Lattice QCD at Fermilab and Argonne

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USQCD Collaboration

Organizes hardware and software infrastructure for lattice gauge theory for the DoE.

Majority of US lattice gauge theorists, ~145 members.

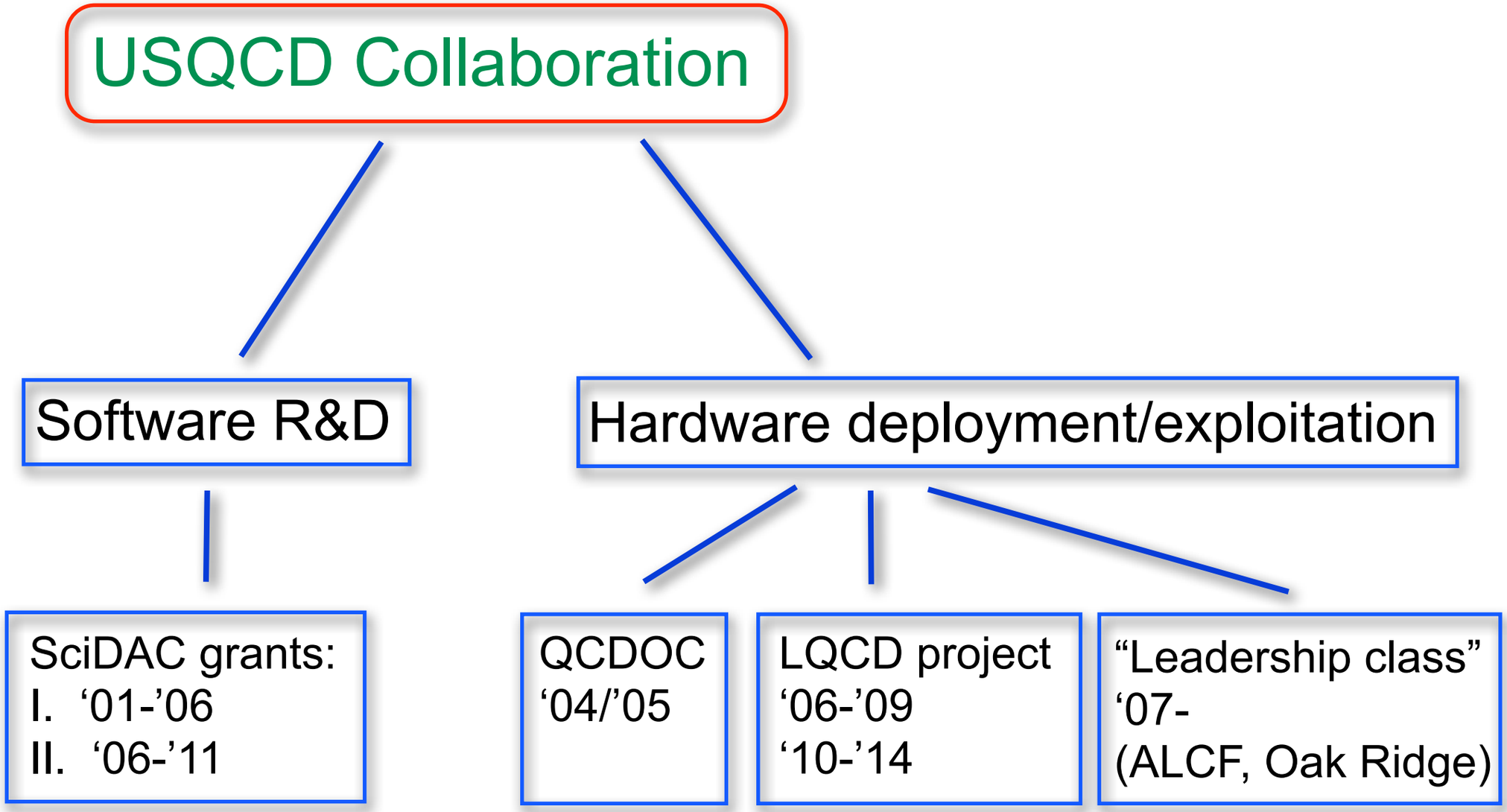
Executive committee:
Paul Mackenzie (chair), Rich Brower, Norman Christ, Mike Creutz, John Negele, Claudio Rebbi, David Richards, Steve Sharpe, Bob Sugar

LQCD Project:
Designs and deploys cluster hardware for USQCD.

