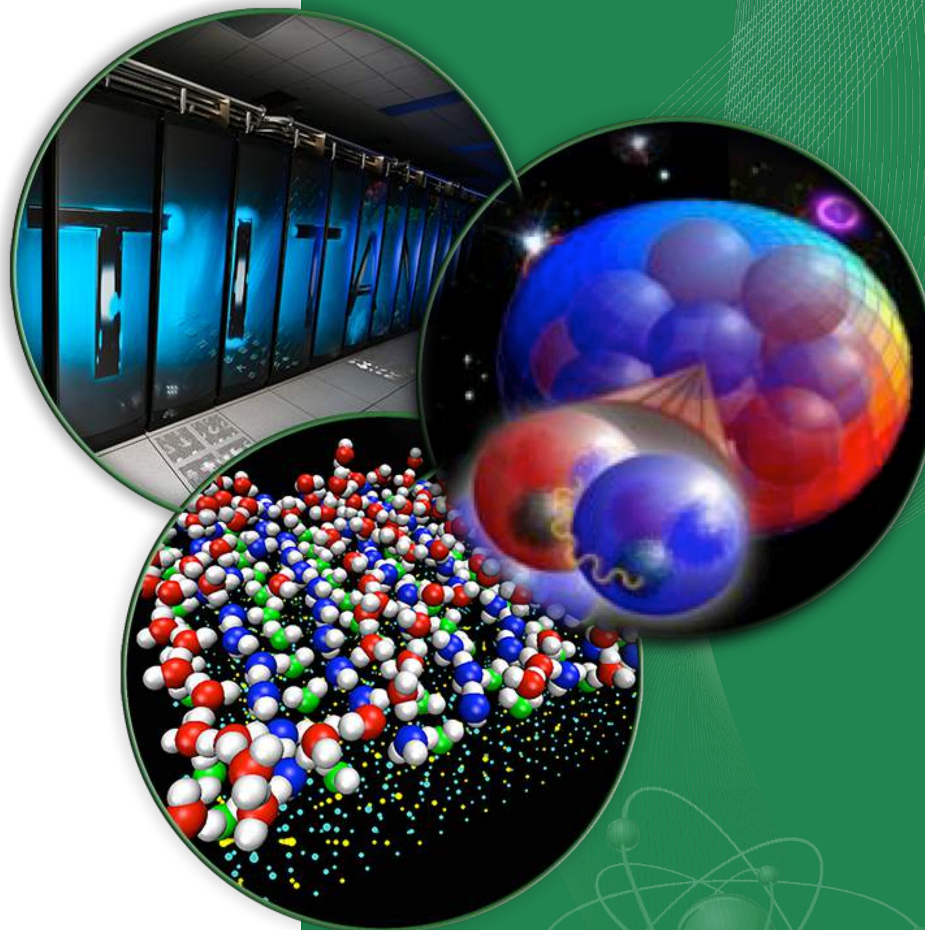
Nuclear Data, Nuclear Theory, and Isotopes

May 28-30, 2015



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Outline

- A brief assessment of nuclear reaction data: errors matter
- ORNL Isotope Program: applications matter

A brief assessment of nuclear reaction data: errors matter

Nuclear data mission and standards

The mission of the United States Nuclear Data Program (USNDP) is to provide current, accurate, authoritative data for workers in pure and applied areas of nuclear science and engineering. This is accomplished primarily through the compilation, evaluation, dissemination, and archiving of extensive nuclear datasets. The USNDP also addresses gaps in the data, through targeted experimental studies and the use of theoretical models.

Begs the question: just how good are the models?

Worldwide network of nuclear data centers:

- Collect nuclear data (experiment and theory)
- Evaluate the quality
- Make the data available in the appropriate form for the user

Data libraries and codes based on models maintained by Centers: IAEA, NNDC,…
Codes and Libraries: TALYS, ENDF, JENDL…

Future requirements:
Uncertainty and reliability measures of the evaluated data, *particularly models/theory*

How do you know what you know?

