Present and Future Computing Requirements for Nuclear Data

Alejandro Sonzogni
National Nuclear Data Center
Brookhaven National Laboratory
www.nndc.bnl.gov

BROOKHAVEN NATIONAL LABORATORY
a passion for discovery

Office of Science
U.S. DEPARTMENT OF ENERGY

US Nuclear Data Project

www.nndc.bnl.gov/usndp

List of Pi's/Institutions

Mike Herman (head), NNDC, BNL
Filip Kondev, ANL
Toshihiko Kawano, LANL
Richard Firestone, LBNL
Neil Summers, LLNL
Balraj Singh, McMaster
Allan Carlson, NIST
Mike Smith, ORNL
John Kelly, TUNL

- Only R. Firestone has used NERSC computers before. Other PI's have said they used their own High Performance computers.
- The NNDC has a 70+ CPU cluster and several high-end power stations, two web servers, two database servers, one GForge server and one production server.

USNDP is funded by DoE Office of Science, Nuclear Physics, Nuclear Theory.

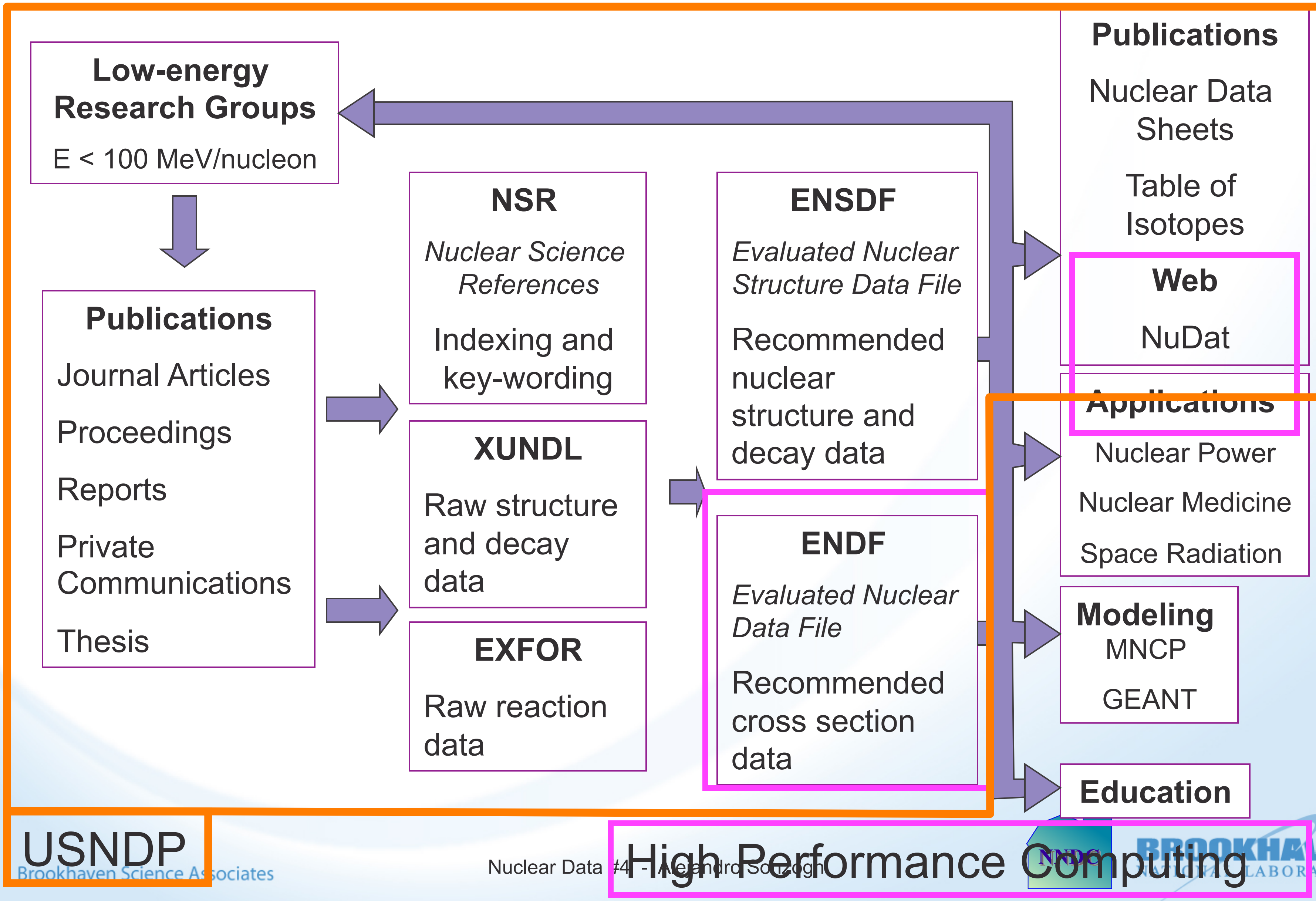
In 2010, 21.35 total FTE's, 12.5 Scientific permanent FTE's, $ 6.5M budget.

