A Database Management System for LCCI

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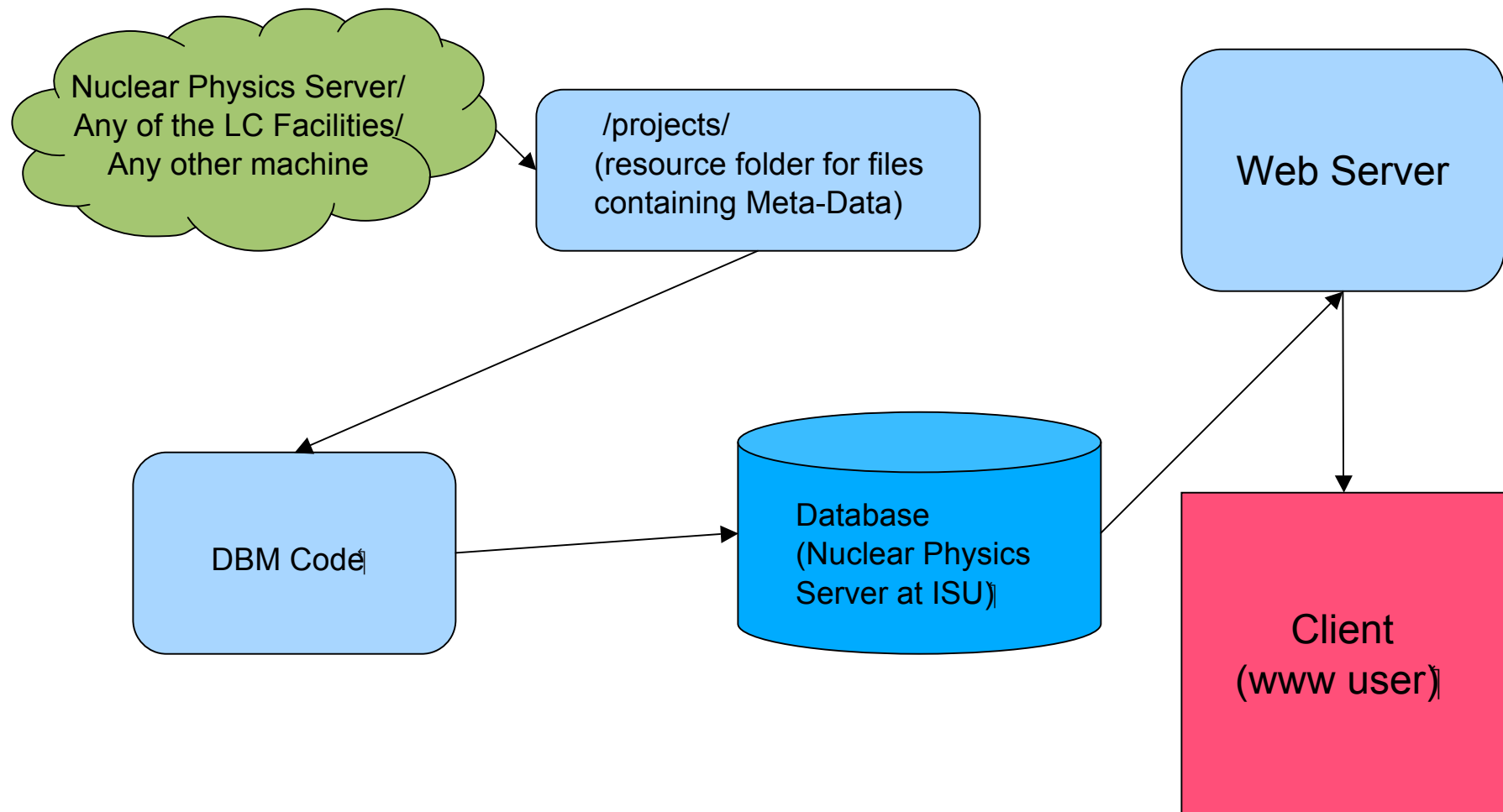### Ames Laboratory

Miles V. Aronnax, Iowa State

Long-term Goal

◆ Efficient tool for retrieving output from ab-initio CI calculations
  – Currently, CI codes run on different platforms, and results are often stored under different usernames and directories

◆ Step towards reproducible research
  – Record not only results, but also how those results are obtained

Current Prototype

◆ Record meta-data of every run in database
  - Data: results from LCCI ab-initio codes, typically stored on platforms where runs are performed (physical observables, OBDMEs, wavefunctions)
  - Meta-data: key information about each run, consolidated and formatted in the .info file

