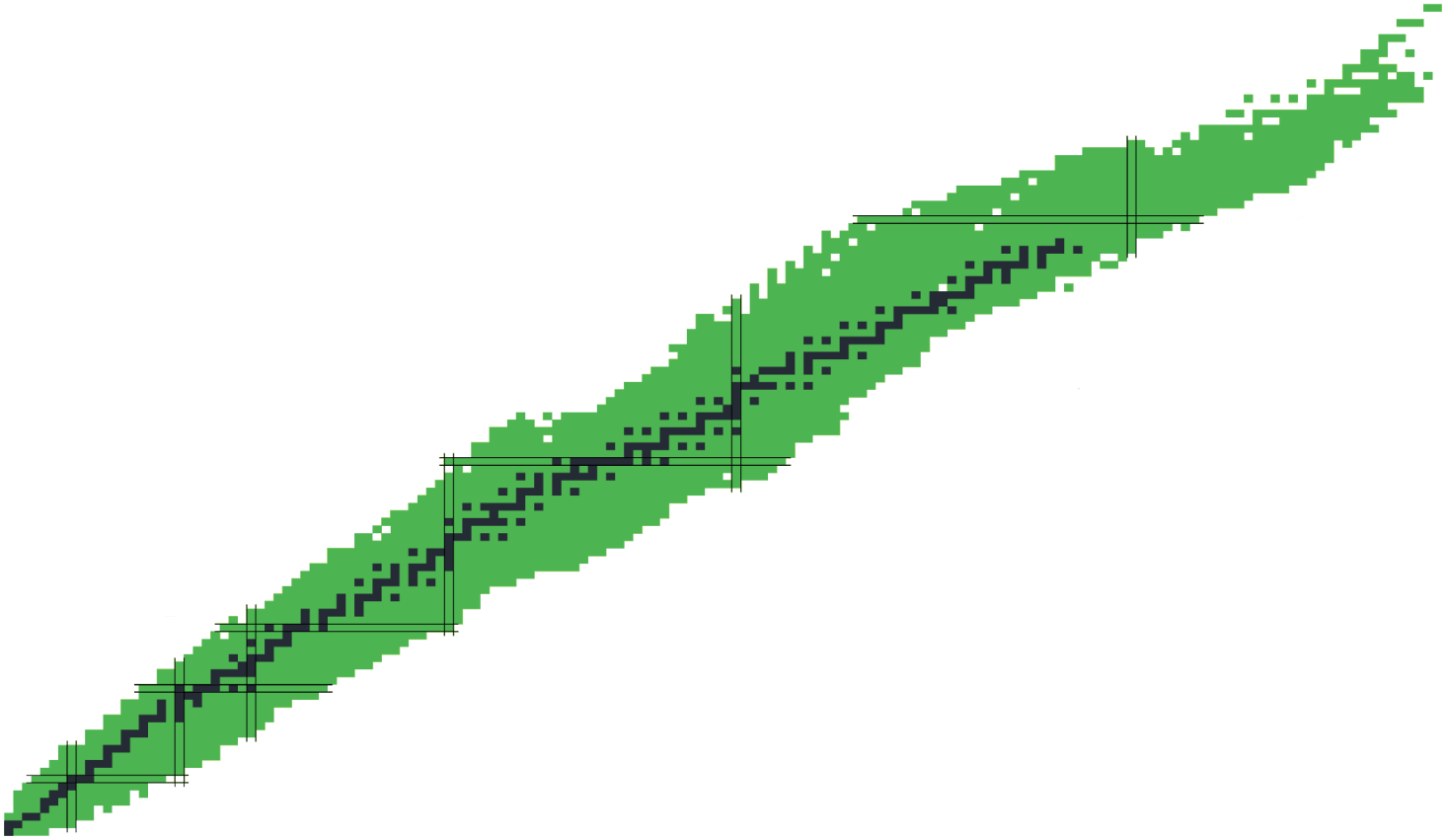
Notre Dame Nuclide Database Project



Matthew Mumpower

University of Notre Dame / Joint Institute for Nuclear Astrophysics

Wednesday Sept. 18th 2013

LANL Nuclear Data Seminar

Motivation

- An attempt to parse nuclear masses from the AME2012

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   This is one file out of a series of 3 files published in:
       "The Ame2012 atomic mass evaluation (I)"  by G.Audi, M.Wang, A.H.Wapstra, F.G.Kondev, M.MacCormick, X.Xu, and B.~Pfeiffer
           Chinese Physics C36 p. 1287-1602, December 2012.
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           Chinese Physics C36 p. 1603-2014, December 2012.
                       for files : mass.mas12 : atomic masses
                                   rct1.mas12 : react and sep energies,  part 1
                                   rct2.mas12 : react and sep energies,  part 2

   All files are 3353 lines long with 124 character per line.
       Headers are 39 lines long.

