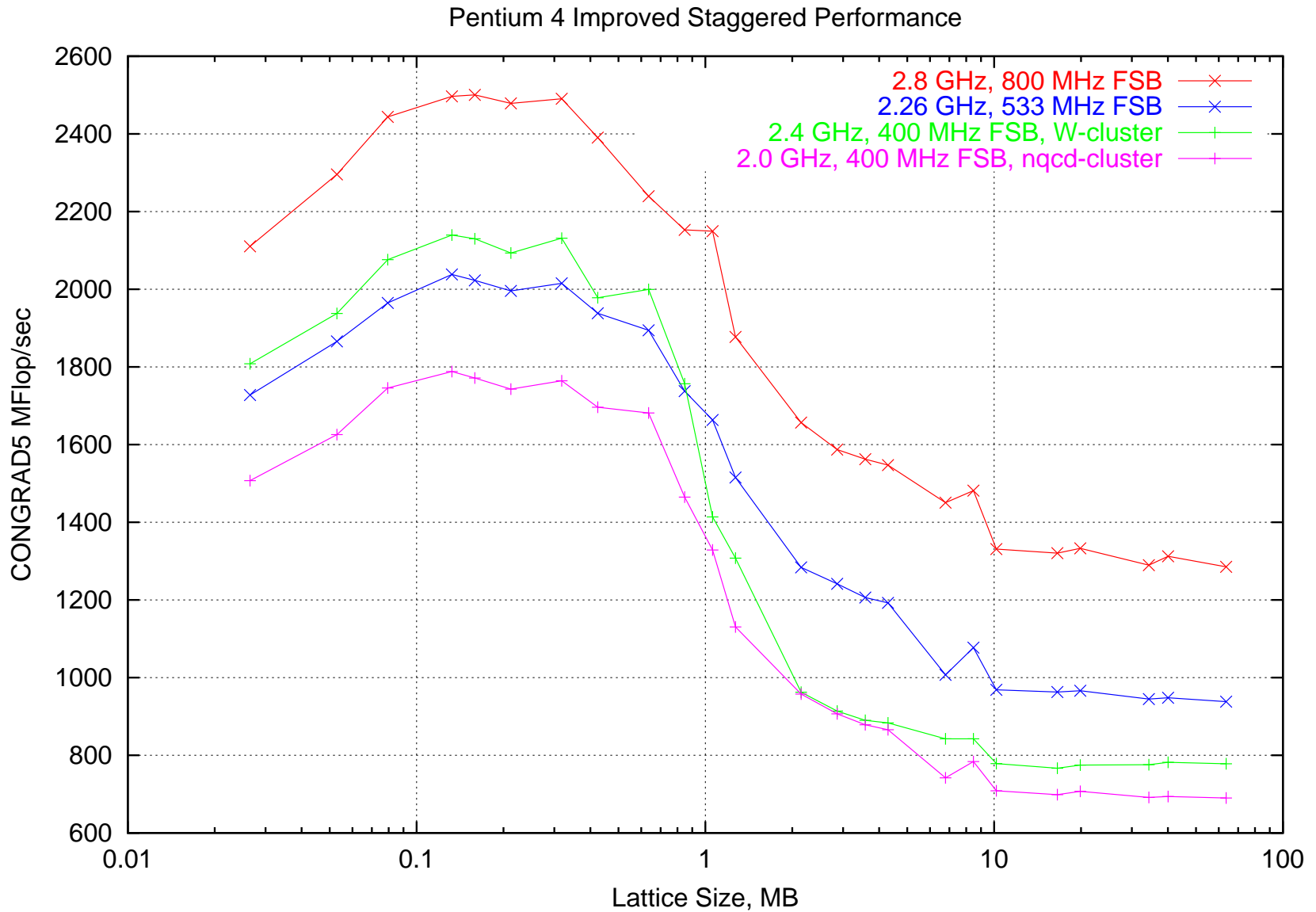
# Hardware Requirements

- The U.S. Lattice QCD Community presently sustains 0.5–1.0 Tflop/s
- It will need to sustain 50 – 100 Tflop/s within the next few years in order to:
  - Support the experimental programs in high energy and nuclear physics in a timely fashion
  - Keep pace with theoretical physicists in Europe and Japan
- Will need to sustain Petaflop/s by the end of the decade

# Processor Challenge

- The basic mathematical operation is the multiplication of a three–component vector by a  $3 \times 3$  complex matrix
  - 1.45 bytes of input data required for each floating point operation
  - 0.36 bytes of output data produced for each floating point operation
  - In current commercial processors, the problem must fit entirely into cache in order for the data movement to keep up with floating point calculations

# Impact of Bus Bandwidth



# Inter-Processor Communication Challenge

- It is necessary to overlap communications and computation to obtain strong performance
  - Assign  $L^4$  lattice points to each processor
  - Because interactions are short range, one needs information from only a few neighboring processors
  - Required inter-processor bandwidth (in Megabytes/s) is approximately  $0.364MF/L$ , where MF is the sustained floating point performance in Megaflop/s
- With current commercial processors and networks, the latency is usually too high to keep the problem in cache
- Balance among memory bandwidth and latency, cache size, floating point performance, and inter-processor bandwidth and latency is critical.

# Hardware Architecture

- Lattice QCD simulations are very well suited to MPP architectures
- Simplifying features of the calculations make custom designed machines very attractive
  - QCDOC (Columbia/IBM/SciDAC)
  - ApeNEXT (Italy)
  - Optimized clusters (FNAL/JLab/SciDAC)
- Price–performance of \$1M per sustained Tflop/s appears to be in reach

# Software

- Open source codes exist for clusters and commercial machines, and for special purpose computers.
- A major effort is in progress under the DOE SciDAC Program to develop a community code that will run with high efficiency on special purpose computers, clusters and commercial machines
- Continued support at least at the level of the SciDAC project will be necessary to enable effective use of petascale computers.
- Participation of software engineers in code development and tuning would be a major asset
- Robust performance diagnostic tools are critical