◆ A curious user can access this database over the web and find out whether the runs of his interest are performed, if yes,
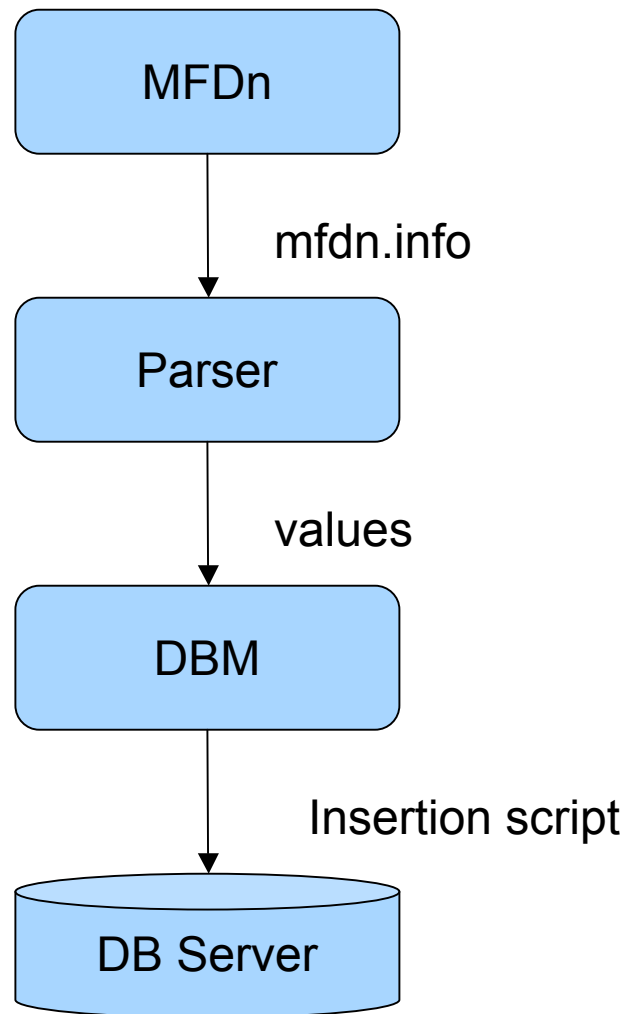
◆ .. where the **results are located.**

Current Prototype

Nuclear Physics Server/
Any of the LC Facilities/
Any other machine

/projects/
(resource folder for files
containing Meta-Data)

Web Server

DBM Code

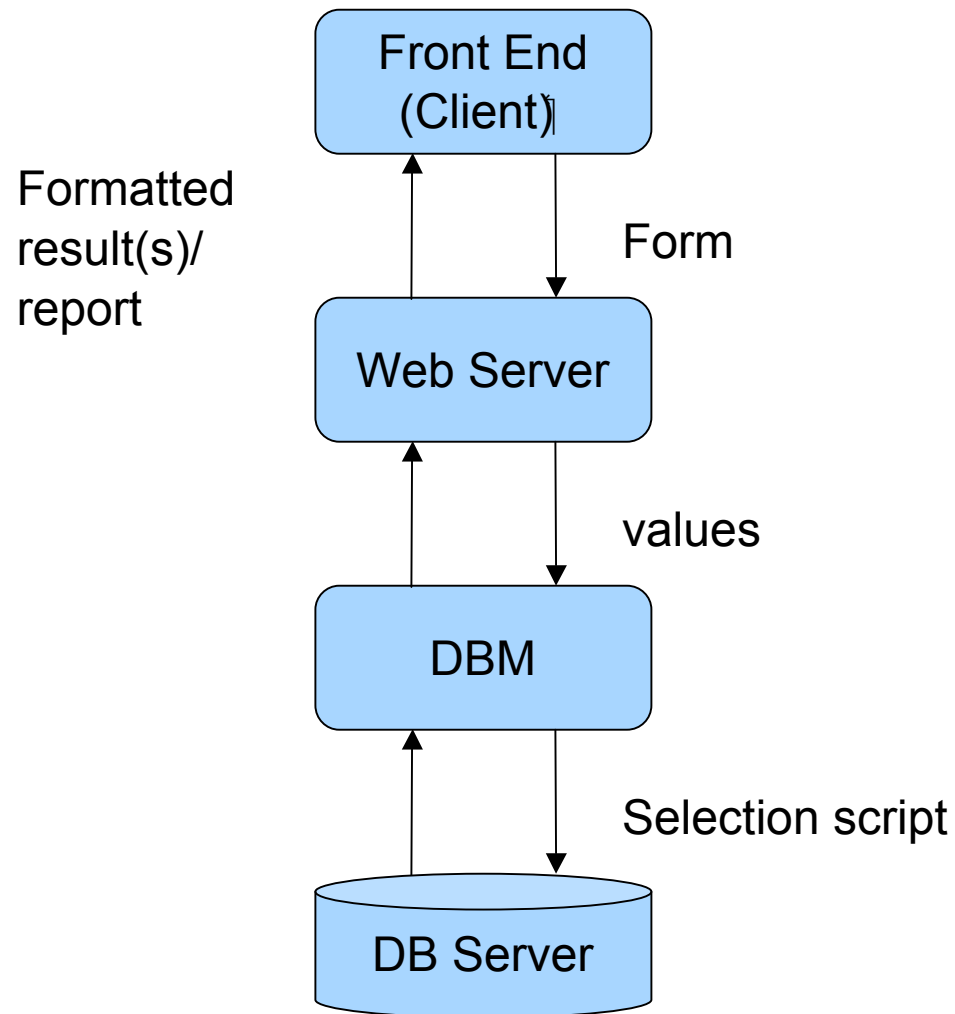Database
(Nuclear Physics
Server at ISU)