Institutions

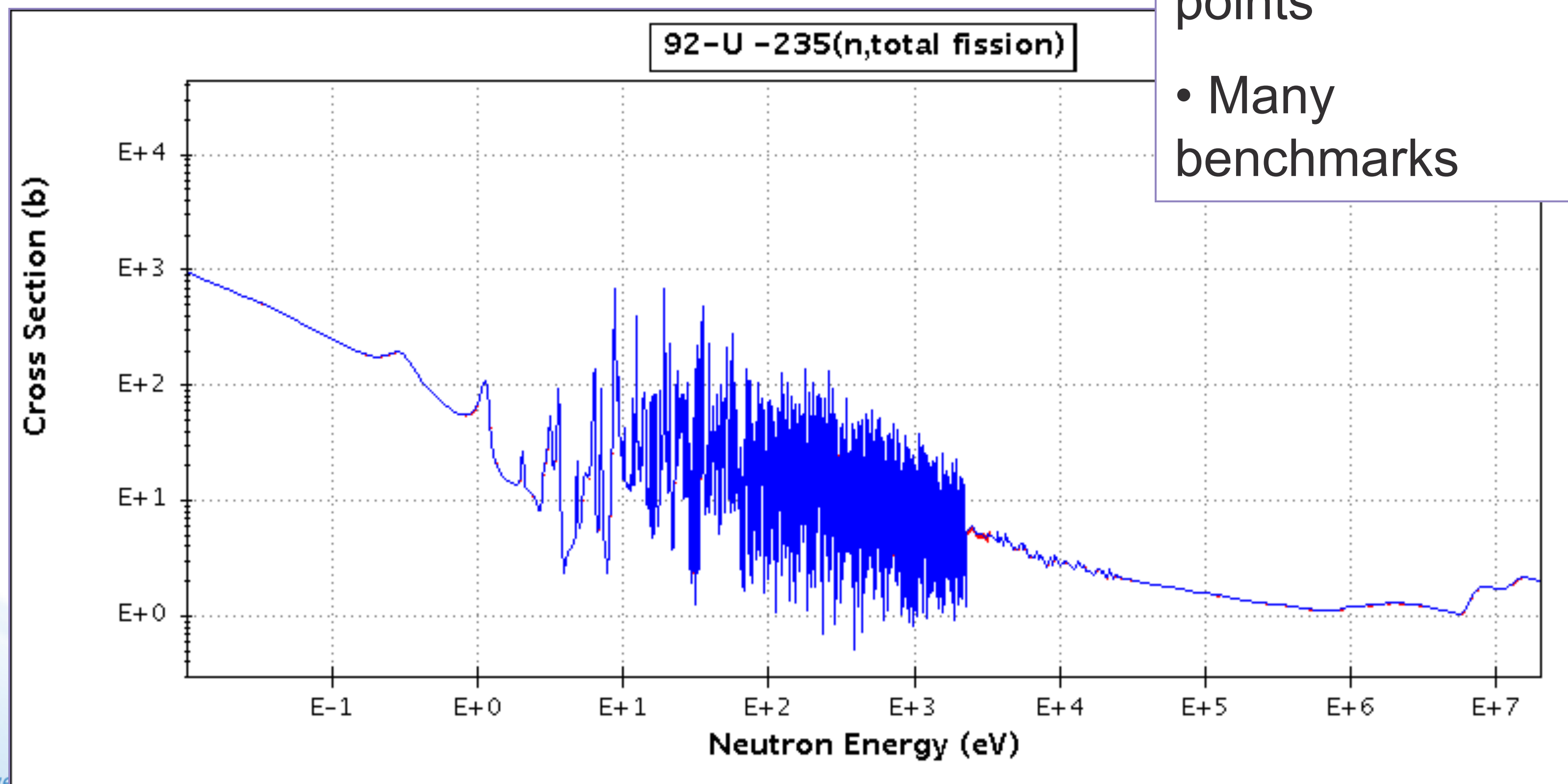
National Nuclear Data Center (12 people)
Argonne National Laboratory
Georgia Tech
Los Alamos National Laboratory
Lawrence Berkeley National Laboratory
Lawrence Livermore National Laboratory
McMaster University
NIST
Texas A&M University
TUNL

Close collaborations with INL, RPI, IAEA (Vienna), OECD-NEA (Paris), Australian Natl. University, KAERI, JAEA.