   Values in all files are unrounded values

   col 1     :  Fortran character control: 1 = page feed  0 = line feed
   format    :  a1,i3,i5,i5,i5,1x,a3,a4,1x,f13.5,f11.5,f11.3,f9.3,1x,a2,f11.3,f9.3,1x,i3,1x,f12.5,f11.5
                cc NZ  N  Z  A    el  o     mass  unc binding unc     B  beta  unc    atomic_mass   unc
   Warnings  :  this format is identical to the one used in Ame2003
                      in particular "Mass Excess" and "Atomic Mass" values are given now, when necessary,
                      with 5 digits after decimal point.

                decimal point is replaced by # for (non-experimental) estimated values.
                * in place of value : not calculable

....+....1....+....2....+....3....+....4....+....5....+....6....+....7....+....8....+....9....+...10....+...11....+...12....


                                                                MASS LIST
                                                               for analysis

1N-Z    N    Z   A  EL    O     MASS EXCESS       BINDING ENERGY/A        BETA-DECAY ENERGY          ATOMIC MASS          V/S
                                    (keV)               (keV)                   (keV)                (micro-u)
0  1    1    0    1  n          8071.31714    0.00046      0.0      0.0   B-    782.347    0.000   1 008664.91585    0.00049
  -1    0    1    1 H           7288.97059    0.00009      0.0      0.0   B-       *               1 007825.03223    0.00009
0  0    1    1    2 H          13135.72174    0.00011   1112.283    0.000 B-       *               2 014101.77812    0.00012
0  1    2    1    3 H          14949.80611    0.00221   2827.266    0.001 B-     18.591    0.001   3 016049.27791    0.00237
  -1    1    2    3 He         14931.21551    0.00233   2572.681    0.001 B- -13736#    2000#     3 016029.32008    0.00250
  -3    0    3    3 Li  -pp    28667#       2000#       -2267#     667#    B-       *               3 030775#       2147#
0  2    3    1    4 H    -n    24621.123     100.000     1720.450   25.000 B-  22196.208  100.000   4 026431.864     107.354
   0    2    2    4 He          2424.91561    0.00006   7073.915    0.000 B- -22898.270  212.132   4 002603.25413    0.00006
  -2    1    3    4 Li   -p    25323.186     212.132     1153.761   53.033 B-       *               4 027185.559     227.733
0  3    4    1    5 H    -nn   32892.440      89.443     1336.360   17.889 B-  21661.208   91.652   5 035311.489      96.020
   1    3    2    5 He   -n    11231.233      20.000     5512.132    4.000 B-   -447.653   53.852   5 012057.224      21.470
  -1    2    3    5 Li   -p    11678.886      50.000     5266.132   10.000 B- -25460#    2003#     5 012537.800      53.677
  -3    1    4    5 Be    x    37139#       2003#         18#      401#    B-       *               5 039870#       2150#
0  4    5    1    6 H    -3n   41875.717     254.127      961.640   42.354 B-  24283.622  254.127   6 044955.433     272.816
   2    4    2    6 He          17592.095      0.053     4878.519    0.009 B-   3505.216    0.053   6 018885.891      0.057
   0    3    3    6 Li          14086.87893    0.00144   5332.331    0.000 B-  -4288.155    5.448   6 015122.88742    0.00155
  -2    2    4    6 Be    -     18375.034      5.448     4487.247    0.908 B- -28945#    2003#     6 019726.411      5.848
  -4    1    5    6 B     x    47320#       2003#       -467#      334#    B-       *               6 050800#       2150#
0  5    6    1    7 H    -nn   49135#       1004#        940#      143#    B-  23062#    1004#     7 052749#       1078#
   3    5    2    7 He   -n    26073.126      7.559     4123.057    1.080 B-  11166.021    7.559   7 027990.654      8.115
   1    4    3    7 Li          14907.10520    0.00423   5606.439    0.001 B-   -861.893    0.071   7 016003.43659    0.00454
  -1    3    4    7 Be          15768.999      0.071     5371.548    0.010 B- -11907.551   25.150   7 016928.717      0.076
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```

