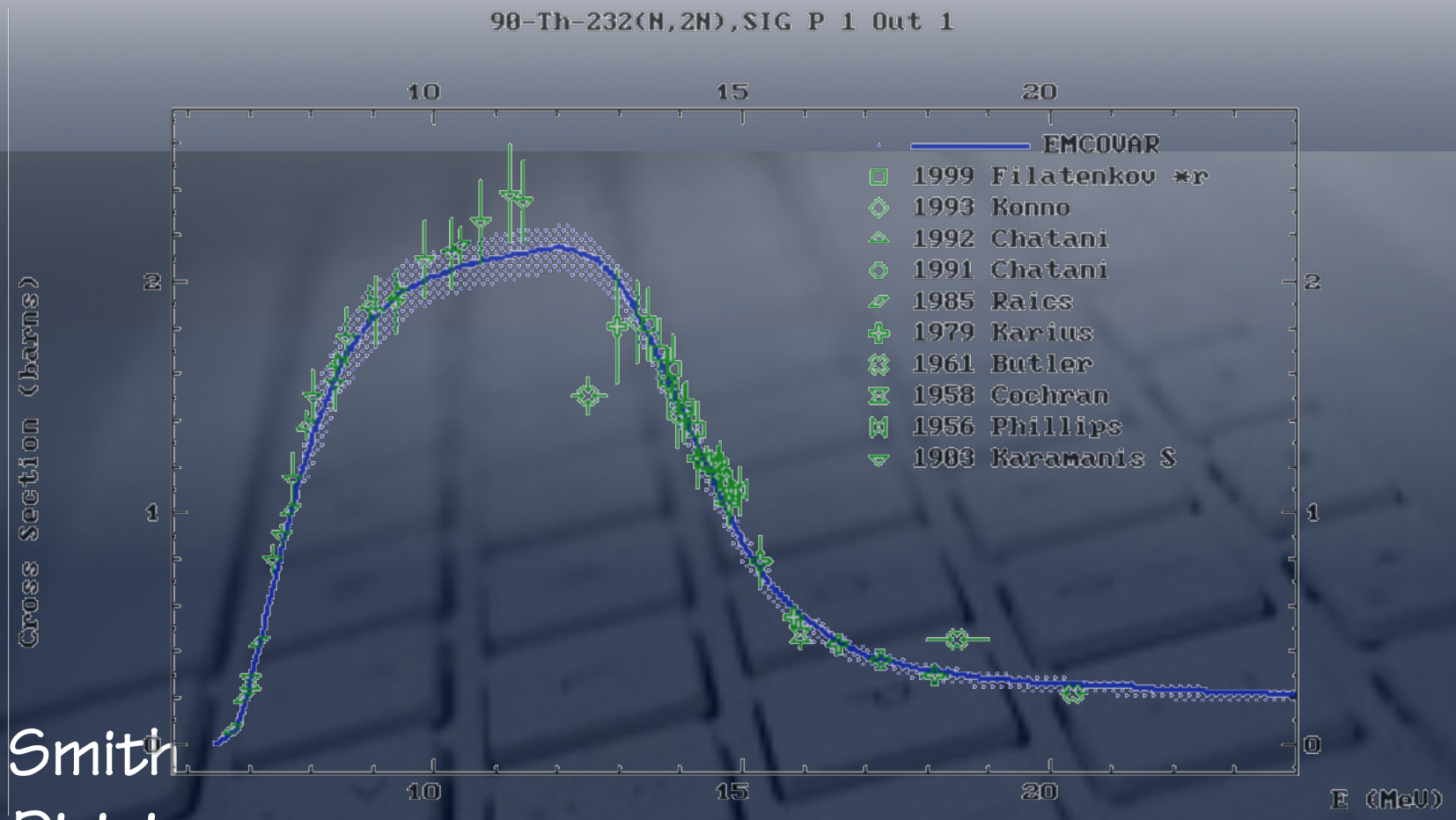
Software for USNDP



Michael Smith

Physics Division

Oak Ridge National Lab

Oak Ridge, Tennessee

Motivation

Optical Model parameters collection and tools
B. Kay, ANL

Plotting tools for nuclear structure
R. Casten, Yale

Collection of theory results and database of theory codes
A. Brown, MSU

Access XUNDL and ENSDF simultaneously
M. Carpenter, ANL

Digitizing cross sections from transfer reactions
B. Kay, ANL

GTNDSE code used to search & plot data (maintain / develop)
M. Allmond, ORNL

Tools for pre-review of manuscripts
Multiple attendees

Generate level schemes with Radware