Nuclear Data

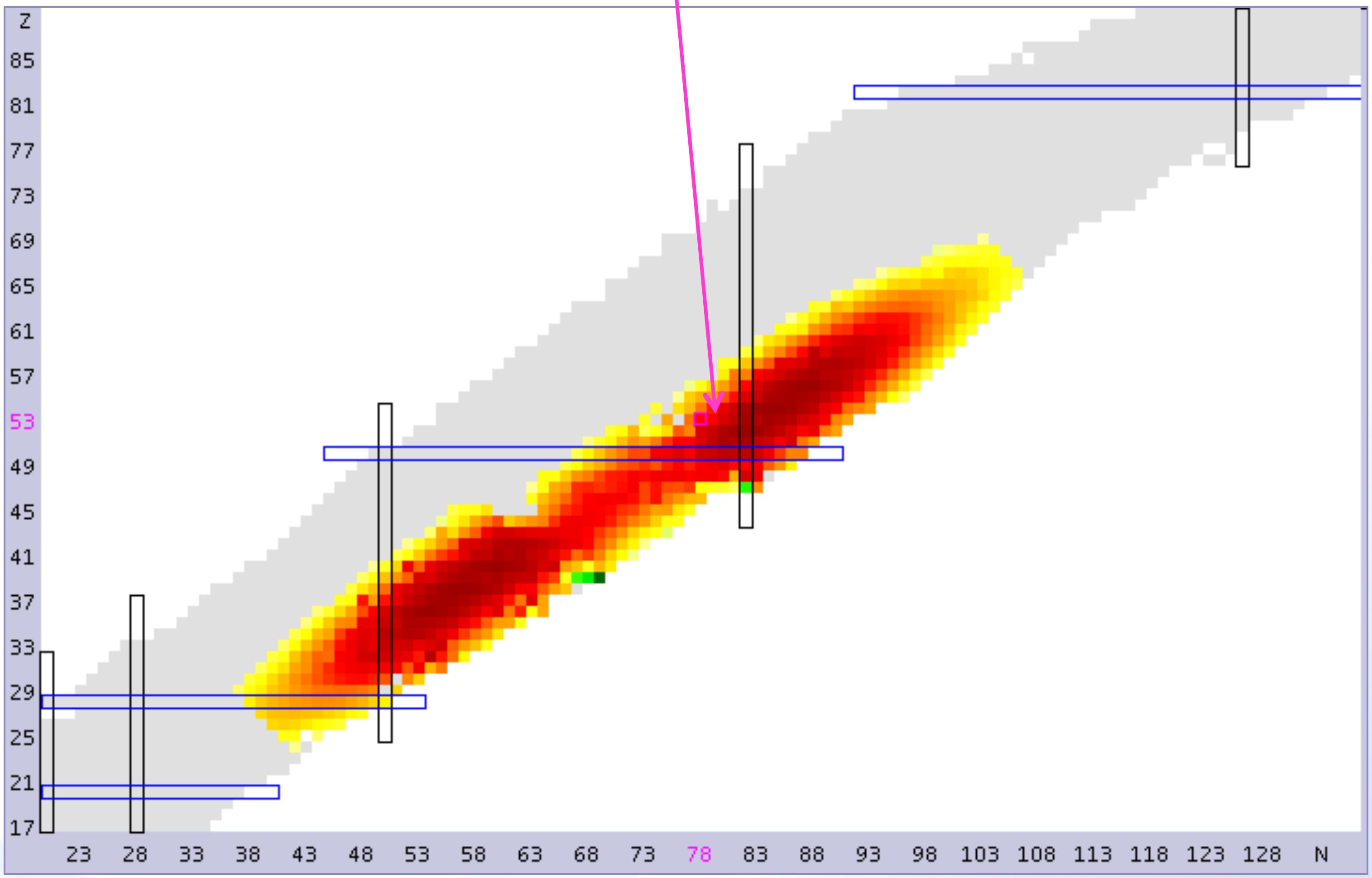


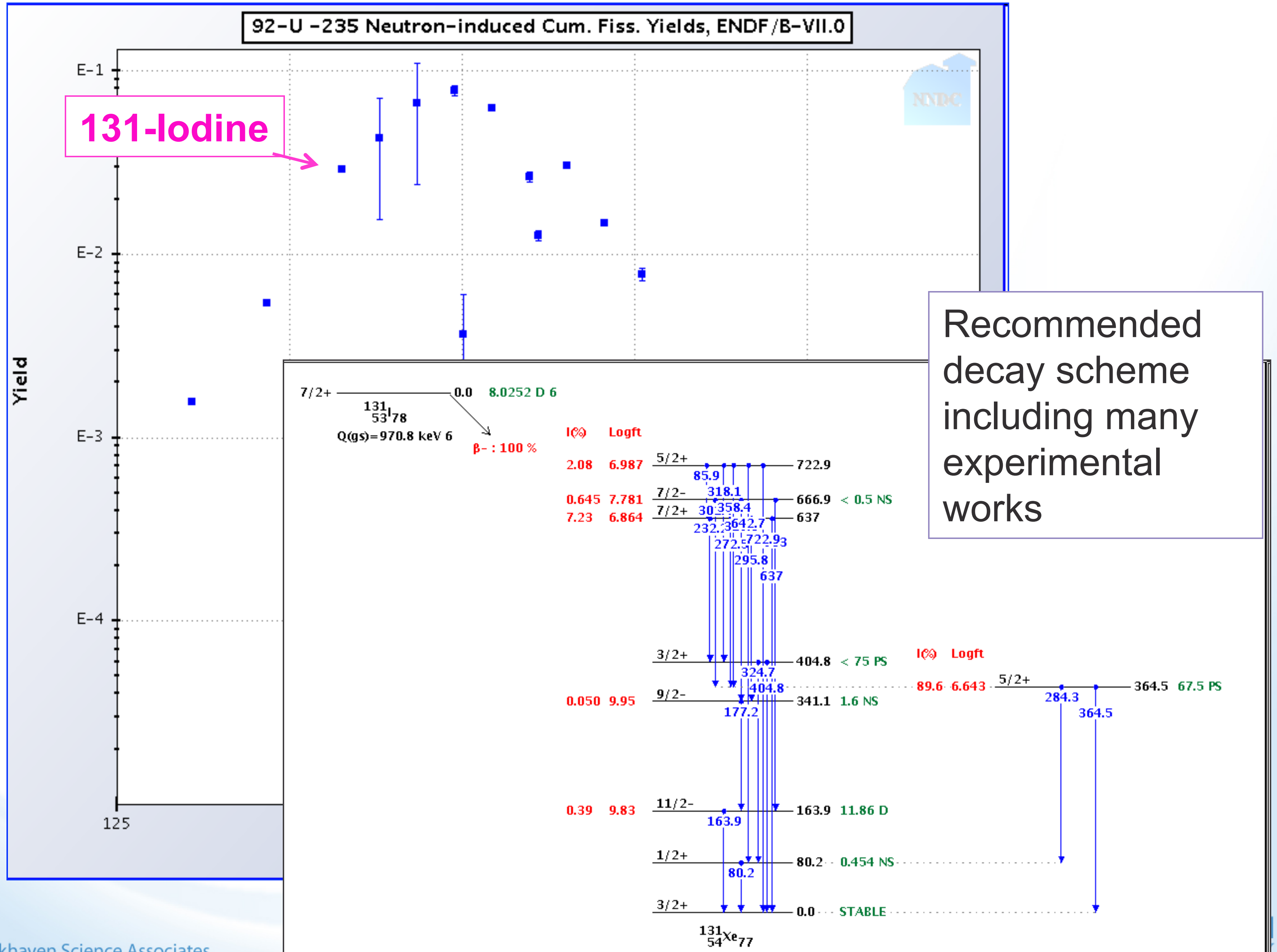
Example
131-Iodine release in Fukushima



- Sophisticated models for three distinct energy regimes