Motivation

- Authors provide one way to parse... Using Fortran

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MASS LIST
for analysis

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Motivation

- What if you only want experimental data (exclude their theory calculations)?
- This is a painful task...
- The easiest way I could find to accomplish this task was to write an OOP Python script

Motivation

- Limitations of the AME2012 dataset
  - Fixed format file (ASCII) – with errors!
  - Authors provide one way to parse... Using Fortran
  - Custom parser must be written even for common data requests
  - No metadata provided in the dataset (one has to go to the booklet and search for this by hand)

Project Goals

- To implement a web-based system which allows users to set criterion for searching, combining and outputting customized datasets of measured nuclear properties

- Intended application: nuclear astrophysics

- Initial plan is to support:
  - Nuclear masses
  - Beta (+/-) decay
  - Beta-delayed neutron emission probabilities

- Expand to other properties in the future

Project Features

- Data in the database is **immutable –** Data in the database is fixed and does not change – however new data can be added at any time

- **Extensible** – stores data in a generalized format so that more properties can be added at later dates

- Also stores **metadata** (data about data) - providing context to data that we use

- Database will be accessible via online (web) and command line terminal interfaces

Backend Technologies Used

Pyramid™

python powered

SQLAlchemy

git

Backend Technologies Used

- **Python**
  - High-level object-oriented programming (OOP) language
  - It affords highly-readable syntax and a large number of freely available libraries and tools, while still maintaining fast and efficient code
  - Basis language for the development of the database
  - Operating system independent

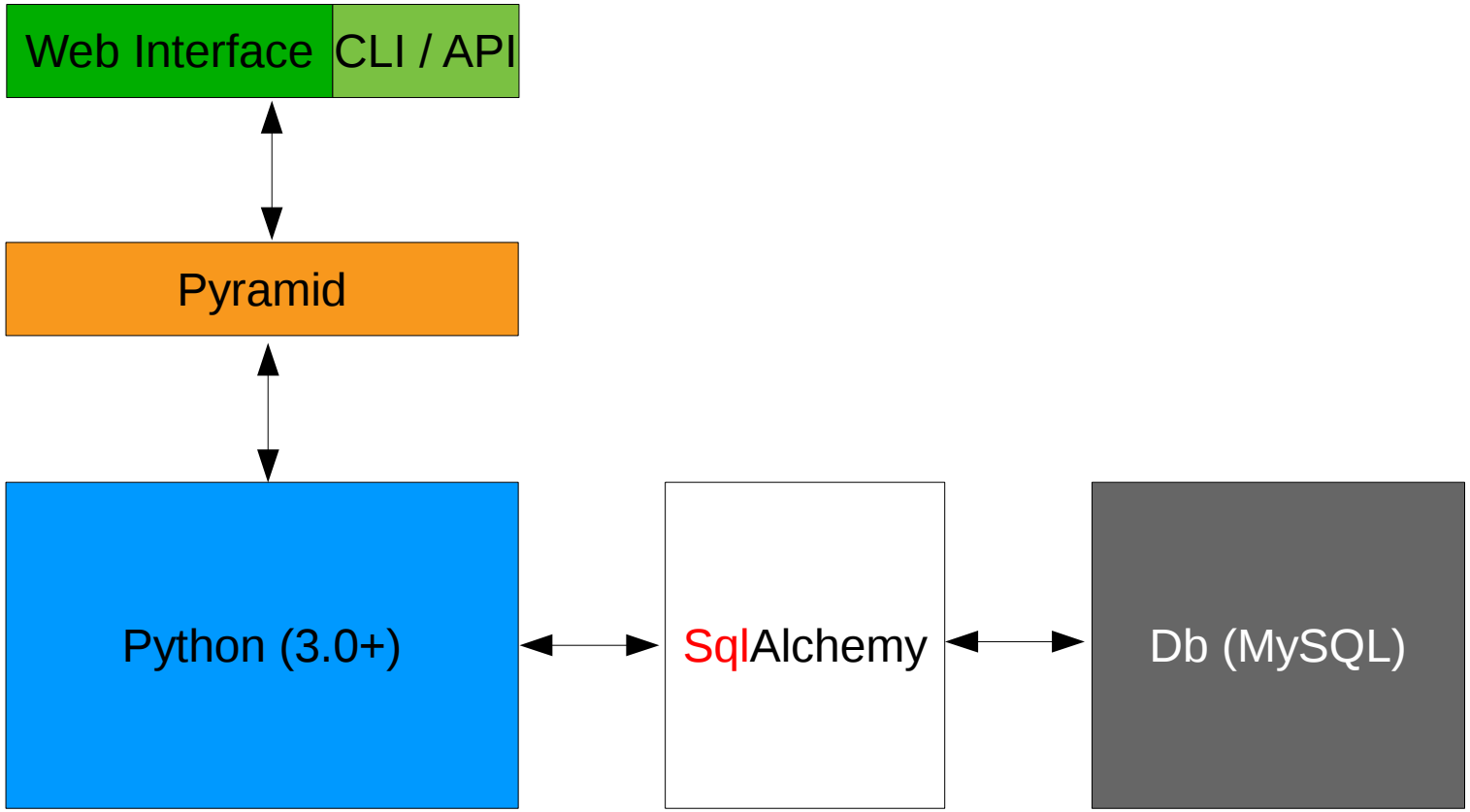
- **Pyramid**
  - Web development framework for Python
  - Handles all processing of requests from a web server
  - Using resource-tree-view design pattern which is a derivative of the model-view-control pattern