Scientific program committee:
Frithjof Karsch (chair)

Software Committee:
Richard Brower (chair)

The USQCD collaboration is funded through SciDAC, through the LQCD project, and through base HEP and NP funds at BNL, Fermilab, and JLab.



USQCD has grants for
- R&D for software development through the SciDAC program.
- Hardware deployment from several sources, including the current LQCD project.

Anatomy of a typical lattice calculation

Near-TB file sizes

Generate gauge configurations on a leadership facility or supercomputer center.
Tens of millions of BG/P core-hours.

Transfer to labs for analysis on clusters.
Comparable CPU requirements.

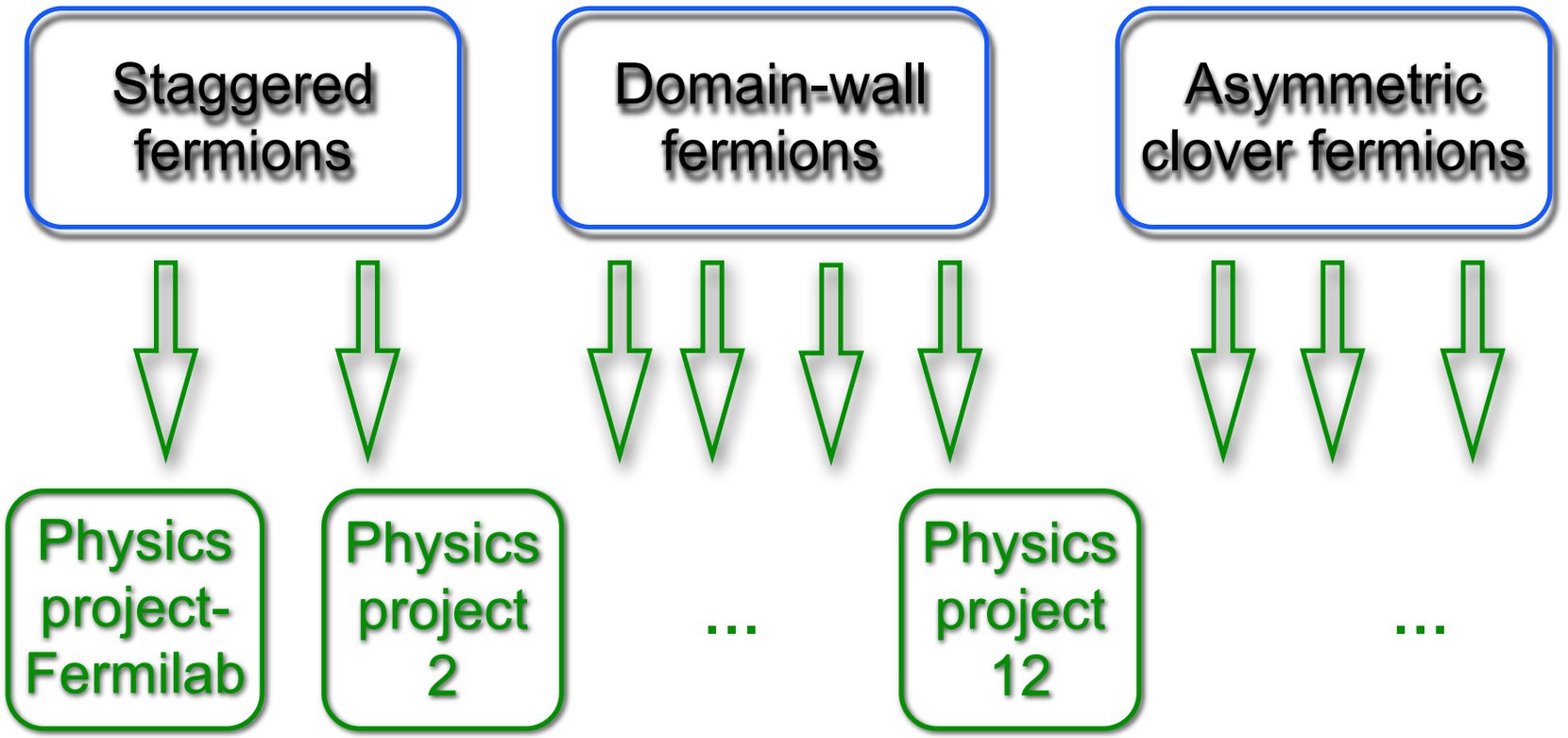
A single highly optimized program, very long single tasks, moderate I/O and data storage.