- Hundreds of experimental points
- Many benchmarks

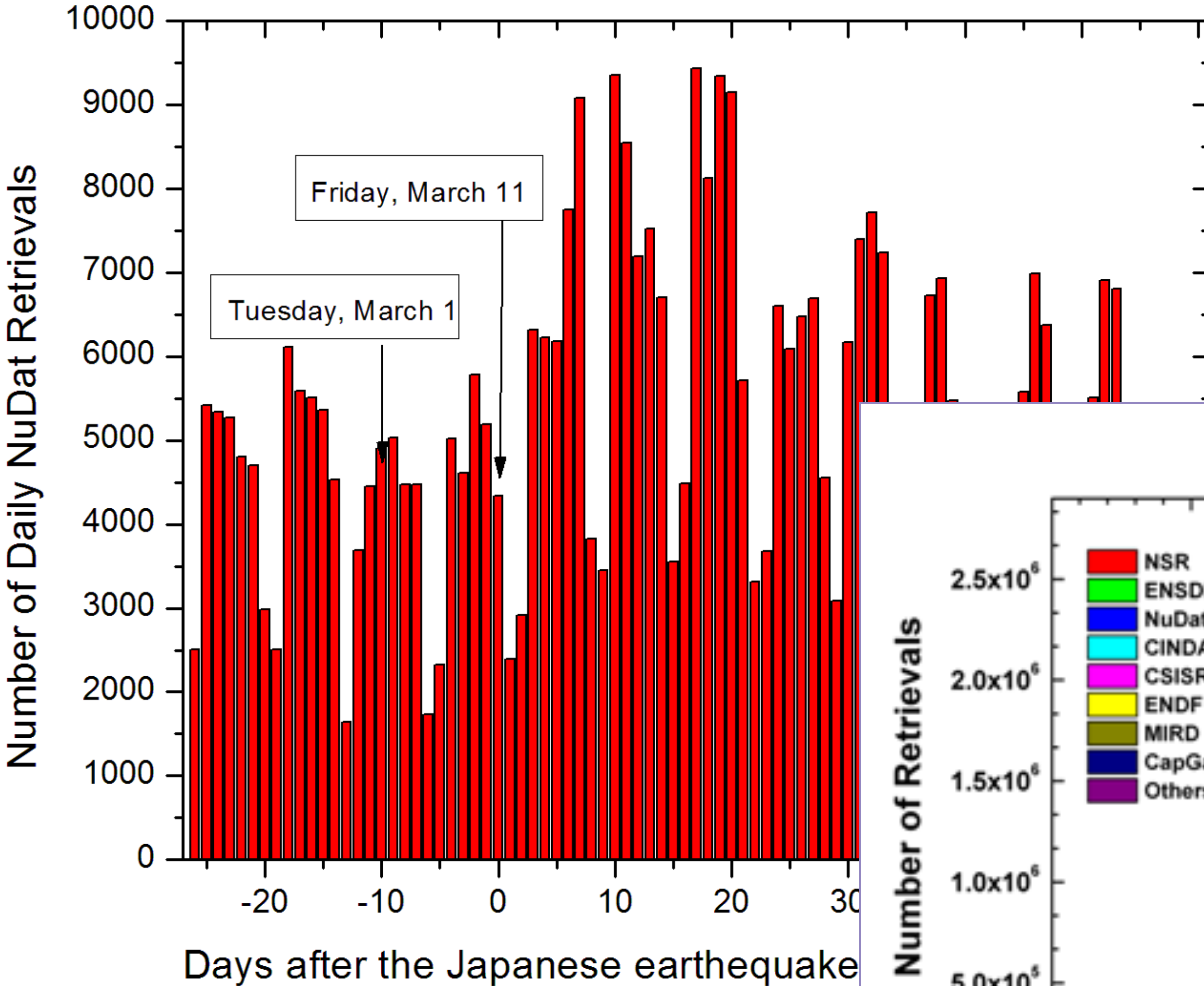
2D fission yield plots. 131-Iodine ground state is just one of the 800+ long lived levels produced.