M. Carpenter, ANL

HSCALC tool extracting band info from ENSDF (generalize)
M. Carpenter, ANL

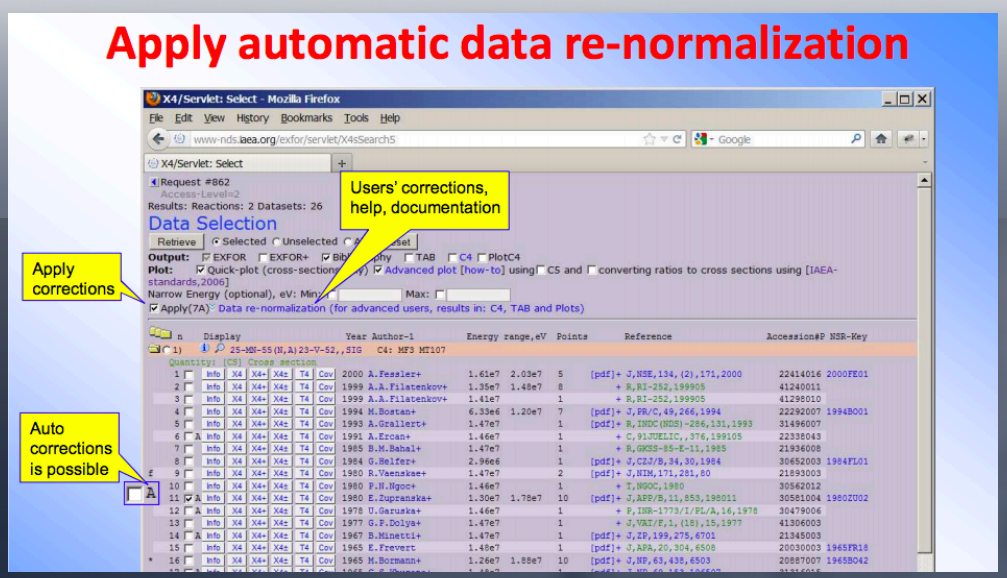
Comprehensive inventory of existing tools located in one place
Multiple attendees

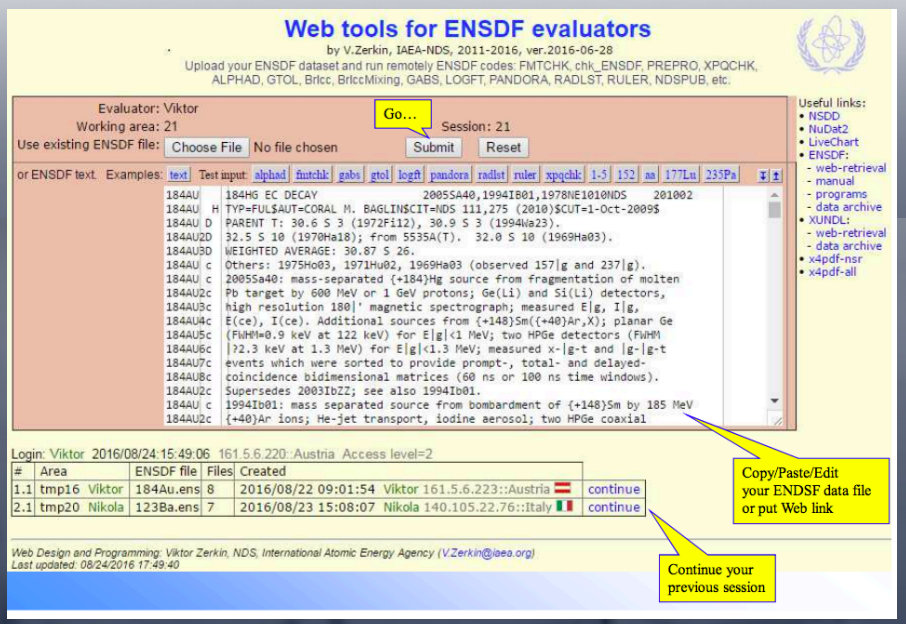
Direct access to databases for data extraction
M. Carpenter, ANL

Structure tools and codes
A. Brown, MSU

- Strong need for new software tools was repeatedly expressed by researchers at the Notre Dame Workshop
  - opportunity for researchers to more fully utilize USNDP products
  - many creative ideas, but lack expertise to implement and resources to maintain