PHYSICAL REVIEW A **83**, 040001 (2011)

Editorial: Uncertainty Estimates

The purpose of this Editorial is to discuss the importance of including uncertainty estimates in papers involving theoretical calculations of physical quantities.

It is not unusual for manuscripts on theoretical work to be submitted without uncertainty estimates for numerical results. In contrast, papers presenting the results of laboratory measurements would usually not be considered acceptable for publication in *Physical Review A* without a detailed discussion of the uncertainties involved in the measurements. For example, a graphical presentation of data is always accompanied by error bars for the data points. The determination of these error bars is often the most difficult part of the measurement. Without them, it is impossible to tell whether or not bumps and irregularities in the data are real physical effects, or artifacts of the measurement. Even papers reporting the observation of entirely new phenomena need to contain enough information to convince the reader that the effect being reported is real. The standards become much more rigorous for papers claiming high accuracy.

The question is to what extent can the same high standards be applied to papers reporting the results of theoretical calculations. It is all too often the case that the numerical results are presented without uncertainty estimates. Authors sometimes say that it is difficult to arrive at error estimates. Should this be considered an adequate reason for omitting them? In order to answer this question, we need to consider the goals and objectives of the theoretical (or computational) work being done. Theoretical papers can be broadly classified as follows:

1. Development of new theoretical techniques or formalisms.
2. Development of approximation methods, where the comparison with experiment, or other theory, itself provides an assessment of the error in the method of calculation.
3. Explanation of previously unexplained phenomena, where a semiquantitative agreement with experiment is already significant.
4. Proposals for new experimental arrangements or configurations, such as optical lattices.
5. Quantitative comparisons with experiment for the purpose of (a) verifying that all significant physical effects have been taken into account, and/or (b) interpolating or extrapolating known experimental data.
6. Provision of benchmark results intended as reference data or standards of comparison with other less accurate methods.

It is primarily papers in the last two categories that require a careful assessment of the theoretical uncertainties. The uncertainties can arise from two sources: (a) the degree to which the numerical results accurately represent the predictions of an underlying theoretical formalism, for example, convergence with the size of a basis set, or the step size in a numerical integration, and (b) physical effects not included in the calculation from the beginning, such as electron correlation and relativistic corrections. It is of course never possible to state precisely what the error is without in fact doing a larger calculation and obtaining the higher accuracy. However, the same is true for the uncertainties in experimental data. The aim is to estimate the uncertainty, not to state the exact amount of the error or provide a rigorous bound.

There are many cases where it is indeed not practical to give a meaningful error estimate for a theoretical calculation; for example, in scattering processes involving complex systems. The comparison with experiment itself provides a test of our theoretical understanding. However, there is a broad class of papers where estimates of theoretical uncertainties can and should be made. Papers presenting the results of theoretical calculations are expected to include uncertainty estimates for the calculations whenever practicable, and especially under the following circumstances:

1. If the authors claim high accuracy, or improvements on the accuracy of previous work.
2. If the primary motivation for the paper is to make comparisons with present or future high precision experimental measurements.
3. If the primary motivation is to provide interpolations or extrapolations of known experimental measurements.

These guidelines have been used on a case-by-case basis for the past two years. Authors have adapted well to this, resulting in papers of greater interest and significance for our readers.