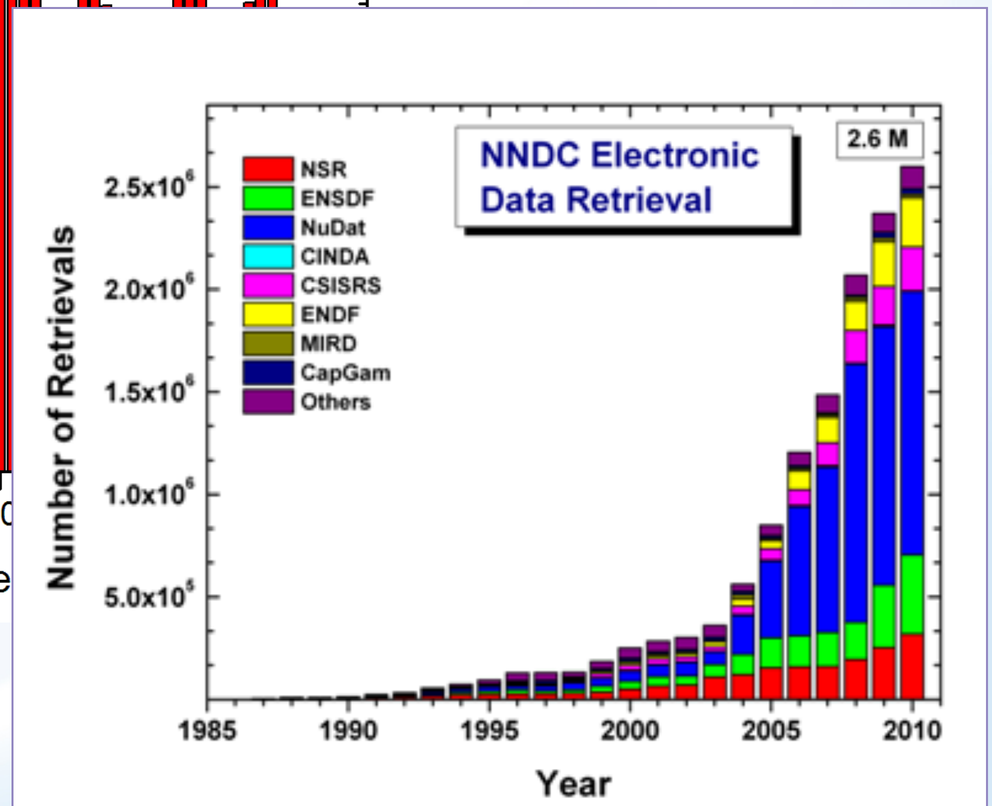




Recommended decay scheme including many experimental works

Effects on Web retrievals





About the data

Original format is from the early 50's. ASCII files with 80 character lines.

There are several well defined formats: ENSDF, ENDF, NSR, EXFOR

Each database is about 1 GB. Some Fortran codes typically load the whole database.

Some disadvantages:
Precision is limited, induces a 2 -5 % numerical noise in calculations
Format is not user friendly, very difficult for a non-expert to deal with it

For the future, XML is the answer:

- Much higher numerical precision
- If designed intelligently, easier to deal with format
- But… databases will get into the TB size… Difficult to put it into disk…Will challenge the legacy Fortran codes

The data archived by the NNDC was collected in more than 100 years of nuclear physics research. Most of those experiments will not be repeated.

More about the data

We save the data using commercial SQL software.

Two database servers. One server can be accessed remotely.

Allows to keep derived data in addition to the original one. For instance:

- In the resonance region, only resonance parameters are given. Cross sections are then calculated in the lab system at room temperature.
- Gamma-gamma coincidences are generated from the ENSDF file
- Atomic radiation following nuclear decay is calculated.

Databases are about 50 GB. Indexing takes about 70%

Cost can be a problem. In early 2000's Oracle cost became too high for us, so we migrated to Sybase, which in turn became too expensive, then migrated to MySQL, which was bought by Oracle…

Must learn SQL, worry about primary keys, foreign keys, store procedures, indexing…