Large, heterogeneous analysis code base, 10,000s of small, highly parallel tasks, heavy I/O and data storage.

Two comparably sized jobs with quite different hardware requirements.

US lattice gauge theory sociology

Currently three main streams of QCD gauge configurations are being generated by USQCD:



Shared among a couple of dozen groups, in both HEP and NP.

Physics projects are done on these configurations by smaller groups of 5-15 members within USQCD.

Around 90 of the 145 members of USQCD have submitted jobs to USQCD hardware.

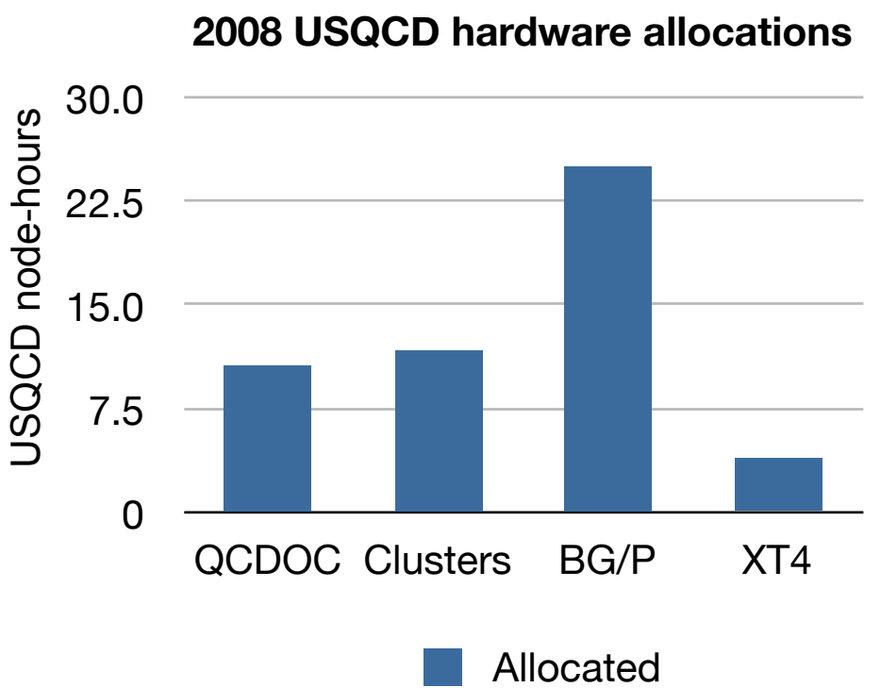
Roles of Fermilab and Argonne

- The Fermilab Computing Division
  - Designs and operates the large clusters for USQCD computing.
  - Works with users to optimize and run their codes.
  - Participates in the work of the USQCD software committee.
- The Argonne Leadership Computing Facility
  - Good for largest computing tasks: ensemble generation.
  - James Osborn, an ALCF “catalyst”, is a lattice gauge theorist.
    - Worked with USQCD to get code ready for the BG/P.
    - Previously has worked with the USQCD software committee.