The Editors

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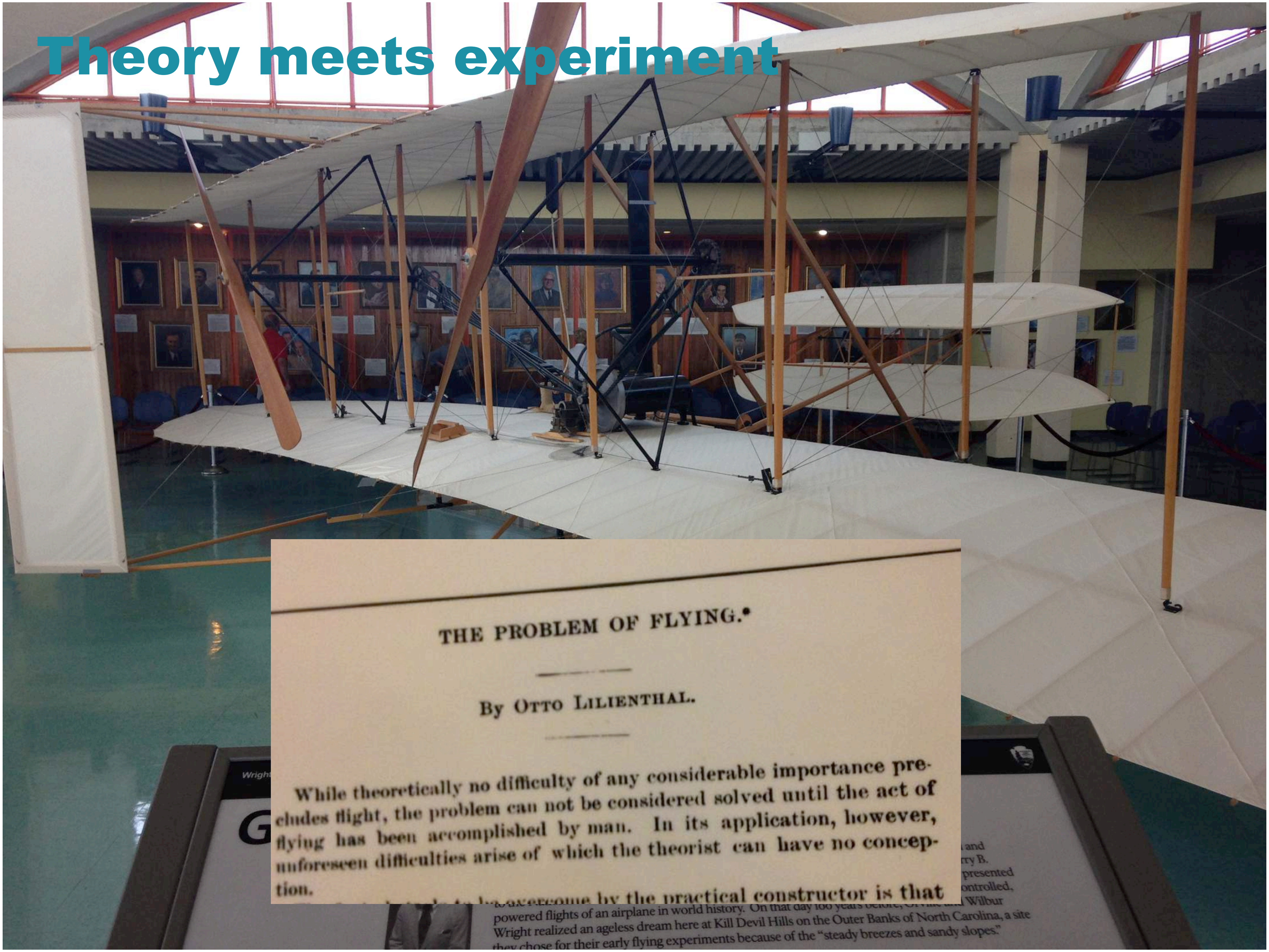
‘It is not unusual for manuscripts on theoretical work to be submitted without uncertainty estimates for numerical results’

‘Papers presenting the results of theoretical calculations are expected to include uncertainty estimates for the calculations whenever practicable.’

- Claim of high accuracy
- Comparison with high precision experimental measurements
- Interpolation or extrapolation of known experimental measurements

Phys. Rev. A 83, 040001 (2011)
(atomic, molecular, optical physics)

Theory meets experiment



THE PROBLEM OF FLYING.*

By OTTO LILIENTHAL.

While theoretically no difficulty of any considerable importance precludes flight, the problem can not be considered solved until the act of flying has been accomplished by man. In its application, however, unforeseen difficulties arise of which the theorist can have no conception.