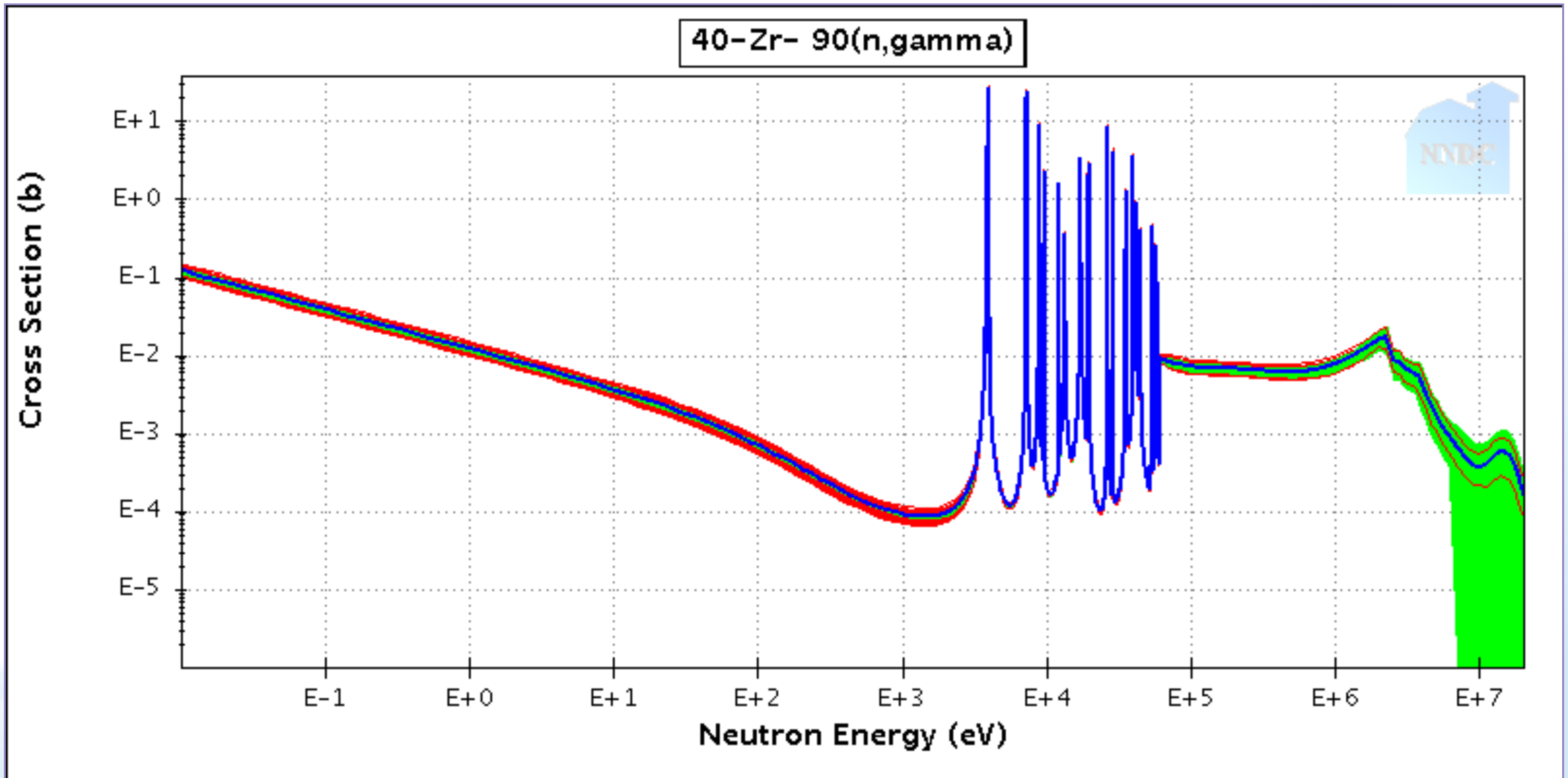
Current HPC Methods & Requirements

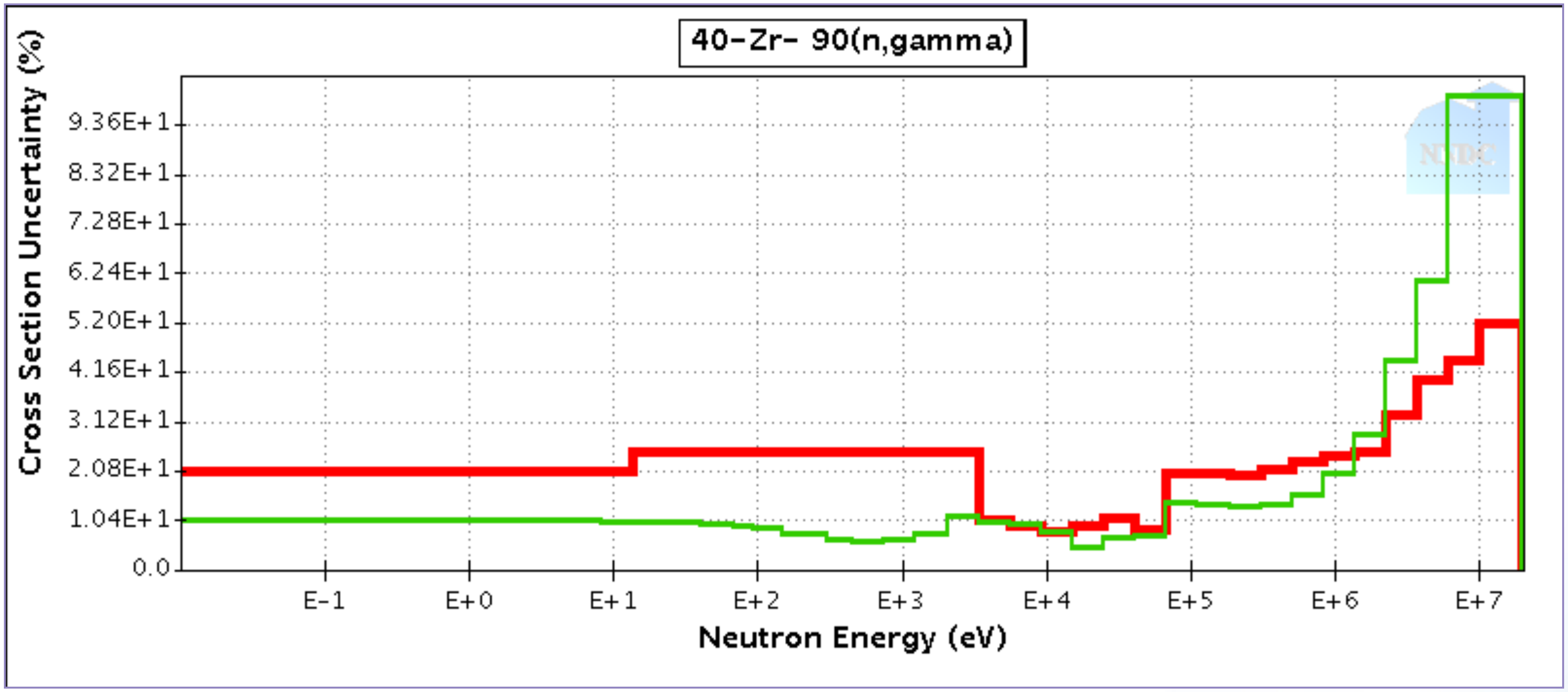
- **Architectures currently used (NNDC):**
- 70+ CPU cluster, each 2.4 GHz dual core with 2 GB RAM per core.   Mainly for:
  - EMPIRE code to calculate cross sections
  - EMPIRE + Kalman filter to calculate covariances
  - NJOY to obtain group cross sections
  - MCNP to validate cross sections
- Linux operating system, Portland Group, Fujitsu, Lahey Fortran compilers
- Several high end Linux and windows power stations.   Many Java codes.
- Two Linux web servers, Apache Tomcat, 4 core Xeon, 2 GB RAM per core.
- Two Linux database servers, MySQL, same specs as web servers
- One Linux server for Gforge
- One Linux server for general purposes, mainly production of Nuclear Data Sheets
- **Compute/memory load**
- 2GB of RAM often limits operations.   Would like to use 4GB