Backend Technologies Used

- **MySQL**
  - Relational database used for data storage
  - Designed for data “normalization”
  - Avoids duplicating data
  - Defines foreign key relationships which connect one value to another

- **SqlAlchemy**
  - An object-relational mapper which handles...
  - Extracting / inserting data from the database
  - Dynamically generating SQL statements and performing queries

Backend Flow



- The backend is unified by Python and its supported technologies

Database Design Goals

- **Exportability**
  - Researchers can export data to nearly any file format. e.g. standard (CSV, XML, JSON, ASCII, Excel, HDF5, etc.) or user custom defined

- **Metadata**
  - All data is tied to information about its origin, such as apparatus, facility, publication, authors, etc.

- **Data Integrity / Database Normalization**
  - Data is stored to minimize unnecessary data duplication and to ensure self-consistency

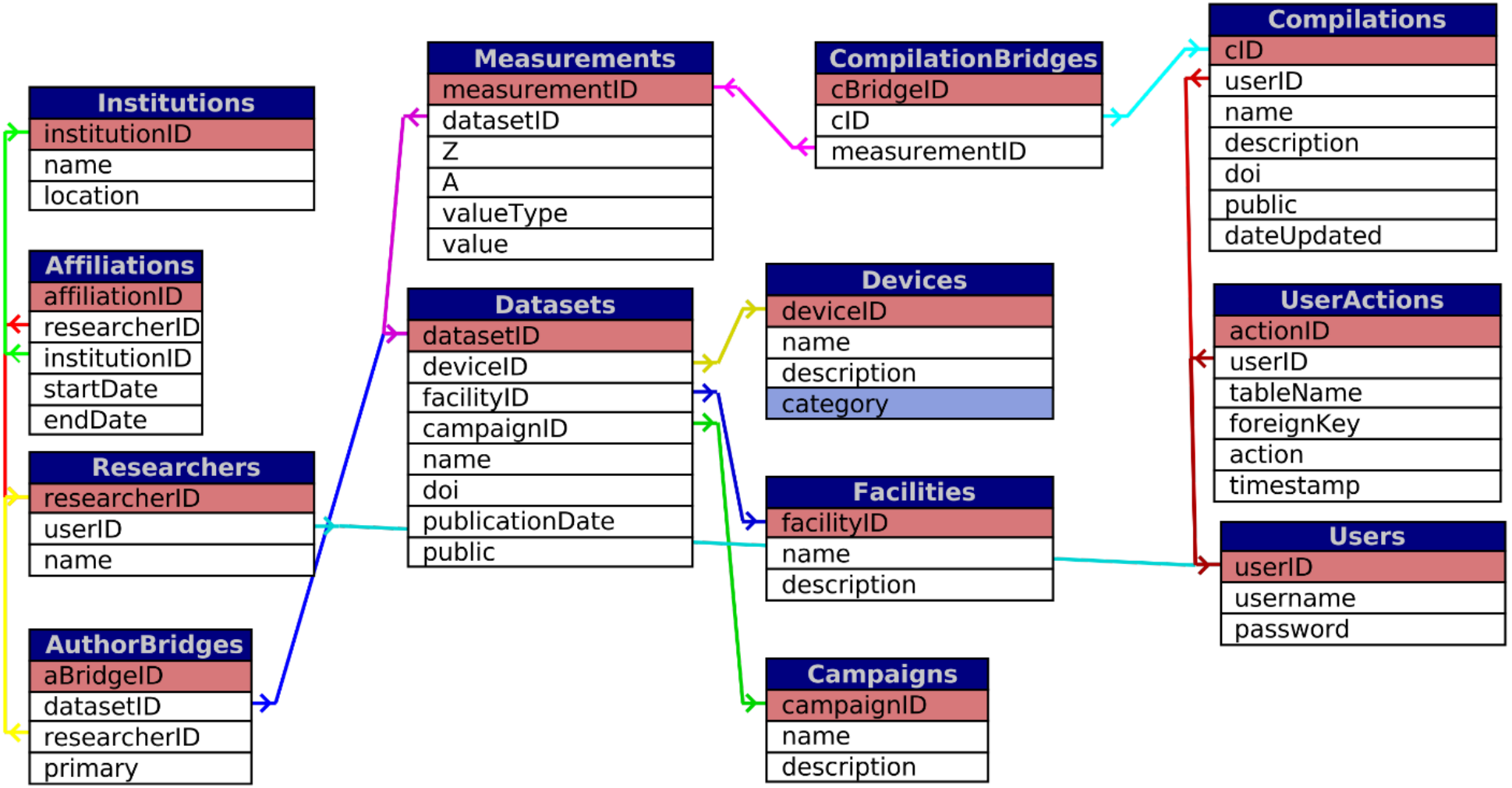
Database Design Goals