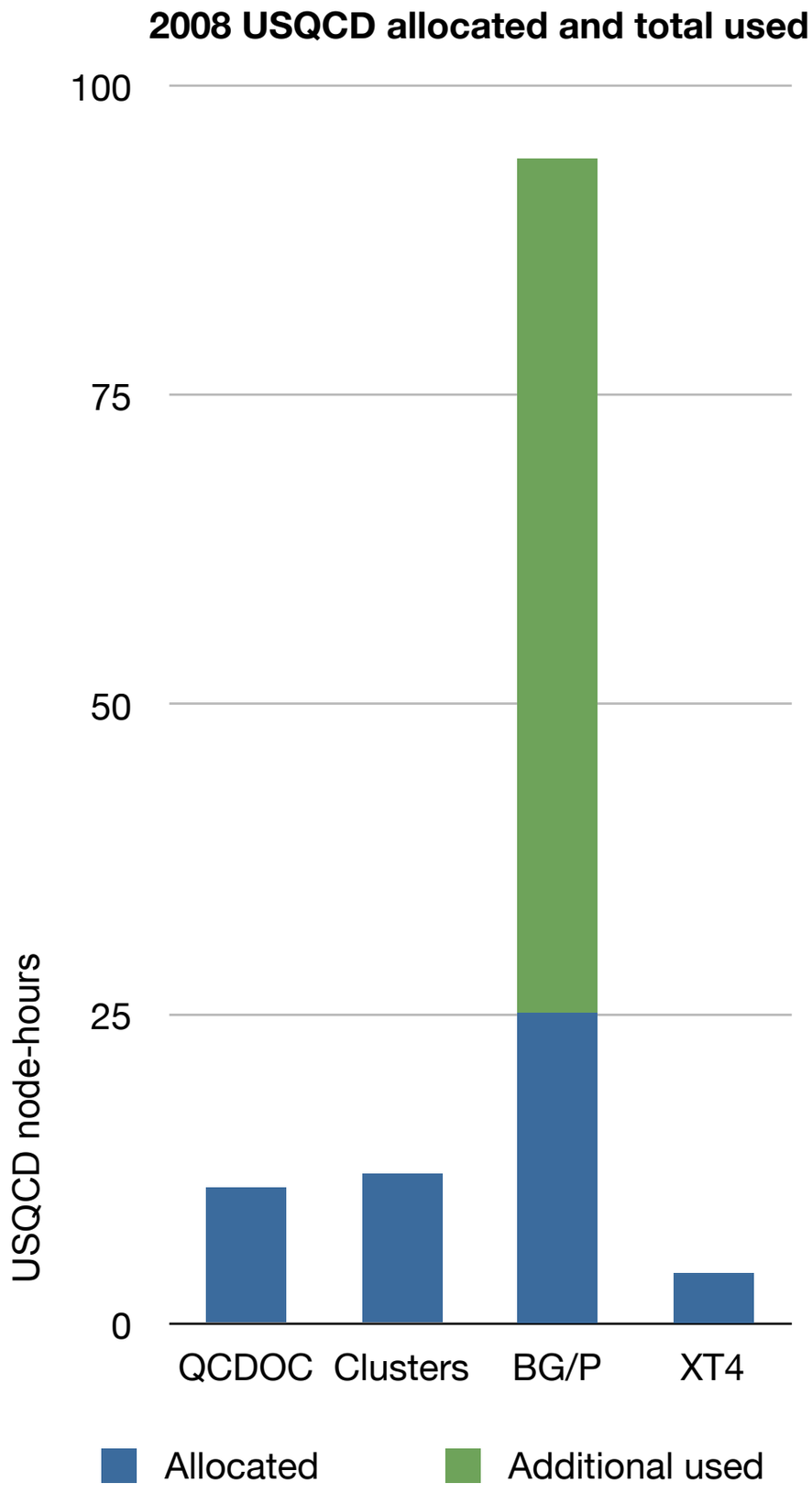
2008 USQCD hardware resources

In 2008, a three year program of gauge configuration generation was planned on the BG/P and the XT4.

USQCD worked with James Osborn and other BG/P experts to ready code for BG/P.



2008 USQCD hardware resources



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USQCD worked with James Osborn and other BG/P experts to ready code for BG/P.