... be overcome by the practical constructor is that

Model (theory) inputs to the reaction problem….

from TALYS – Calculational Scheme

Loop possible over
- incident energies
- Natural isotopes

Input:
projectile p
element Fe
size 16
energy 22

Optical Model:
- Phenomenology
  local/global

Direct Reaction:
- Spherical Optical model
- DWBA
- Rotational CC
- Giant Resonances
- Vibrational CC
- Weak coupling

Pre-equilibrium:
- Exciton model
  1+2 component
- p-h LD phenom.
  surface effects
- Kalbach systematics
  - angular distributions
  - cluster emission
  - surface effects
- γ-ray emission

Nucl. Structure
- Abundances
- Discrete levels
- Deformations
- Masses
- Level density par.
- Resonance par.
- Fission barrier par.
- Thermal XS
- Microscopic LD
- Pre-scission shapes

Compound:
- Width fluctuations
  - Moldauer
  - GOE trip. Int.
  - HRTW
- Hauser-Feshbach
- Fission competition
  -- Isotopic Yields
- γ-ray emission
- GC+ Ignatyuk

Multiple emission:
- Exciton (any order)
- Hauser-Feshbach
- Fission competition
- All flux depleted
- γ-ray cascade
- Exclusive channels
- Recoils

Output:
- File containing
  useful output.

ENDF:
- transport libs.
- activation libs.

Talys User Manual, 2013

The physics problem challenge

$$H\left|\Psi\right\rangle = E\left|\Psi\right\rangle$$

$$i\partial_t\left|\Psi\right\rangle = H\left|\Psi\right\rangle$$

Deceptively simple

Some of the difficulties

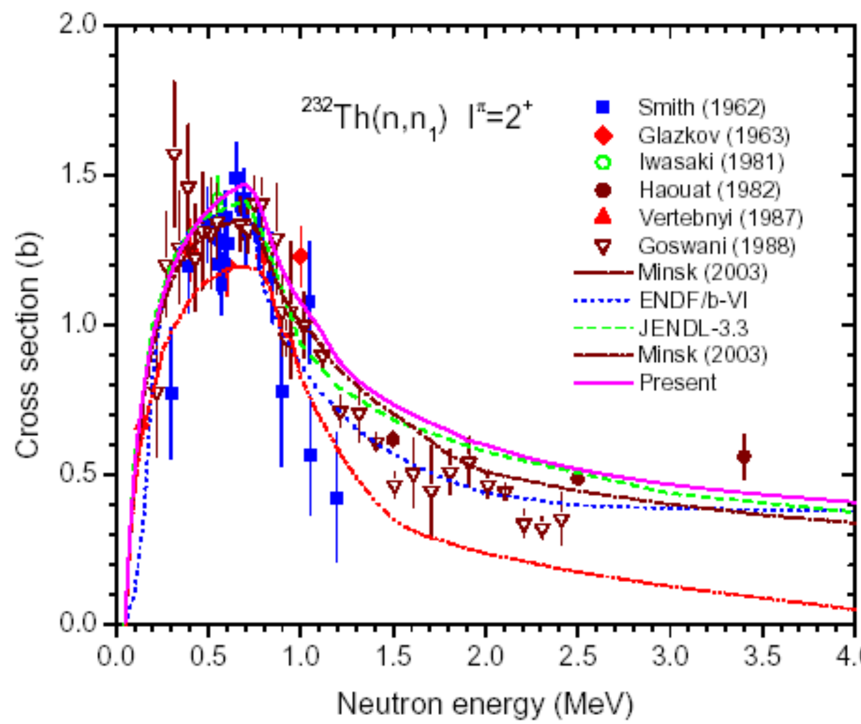
- 2N+3N interaction approaches
  - Precision of V (even the most modern)
- Density Functional Theory
  - Precision of Energy Density Functional
  - Coupling of DFT to reaction theory
- Coupling of bound-state problem to continuum problem
- Non equilibrium emission
- Non statistical decay modes
- What is the appropriate optical model?

How do these problems manifest in data compilations?