- **Extensibility / Modularity**
  - It should be simple to add new measurements to the database
  - Also, new types of measurements should be easy to add in the future

- **Multiple Interfaces**
  - Data should be accessible from several different interfaces
  - Web or command line initially supported
  - Web API (custom applications) in the future

Oversimplified View of The Database

Star Schema Structure Employed



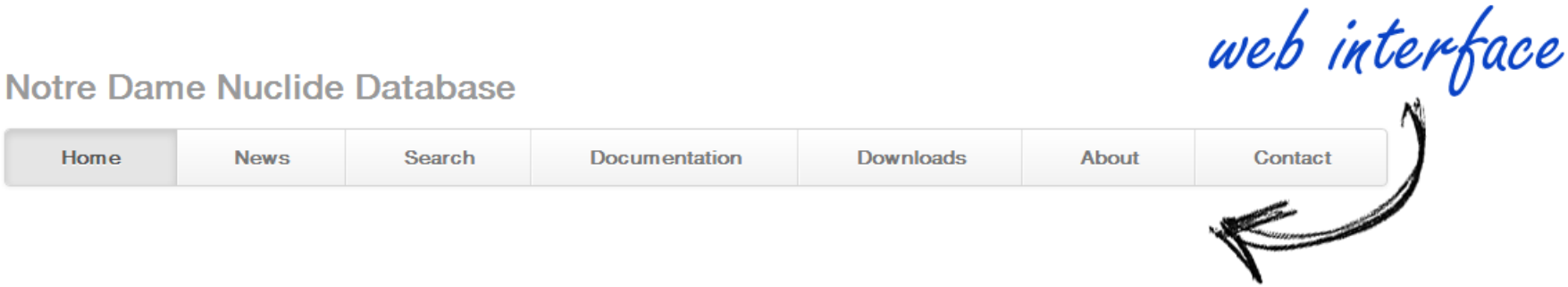
Search Criterion & Usability

- Search by metadata – nuclide, Z, N or A, researcher or team that performed the experiment / measurements, equipment used, facility, date, publication information or combination of these

- User can select from a variety of custom output data formats that fits their needs

- Example output formats: HDF5, XML, ASCII, HTML, CSV, Excel

Front Page Design Mockup



Welcome!

The Notre Dame Nuclide Database $(ND)^2$ is a publicly available suite of tools to assist researchers in nuclear astrophysics.