Client
(www user)

System Components

◆ **DB Manager:** parses the mfdn.info file and inserts the run record to database; serves as the backend for web-based retrieve functions.

◆ **Web based front end:** searches and lists the existing run, and allows the update on file paths.

◆ **DB Server:** stores all the related metadata for each run of MFDn.

Workflow (Insert)

MFDn

mfdn.info

Parser

values

DBM

Insertion script

DB Server

Workflow (Search)

Front End (Client)

Web Server

DBM

DB Server

Formatted result(s)/ report

Form

values

Selection script

Strengths and Advantages

◆ Running of insert script can be done manually or automatically at nuclear physics server.
  - Levels of control are defined for handling the data.
◆ Insert code bundled in C script and separate query library: allows for future changes in database and platform.
◆ Flexibility of PHP scripting with mysql: Can accommodate any kind of customized query and optimize for efficiency. Expect better user interaction and presentation on user end with php-mysql dynamic server side scripting: scripts can be carefully isolated from schema to a large extent.

Next Steps of Action

◆ Query optimization

◆ User interface improvements

◆ Extend implementation to other LCCI codes
   – Other CI codes (BIGSTICK, NuShellX)

◆ Accommodation as much data as possible in a relational database (RDB)
   – RDB has better organization and accessibility than a DB in plain text format