Motivation





- Strong need for new software tools has also been requested by SOME evaluators
  - opportunity for evaluators to benefit from recent software innovations to increase productivity, accuracy, reliability …
  - some new tools are being developed (JAVA NDS)
  - IAEA has moved in this direction (MyENSDF, X4 tools …)

Categories of Software

	Visualization	Data Diving	Workflow	Executable
Access Codes	●	●		
Science Codes and Pipelines	●	●	●	●
Evaluator Tools	●	●	●	●

- Many different types of software used in nuclear science
- Matrix of code categories suggests gains from parallel development of multiple tools by reusing code components

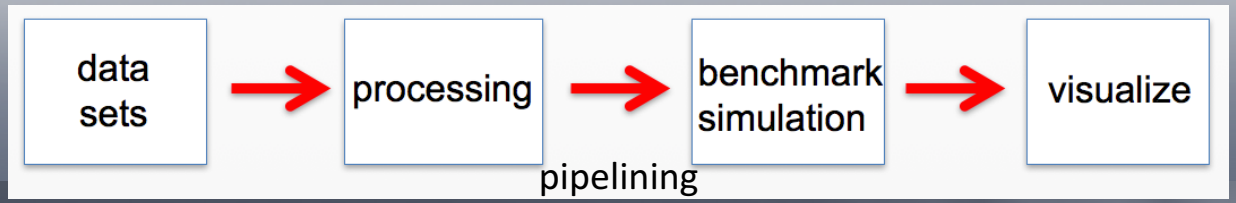
Meeting the Needs

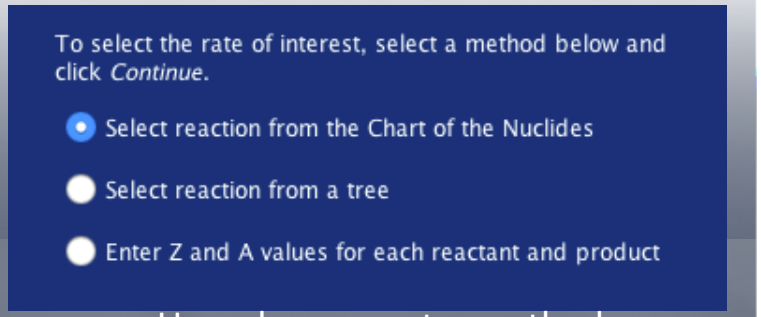
- "Software business as usual" will not meet community requests for new tools or realize possible gains in productivity, ease-of-use …
  - Software has a lower priority than evaluation work
  - Software development requires different skill set
  - Any proposal for incremental software work within the USNDP will compete for funds with evaluations
- Significant progress will require a new approach

New Data Software Project

- Suggested Key Features
  - finite performance period (such as 3 years)
  - focus on projects rated highest priority
  - realistic milestones and deliverables
  - well managed effort with project controls
  - separate funding
  - not replace / conflict with ongoing work
  - involve professional level coders advised by data experts

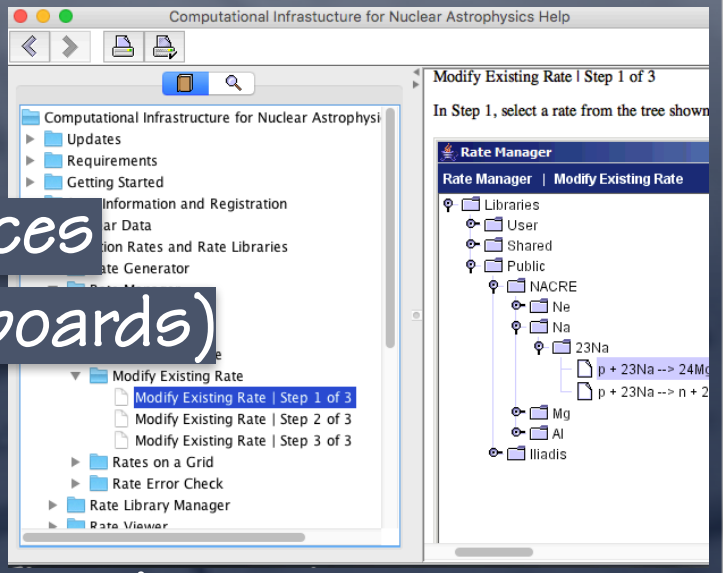
New Data Software Project





User chooses entry method

- Things to do
  - query Users for projects
  - prioritize projects
  - query Users for features / preferences
  - pay attention to interfaces (storyboards)
  - emphasize pipelining when possible
  - include heavy documentation
  - provide multiple views / paths / approaches
  - provide in-system help / guides / manuals
  - provide upgrade paths