Learn more about $(ND)^2$

Latest AME Data

The latest Atomic Mass Evaluation (AME) data was released in December of 2012. A compilation of this dataset is provided in several convenient formats.

Download now »

Getting Started

The $(ND)^2$ maintains information on nuclides. In addition the database holds metadata, such as publication information. This means data stored in this database has *context*.

Learn how to use search »

Commandline Tools

In addition to this site, a commandline interface (CLI) is provided for data access. This python toolkit communicates with the database, providing the data you need right at your terminal.

learn more about the CLI »

Dynamic CSS Viewports

- Can access the web interface on any device
- Without loss of functionality

Example Search (Excel Format)

- Wanted to find recent mass measurements @ Jyvaskyla
- Searched by metadata
- Requested custom units for the masses (mass excess)
- Output format: Excel

42	104	104Mo	-80354	12	Jyväskylä	JYFLTRAP	U. Hager	10.1103/PhysRevLett.96.042504	Hag06
42	105	105Mo	-77341	10	Jyväskylä	JYFLTRAP	U. Hager	10.1103/PhysRevLett.96.042504	Hag06
42	106	106Mo	-76139	10	Jyväskylä	JYFLTRAP	U. Hager	10.1103/PhysRevLett.96.042504	Hag06
42	107	107Mo	-72556	10	Jyväskylä	JYFLTRAP	U. Hager	10.1103/PhysRevLett.96.042504	Hag06
42	108	108Mo	-70760	10	Jyväskylä	JYFLTRAP	U. Hager	10.1103/PhysRevLett.96.042504	Hag06
42	109	109Mo	-66670	7	Jyväskylä	JYFLTRAP	U. Hager	10.1103/PhysRevLett.96.042504	Hag06
42	110	110Mo	-64547	10	Jyväskylä	JYFLTRAP	U. Hager	10.1103/PhysRevLett.96.042504	Hag06
43	106	106Tc	-79736	5	Jyväskylä	JYFLTRAP	U. Hager	10.1103/PhysRevC.75.054302	Hag07a
43	107	107Tc	-78743	9	Jyväskylä	JYFLTRAP	U. Hager	10.1103/PhysRevC.75.054302	Hag07a
43	108	108Tc	-75916	9	Jyväskylä	JYFLTRAP	U. Hager	10.1103/PhysRevC.75.054302	Hag07a
43	109	109Tc	-74276	10	Jyväskylä	JYFLTRAP	U. Hager	10.1103/PhysRevC.75.054302	Hag07a
43	110	110Tc	-71028	10	Jyväskylä	JYFLTRAP	U. Hager	10.1103/PhysRevC.75.054302	Hag07a
43	111	111Tc	-69018	11	Jyväskylä	JYFLTRAP	U. Hager	10.1103/PhysRevC.75.054302	Hag07a
43	112	112Tc	-65250	6	Jyväskylä	JYFLTRAP	U. Hager	10.1103/PhysRevC.75.054302	Hag07a
44	106	106Ru	-86311	9	Jyväskylä	JYFLTRAP	U. Hager	10.1103/PhysRevC.75.054302	Hag07a
44	107	107Ru	-83856	9	Jyväskylä	JYFLTRAP	U. Hager	10.1103/PhysRevC.75.054302	Hag07a
44	108	108Ru	-83655	9	Jyväskylä	JYFLTRAP	U. Hager	10.1103/PhysRevC.75.054302	Hag07a
44	109	109Ru	-80732	10	Jyväskylä	JYFLTRAP	U. Hager	10.1103/PhysRevC.75.054302	Hag07a
44	110	110Ru	-80067	10	Jyväskylä	JYFLTRAP	U. Hager	10.1103/PhysRevC.75.054302	Hag07a
44	111	111Ru	-76778	10	Jyväskylä	JYFLTRAP	U. Hager	10.1103/PhysRevC.75.054302	Hag07a
44	112	112Ru	-75624	10	Jyväskylä	JYFLTRAP	U. Hager	10.1103/PhysRevC.75.054302	Hag07a
44	113	113Ru	-71819	12	Jyväskylä	JYFLTRAP	U. Hager	10.1103/PhysRevC.75.054302	Hag07a
44	114	114Ru	-70213	13	Jyväskylä	JYFLTRAP	U. Hager	10.1103/PhysRevC.75.054302	Hag07a
44	115	115Ru	-66071	8	Jyväskylä	JYFLTRAP	U. Hager	10.1103/PhysRevC.75.054302	Hag07a
45	108	108Rh	-85037	15	Jyväskylä	JYFLTRAP	U. Hager	10.1103/PhysRevC.75.054302	Hag07a