- Theory progress made through
  - Topical collaborations (TORUS)
  - SciDAC (NUCLEI)
  - Individual investigators
  - NNSA campaigns
- Experimental progress
  - Data on specific nuclei of interest to both theory and experiment (A-chains, neutron rich)
- Theory and experiment
  - Targeted joint programs addressing particular nuclei (e.g., surrogate reactions)
  - Reactor neutrino anomaly (KR)

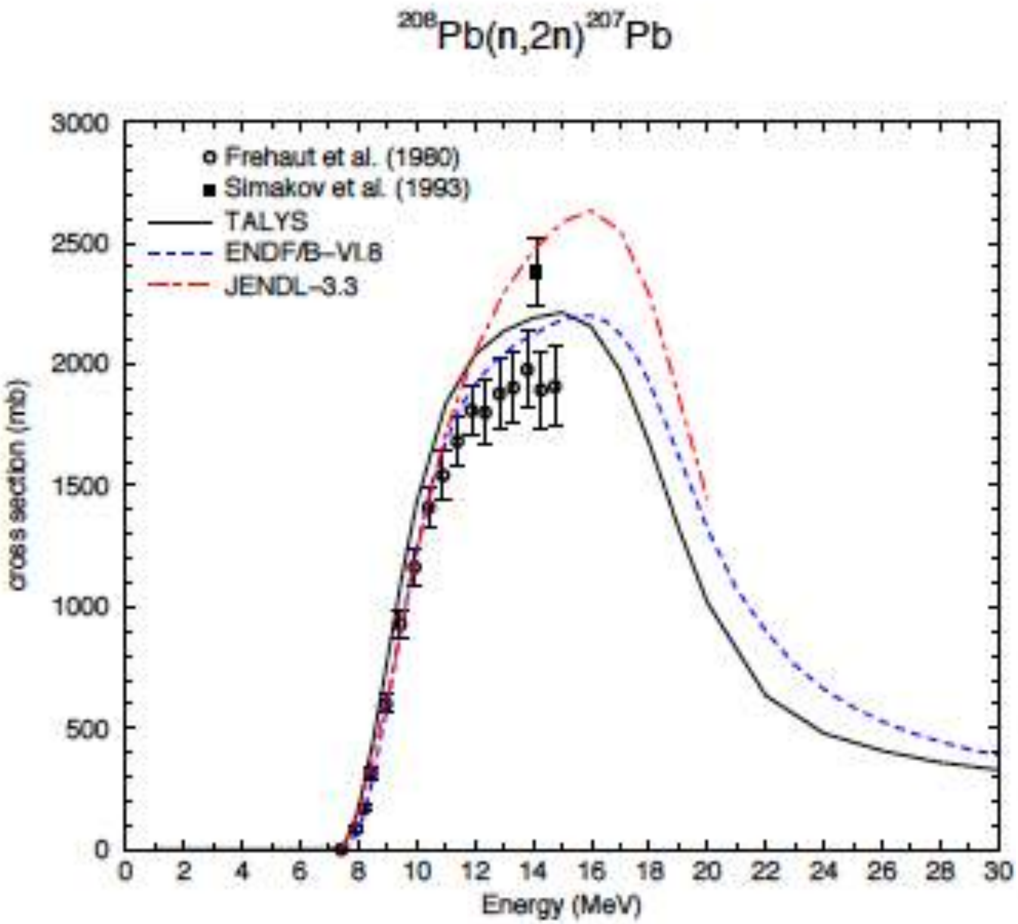
Theory and experiment…

- Incomplete experiments points to a need for
  - Nuclear theory with higher predictive power
  - Reliable estimates of the quality of the nuclear theory
  - Realistic margins for calculated observables
- Reason for improved theory:
  - Significant increase in open channels in heavy nuclei
  - Limited number of validation experiments exist
- Reason for improved experiments
  - Constrain the theory