Online help

New Data Software Project

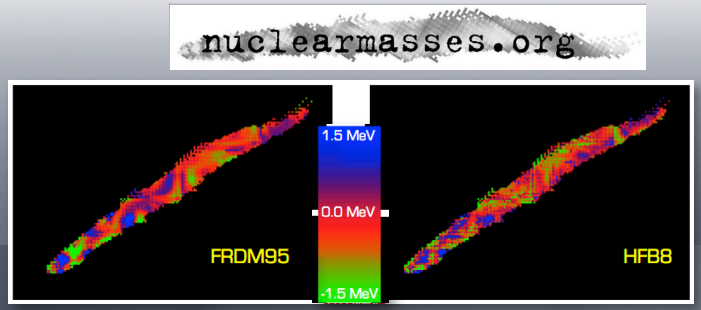
- Things to avoid … don't
  - develop tools that aren't needed
  - duplicate efforts
  - focus on new formats (too controversial)
  - work with proprietary architectures
  - assume all Users want the same features
  - keep codes proprietary

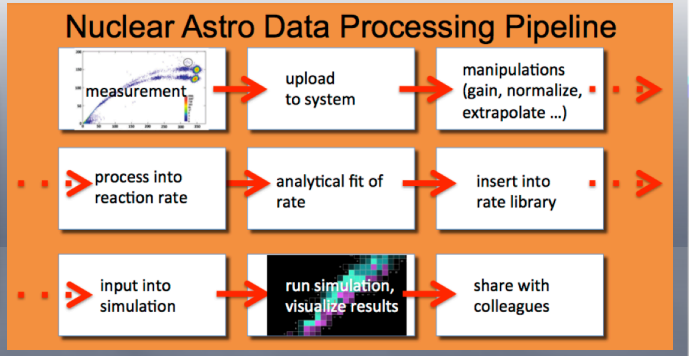
New Data Software Project

- More things to avoid … don't
  - build for a single platform
  - exclusively use old paradigms (downloads)
  - ignore cloud-based solutions
  - develop in a vacuum (ignore other products)
  - assume others will develop tools we request
  - assume that one solution will work for all

Pioneering Efforts at ORNL

nucastrodata.org

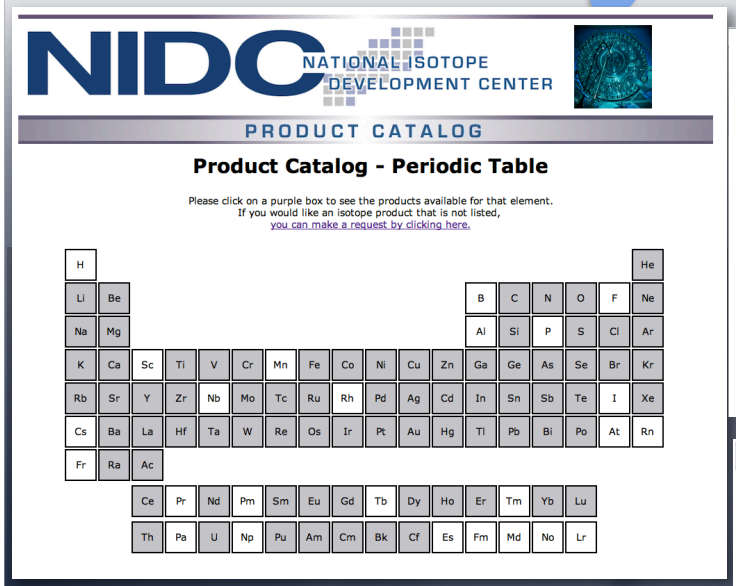




- Computational Infrastructure for Nuclear Astrophysics
  - Cloud-based solution offering unique capabilities in the field that span the range from nuclear data to reaction rates to simulations
  - Enables users to upload, manipulate, manage, visualize, share nuclear information and complex simulations
- Nuclear Mass Toolkit
  - Cloud-based solution offering unique comparisons between mass data sets from evaluations, compilations, experiments, and theory
- Big Bang Nucleosynthesis
  - Users can set up and run custom simulations of element creation in the early universe
- Cloud Computing
  - Plenary talk at ND2010 on Cloud Computing for Nuclear Data envisioned a new paradigm for data activities
  - NDC3.net established to host future work
- Bellerophon*
  - Huge expansion of CINA for supernova simulations on ORNL Supercomputers
- BEAM*
  - Expansion of Bellerophon for materials science research at ORNL, spanning desktops, clusters, supercomputers with drag-and-drop queueing and file transfers

* Led by Eric Lingerfelt

Pioneering Efforts at ORNL


NIDO NATIONAL ISOTOPE DEVELOPMENT CENTER

PRODUCT CATALOG

Product Catalog - Periodic Table

Please click on a purple box to see the products available for that element.
If you would like an isotope product that is not listed,
you can make a request by clicking here.