Usage Demo

◆ **Input record to database**

host: nuclear.physics.iastate.edu

- ◆ /project is the *Drop-box* for new .info files.
- ◆ New .info files are automatically inserted in database
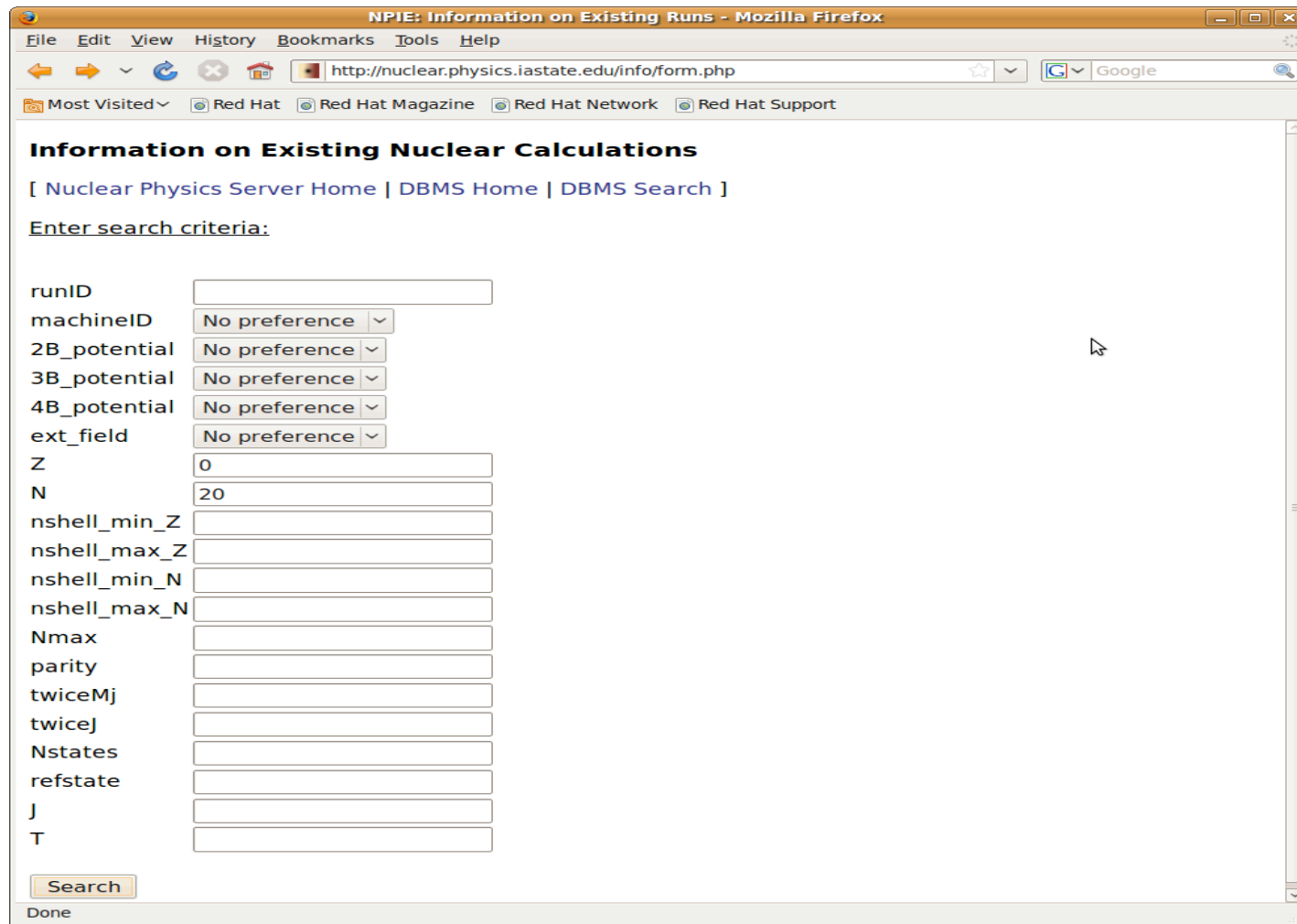- ◆ All processed files are stored in /project/info/

◆ **View the records**

access online:

http://nuclear.physics.iastate.edu/info

- ◆ View all runs – list all records in the database
  - ◆ Each record has a link to the detailed information for the run
- ◆ Search for specific runs
  - ◆ User may specify search criteria to retrieve runs

Search for runs (Z=0 and N=20)

Search Results

NPIE: Information on Existing Runs - Mozilla Firefox

File Edit View History Bookmarks Tools Help

http://nuclear.physics.iastate.edu/info/search.php?var[0]=&var[3]=&var[6]=&var[7]=&var[8]=&var[10]=&var[11]=(