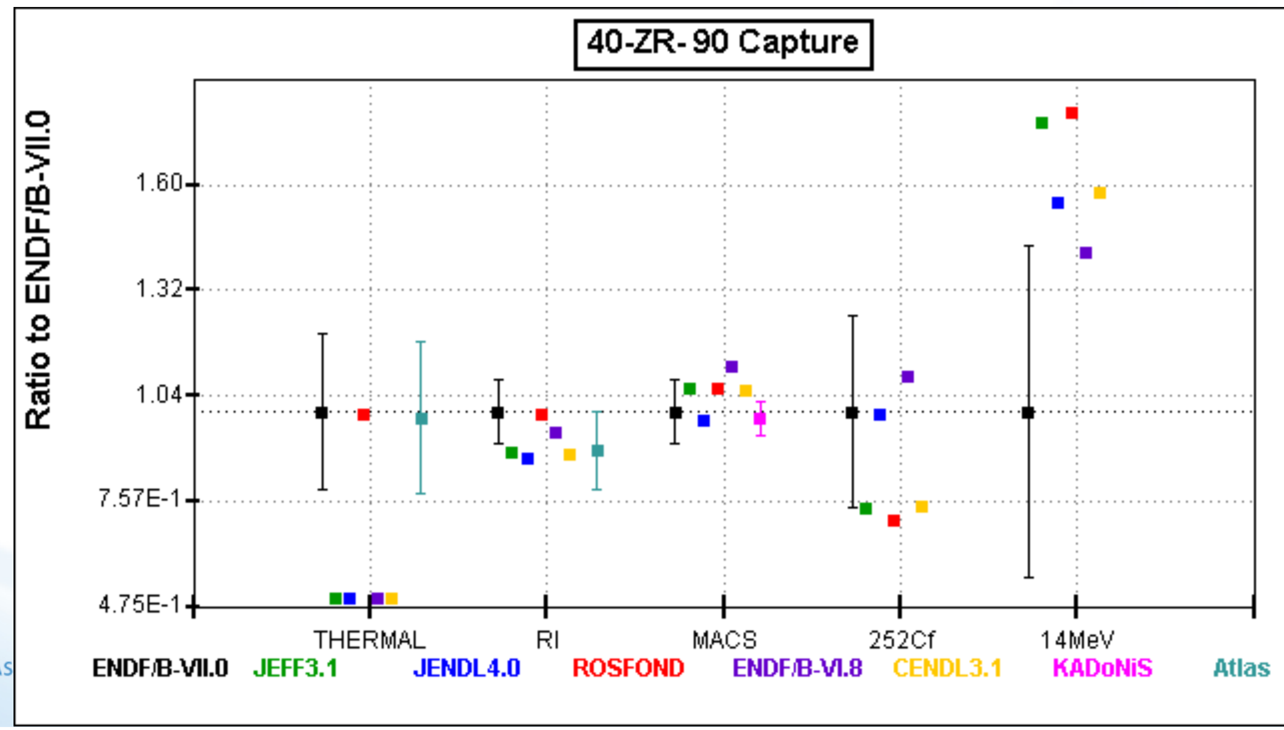
HPC Usage and Methods for the Next 3-5 Years

Currently working on the release of the ENDF/B-VII.1 library. The NNDC cluster is running MCNP constantly. We will add the code SCALE in the near future.

Key area is covariance matrices, in particular, realistic uncertainties.