H																	He
Li	Be											B	C	N	O	F	Ne
Na	Mg											Al	Si	P	S	Cl	Ar
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe
Cs	Ba	La	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn
Fr	Ra	Ac															

Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu
Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr

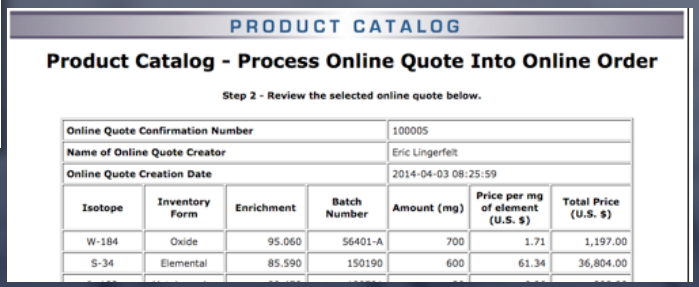

NIDO NATIONAL ISOTOPE DEVELOPMENT CENTER

PRODUCT CATALOG

Silver

Back

Isotope	Natural abundance (atom %)	Isotopic enrichment (atom %)	Request a Quote
Ag-107	51.35	>99	Request a Quote for This Ag-107 Product
Ag-109	48.65	>99	Request a Quote for This Ag-109 Product
PRODUCT FORM			
Inventory Form	metal		
Alternate Form	chloride, nitrate, acetate		

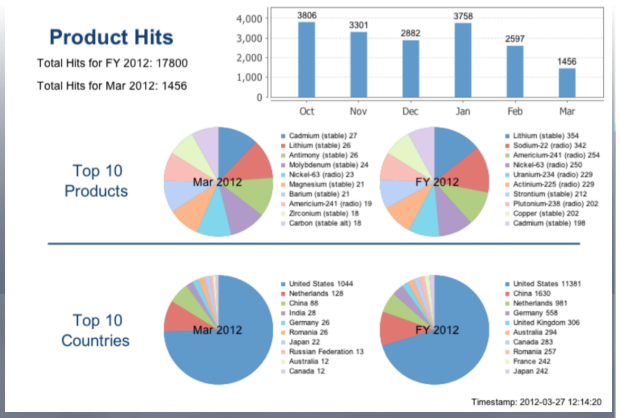

PRODUCT CATALOG

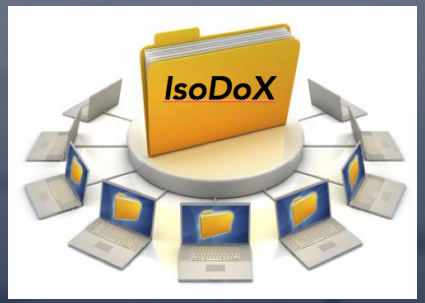
Product Catalog - Process Online Quote Into Online Order

Step 2 - Review the selected online quote below.

Online Quote Confirmation Number	100005
Name of Online Quote Creator	Eric Lingerfelt
Online Quote Creation Date	2014-04-03 08:25:59

Isotope	Inventory Form	Enrichment	Batch Number	Amount (mg)	Price per mg of element (U.S. $)	Total Price (U.S. $)
W-184	Oxide	95.060	56401-A	700	1.71	1,197.00
S-34	Elemental	85.590	150190	600	61.34	36,804.00





- Isotopes.gov
  - Modernized DOE's isotope program IT infrastructure
  - Cloud solution features catalog with multiple entry methods, ordering, preferred customers "one click" ordering features, top-notch security, tool kit and interface custom designed for Isotope Business Office, custom permissions, associated expansive website …
  - Time-saving "snapshots" of data activities can do a weeks work with a few clicks … duplicates functions of excel, powerpoint, pdf exports
  - Done as separate DOE Project with milestones & project controls

Path Forward

- identify sponsors
- gather interested parties
- discuss possible projects
- solicit project suggestions from community
- prioritize projects
- write and submit proposal