Most Visited ⌄   Red Hat   Red Hat Magazine   Red Hat Network   Red Hat Support

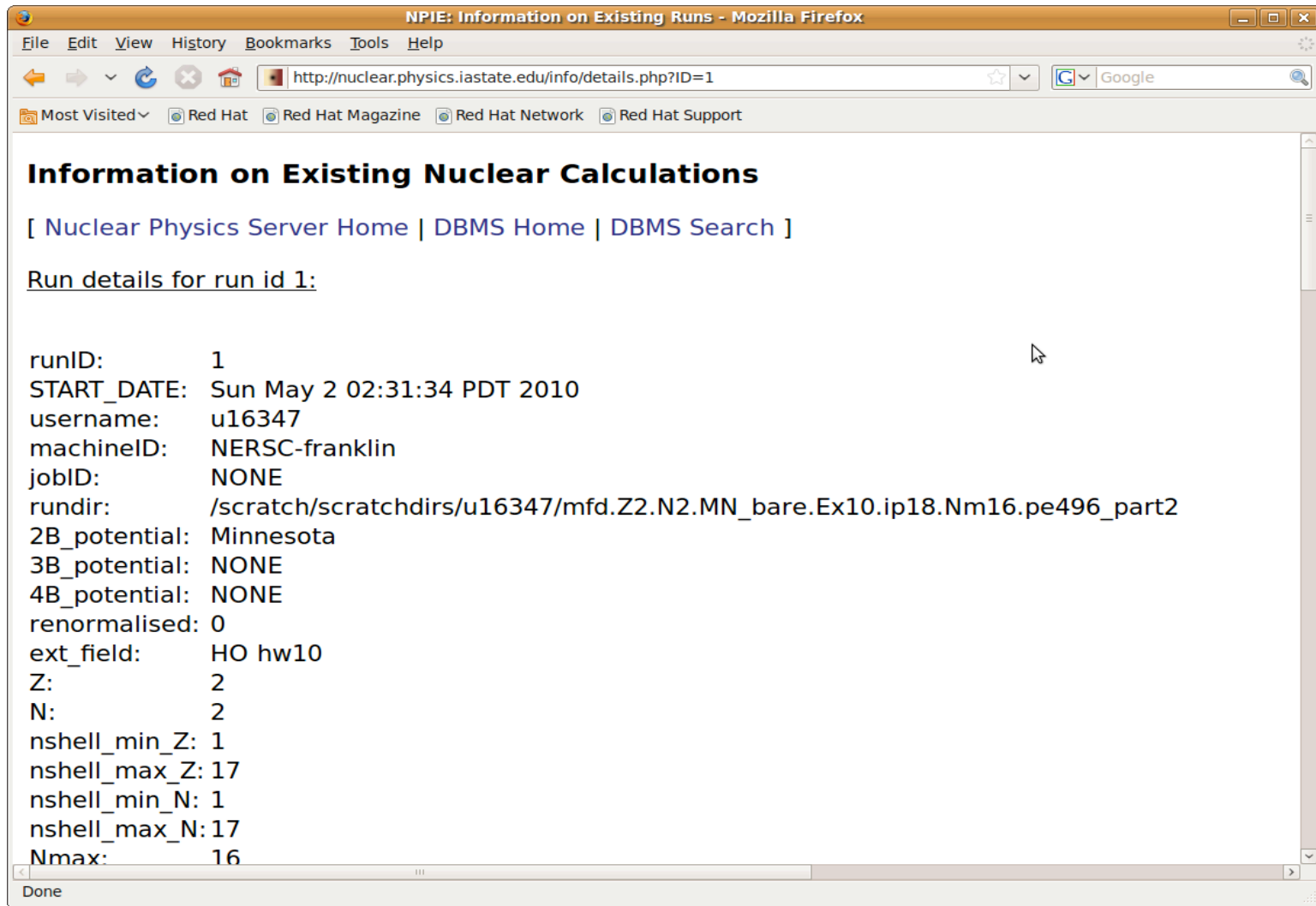## Information on Existing Nuclear Calculations

[Nuclear Physics Server Home | DBMS Home | DBMS Search]

runID	username	Z	N	nshell_min_Z	nshell_max_Z	nshell_min_N	nshell_max_N	Nmax	Nstates	twiceJ	twiceMj	START_DATE
131	u16347	0	20	0	0	1	5	2	5	-1	0	Sat May 29 18:02:25 PDT 2010
132	u16347	0	20	0	0	1	5	2	5	-1	0	Sat May 29 18:03:16 PDT 2010
133	u16347	0	20	0	0	1	5	2	5	-1	0	Sat May 29 19:55:43 PDT 2010
134	u16347	0	20	0	0	1	5	2	5	-1	0	Sat May 29 19:56:30 PDT 2010
135	u16347	0	20	0	0	1	5	2	5	-1	0	Sat May 29 20:02:34 PDT 2010
136	u16347	0	20	0	0	1	5	2	5	-1	0	Sat May 29 20:03:17 PDT 2010
137	u16347	0	20	0	0	1	7	4	5	-1	0	Sat May 29 20:26:29 PDT 2010
138	u16347	0	20	0	0	1	7	4	5	-1	0	Sat May 29 20:42:16 PDT 2010
139	u16347	0	20	0	0	1	7	4	5	-1	0	Sat May 29 20:58:16 PDT 2010
140	u16347	0	20	0	0	1	7	4	5	-1	0	Sat May 29 21:13:55 PDT 2010
141	u16347	0	20	0	0	1	7	4	5	-1	0	Sat May 29 21:29:55 PDT 2010
142	u16347	0	20	0	0	1	7	4	5	-1	0	Sat May 29 21:45:38 PDT 2010
144	u16347	0	20	0	0	1	9	6	3	-1	0	Sun May 30 09:10:16 PDT 2010
145	u16347	0	20	0	0	1	9	6	3	-1	0	Sun May 30 09:37:49 PDT 2010
146	u16347	0	20	0	0	1	9	6	3	-1	0	Sun May 30 10:28:35 PDT 2010
147	u16347	0	20	0	0	1	9	6	3	-1	0	Sun May 30 10:56:41 PDT 2010
148	u16347	0	20	0	0	1	9	6	3	-1	0	Sun May 30 12:12:15 PDT 2010
149	u16347	0	20	0	0	1	9	6	3	-1	0	Sun May 30 12:41:11 PDT 2010
163	u16347	0	20	0	0	1	11	8	3	-1	0	Mon Jun 7 17:03:05 PDT 2010

19 records found.