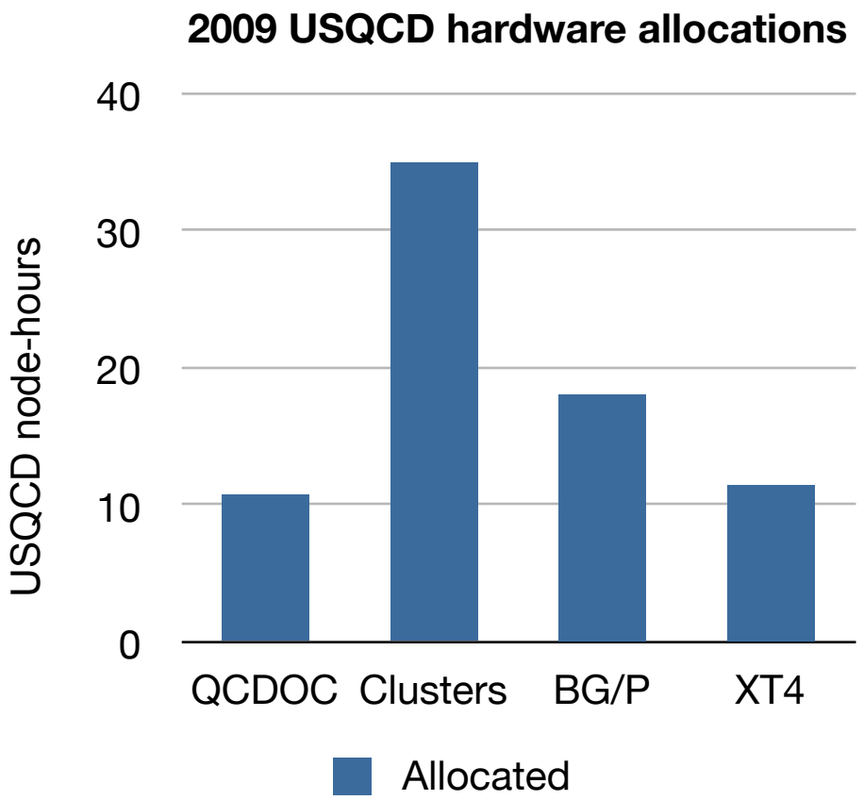
This process has worked well.

USQCD was one of two or three ALCF projects ready from the beginning, and the only one with a three-year program mapped out.

The three-year program of configuration generation was accomplished in nine months on the BG/P.

2009 USQCD hardware resources

In 2009, now working to port a subset of analysis codes to BG/P.



Fermilab/MILC CMK on the lattice program

	a (fm)	ml/ms	V	V		M 6n node-hours
Fine	0.09					
		0.3	28^3*96	2,107,392		0.72
		0.2	28^3*96	2,107,392		0.72
		0.15	32^3*96	3,145,728		1.08
		0.1	40^3*96	6,144,000		2.11
		0.05	64^3*96	25,165,824		8.64
Superfine	0.06					
		0.3	48^3*144	15,925,248		5.48
		0.2	48^3*144	15,925,248		5.48
		0.14	56^3*144	25,288,704		8.7
		0.1	64^3*144	37,748,736		12.99
Anchor point	0.045					
		0.2	64^3*192	50,331,648		5
					Total	50.92

In 2009, now working to port a subset of analysis codes to BG/P.

Resource needs/ensemble for the Fermilab/MILC heavy-light project, , including leptonic decays, B->D, B->pi, D->{K,pi}, BBbar and DDbar mixing.*

Summary

- Fermilab and Argonne computing play complementary, essential roles in the USQCD computing program.
- The cooperation between the labs is working well.
- We look forward to continued close cooperation.

Extra slides

Role of Fermilab

Fermilab theorists work with the Computing Division to develop and operate new hardware for the national lattice QCD program, such as the “Kaon” cluster at Fermilab.

The Fermilab Computing Division supplies space, electricity, communications infrastructure, and especially top-notch personnel to make this happen.