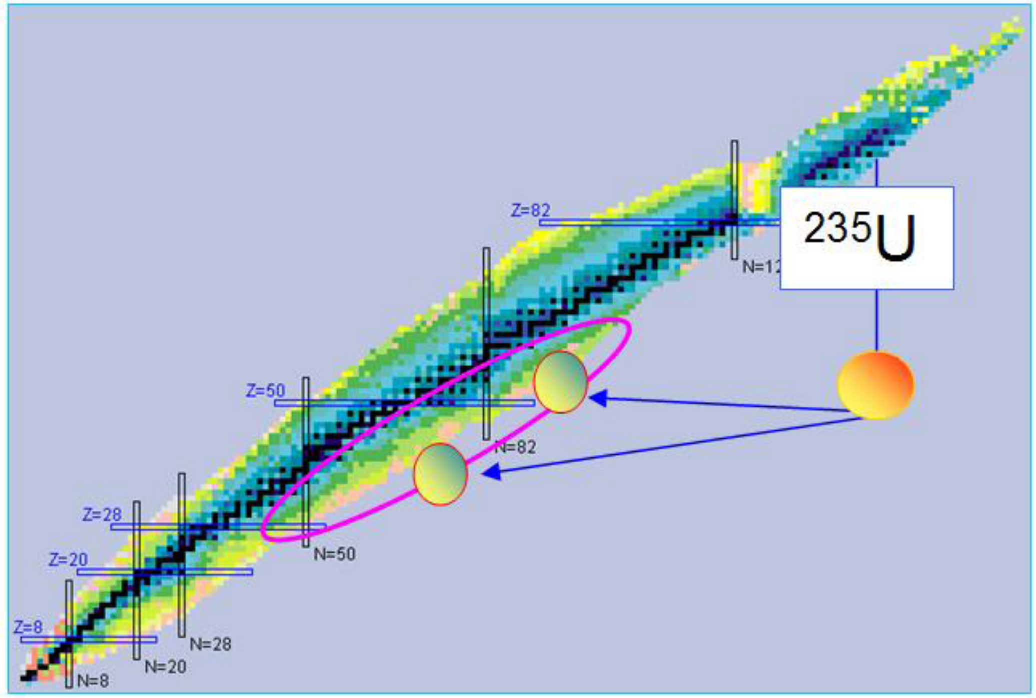


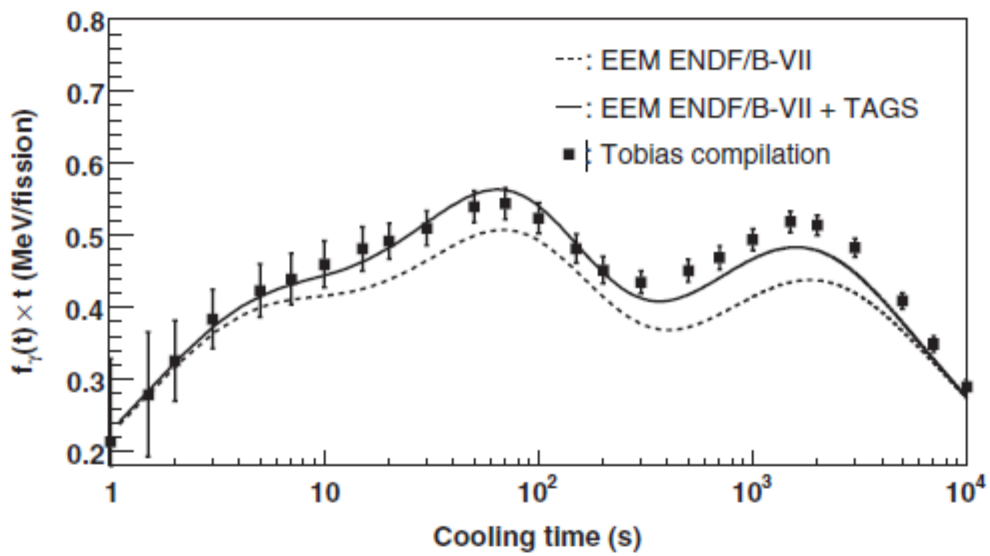

40-Zr- 90(n,gamma)
Cross Section Uncertainty (%)
9.36E+1
8.32E+1
7.28E+1
6.24E+1
5.20E+1
4.16E+1
3.12E+1
2.08E+1
1.04E+1
0.0
E-1
E+0
E+1
E+2
E+3
E+4
E+5
E+6
E+7
Neutron Energy (eV)


40-ZR-90 Capture
Ratio to ENDF/B-VII.0
1.60
1.32
1.04
7.57E-1
4.75E-1
THERMAL
RI
MACS
252Cf
14MeV
ENDF/B-VII.0
JEFF3.1
JENDL4.0
ROSFOND
ENDF/B-VI.8
CENDL3.1
KADoNiS
Atlas

Another project the NNDC is involved, nuclear decay heat following the neutron-induced fission of an actinide nucleus.

A recent PRL reported that detailed study of a few nuclides can improved the calculation of decay heat for 239Pu. Experiments performed in CERN and Jyvaskyla. Calculations at the NNDC.





The NNDC is planning to calculate decay heat uncertainties using a MonteCarlo method.

Codes were written in Java.

HPC Usage and Methods for the Next 3-5 Years

- The NNDC cluster will become obsolete in about 3 years.

- The web and database servers will be replaced in about 3 years.

- RAM, 2 GB/processor is at the moment a limiting factor.

- Could NERSC provide some help in these areas?

- Every year since the mid-60's, there is a week-long meeting in Brookhaven during the Fall. This year will be Nov. 14-18. Perhaps a NERSC presentation will help to bring awareness to the Nuclear Data community.