Command Line Interface (CLI)

- Will be based on a python script – download will be available on the website (once live)
- Use command line to download custom datasets direct to your machine
- Full search capability just as with the web interface
- Version control of these datasets provided locally by git and globally via the web

Command Line Interface (CLI)

Usefulness of git

- Powerful local version control of datasets provided by git (distributed version control system)
- Example: you download mass dataset of Sn isotopes
- You can modify these files as you like (local version control via git)
- Later... you use the CLI to check for updates to the mass measurements
- Can then merge what is new from the database to your local machine effortlessly with git

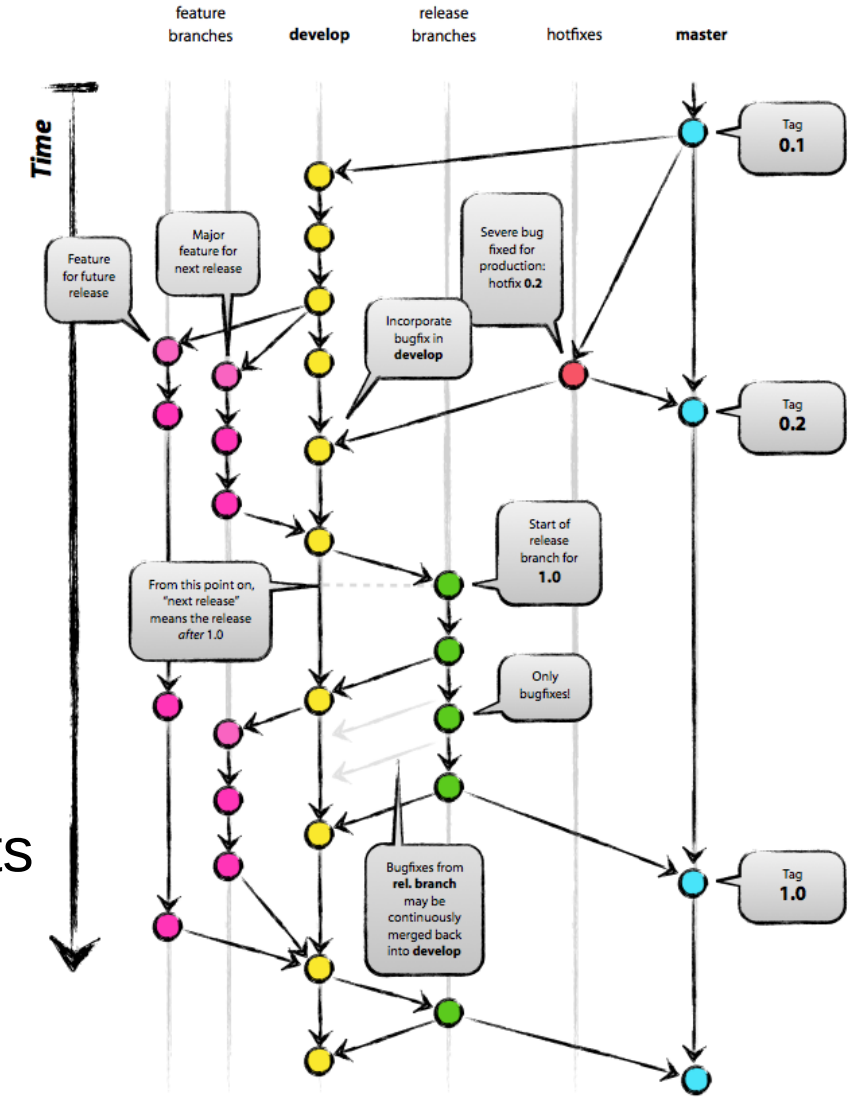


Image from http://nvie.com

Summary & Outlook

The Notre Dame Nuclide Database Project

- We've solved a lot of technical hurdles in designing the database structure
- We've designed the database in a way that any property can be stored and retrieved
- Searches can be performed on data or metadata
- We are currently working on polishing the web page and completing the command line interface
- Release date...?
- We are open to any suggestions or collaborations