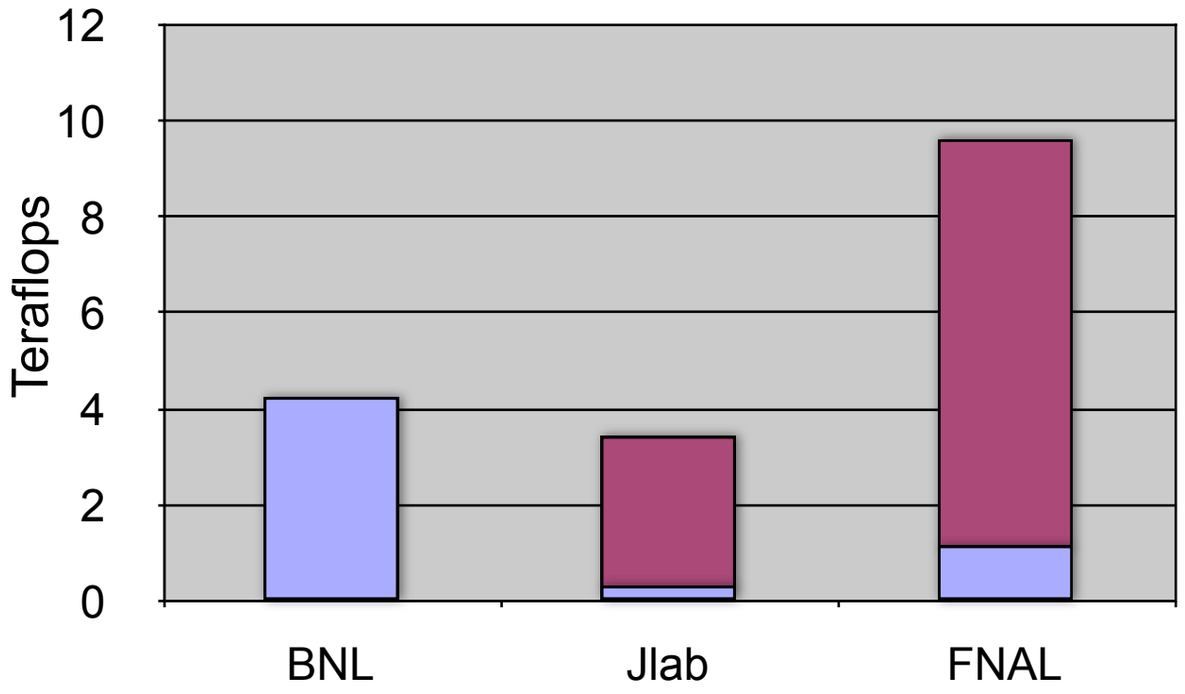
“Kaon” cluster, installed at Fermilab in 2006.

17.5 TF at the end of the 08/09 installation.

Final installation of the 2006-2009 project.
Delivered teraflops using standard benchmarks of “asqtad” and “domain-wall” lattice codes, used in our reporting to the DOE. (Multiply by 5 or 6 to compare peak teraflops used in Top 500 lists, etc.)

Maroon: constructed and operated through LQCD project,

Blue: operated through LQCD project, constructed with other DOE funding.



The computational challenge of lattice QCD

Lattice	Quark			Gauge	ensembles		Analysis propagators, correlators		
spacing *a (fm)*	mass *ml/ms*	Volume (sites)	Configu rations	Core-hours (M)	TB/ ensemble	Files/ ensemble	Core-hours (M)	TB/ ensemble	Files/ ensemble
0.06	0.1	64^3*144	1000	32.36	10.9	1,000	32	696	155,000
	0.15	56^3*144	1000	14.04	7.3	1,000	14	466	“
	0.2	48^3*144	1000	6.74	4.6	1,000	7	294	“
	0.4	48^3*144	1000	3.66	4.6	1,000	4	294	“
0.09	0.1	40^3*96	1000	3.43	1.8	1,000	3	113	155,000
	0.15	28^3*96	1000	0.81	0.6	1,000	0.8	39	“
	0.2	28^3*96	1000	0.62	0.6	1,000	0.6	39	“
	0.4	28^3*96	1000	0.36	0.6	1,000	0.4	39	“
0.12	0.1	24^3*64	1000	0.38	0.3	1,000	0.4	16	155,000
	0.15	20^3*64	1000	0.15	0.1	1,000	0.2	9	“
	0.2	20^3*64	1000	0.12	0.1	1,000	0.1	9	“
	0.4	20^3*64	1000	0.07	0.1	1,000	0.1	9	“

Example gauge ensemble library.

CPU times normalized in BG/P core-hours.

Operationally, lattice QCD computations consist of

1) Sampling a representative set of gauge configurations with Monte Carlo methods,

   E.g., the Metropolis method, the hybrid Monte Carlo algorithm, ...
   Consists of one long Markov chain.

2) Calculating the propagation of quarks through the gauge configurations,

   Solve the Dirac equation on each configuration with relaxation methods, e.g., biconjugate gradient algorithm, etc

3) Constructing hadron correlation functions from the quark propagators.

IV. The USQCD Collaboration

Because of the great potential for lattice calculations to advance the goals of the HEP and NP experimental programs, DoE asked the US lattice gauge theory community to organize itself to create software and hardware infrastructure for lattice calculations.

The USQCD Collaboration was the result.