Done

Run Details

View all runs

Information on Existing Nuclear Calculations

[Nuclear Physics Server Home | DBMS Home | DBMS Search]

runID	username	Z	N	nshell_min_Z	nshell_max_Z	nshell_min_N	nshell_max_N	Nmax	Nstates	twiceJ	twiceMj	START_DATE
1	u16347	2	2	1	17	1	17	16	0	-1	0	Sun May 2 02:31:34 PDT 2010
2	pmaris	3	4	1	6	1	6	4	10	-1	1	Tue Apr 13 10:33:08 CDT 2010
3	jvary	2	2	1	11	1	11	10	10	-1	0	Wed Apr 14 08:13:10 CDT 2010
4	jvary	2	2	1	11	1	11	10	10	-1	0	Wed Apr 14 09:39:10 CDT 2010
5	jvary	2	2	1	11	1	11	10	10	-1	0	Tue Apr 20 10:56:05 CDT 2010
6	jvary	2	2	1	11	1	11	10	10	-1	0	Tue Apr 20 19:34:28 CDT 2010
7	jvary	2	2	1	11	1	11	10	10	-1	0	Wed Apr 21 22:36:15 CDT 2010
8	jvary	2	2	1	11	1	11	10	10	-1	0	Thu Apr 22 05:46:55 CDT 2010
9	jvary	2	2	1	11	1	11	10	10	-1	0	Thu Apr 22 07:33:34 CDT 2010
10	jvary	2	2	1	11	1	11	10	10	-1	0	Thu Apr 22 16:03:15 CDT 2010
11	jvary	2	2	1	11	1	11	10	10	-1	0	Thu Apr 22 22:52:05 CDT 2010
12	jvary	2	2	1	11	1	11	10	10	-1	0	Fri Apr 23 06:05:29 CDT 2010
13	jvary	2	2	1	9	1	9	8	10	-1	0	Fri Apr 23 07:49:00 CDT 2010
14	jvary	2	2	1	9	1	9	8	10	-1	0	Fri Apr 23 08:01:29 CDT 2010
15	jvary	2	2	1	9	1	9	8	10	-1	0	Fri Apr 23 09:03:43 CDT 2010
16	jvary	2	2	1	9	1	9	8	10	-1	0	Fri Apr 23 09:15:47 CDT 2010
17	jvary	2	2	1	9	1	9	8	10	-1	0	Fri Apr 23 09:52:30 CDT 2010
18	jvary	2	2	1	9	1	9	8	10	-1	0	Fri Apr 23 10:07:24 CDT 2010
19	jvary	2	2	1	9	1	9	8	10	-1	0	Fri Apr 23 10:27:22 CDT 2010
20	jvary	2	2	1	9	1	9	8	10	-1	0	Fri Apr 23 11:15:37 CDT 2010
21	jvary	2	2	1	7	1	7	6	10	-1	0	Mon Apr 26 03:17:49 CDT 2010
22	jvary	2	2	1	7	1	7	6	10	-1	0	Mon Apr 26 03:21:28 CDT 2010
23	jvary	2	2	1	7	1	7	6	10	-1	0	Mon Apr 26 03:39:10 CDT 2010
24	jvary	2	2	1	7	1	7	6	10	-1	0	Mon Apr 26 03:47:01 CDT 2010
25	jvary	2	2	1	7	1	7	6	10	-1	0	Mon Apr 26 03:55:19 CDT 2010
26	jvary	2	2	1	7	1	7	6	10	-1	0	Mon Apr 26 04:01:20 CDT 2010
27	jvary	2	2	1	7	1	7	6	10	-1	0	Mon Apr 26 04:12:20 CDT 2010
28	jvary	2	2	1	7	1	7	6	10	-1	0	Mon Apr 26 04:16:20 CDT 2010
29	u16347	2	2	1	13	1	13	12	0	-1	0	Tue Apr 27 00:10:10 PDT 2010
30	u16347	2	2	1	13	1	13	12	0	-1	0	Tue Apr 27 06:31:17 PDT 2010

Done