Consists of the great majority of US lattice gauge theorists, ~145 members.
Purpose: develop hardware and software infrastructure for the US lattice community. (Physics projects are done by individual groups within USQCD.)

USQCD Collaboration

SciDAC lattice QCD computing R&D

Executive committee:
Paul Mackenzie (chair), Rich Brower, Norman Christ, Mike Creutz, John Negele, Claudio Rebbi, David Richards, Steve Sharpe, Bob Sugar

Software Committee:
Richard Brower (chair), Boston University, Carleton DeTar, University of Utah, Robert Edwards, JLab
Rob Fowler, UNC, Donald Holmgren, Fermilab, Robert Mawhinney, Columbia University, Pavlos Vranas, Lawrence Livermore Lab, Chip Watson, JLab

The Executive Committee outlined software tasks and a five-year schedule in the SciDAC II proposal.

The goals and schedule evolve year by year as the program has progressed in response to grass-roots feedback.

The Executive Committee believes that this process is working very well and is producing highly optimized, mission-critical software.

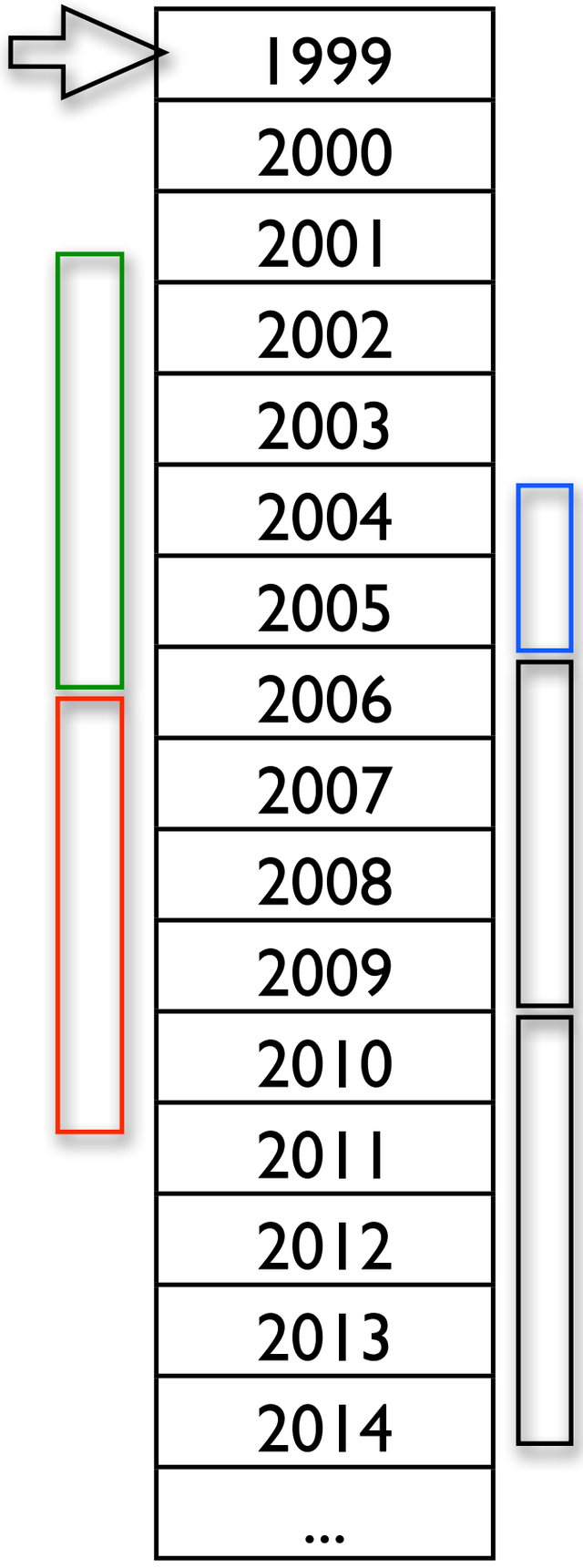
USQCD timeline

USQCD Executive Committee formed.

Software grants

First five-year SciDAC grant for lattice computing R&D.

Second five-year SciDAC grant for R&D (this review).



Hardware grants

Construction of the QCDOC.

First cycle of continuous HEP and NP funding for hardware through LQCD project.

Proposed LQCD II hardware project in 2010-2014.