Ignatyuk et al., ATI-NDC 2005-01

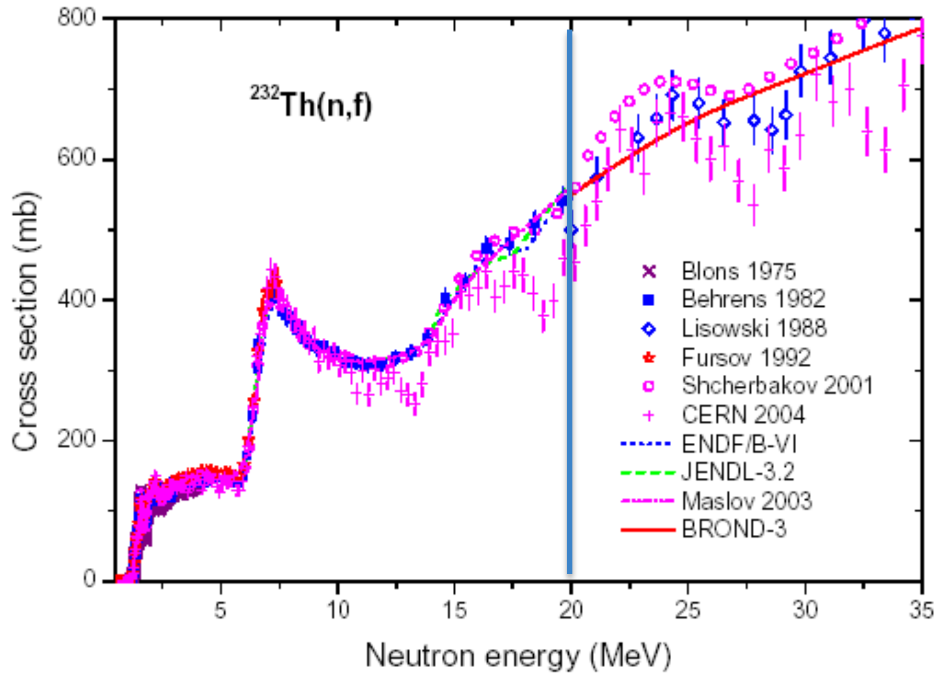
What does a comparison of data codes indiate?



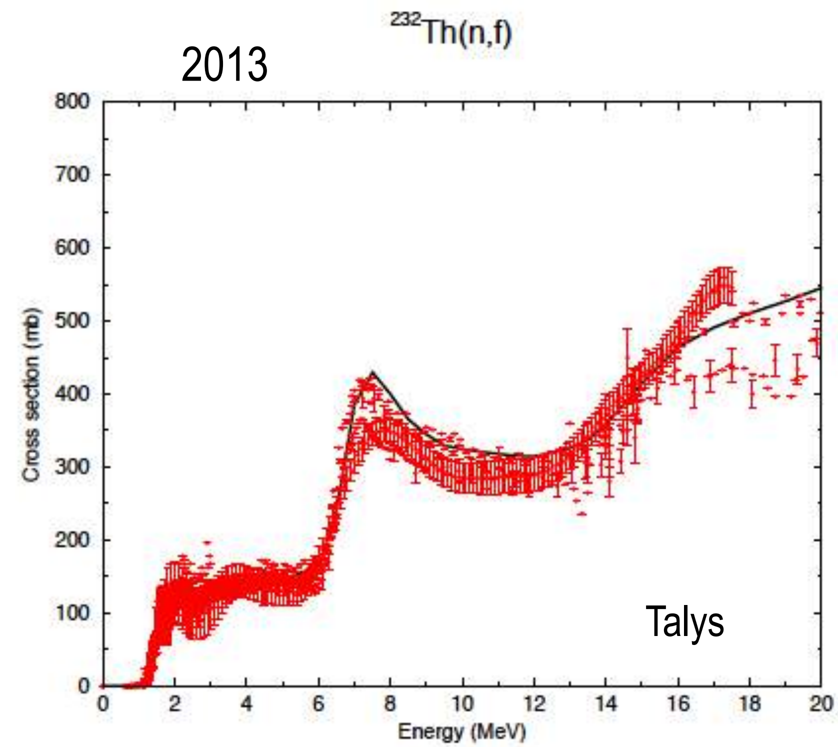
Today: compare three data compilations and conclude that the error is +/-500 mb at 16 MeV
In the future: enhance capability by adding theoretical error estimates

Has there been progress in time?

2005



2013



It is not so clear…

Medium energy example

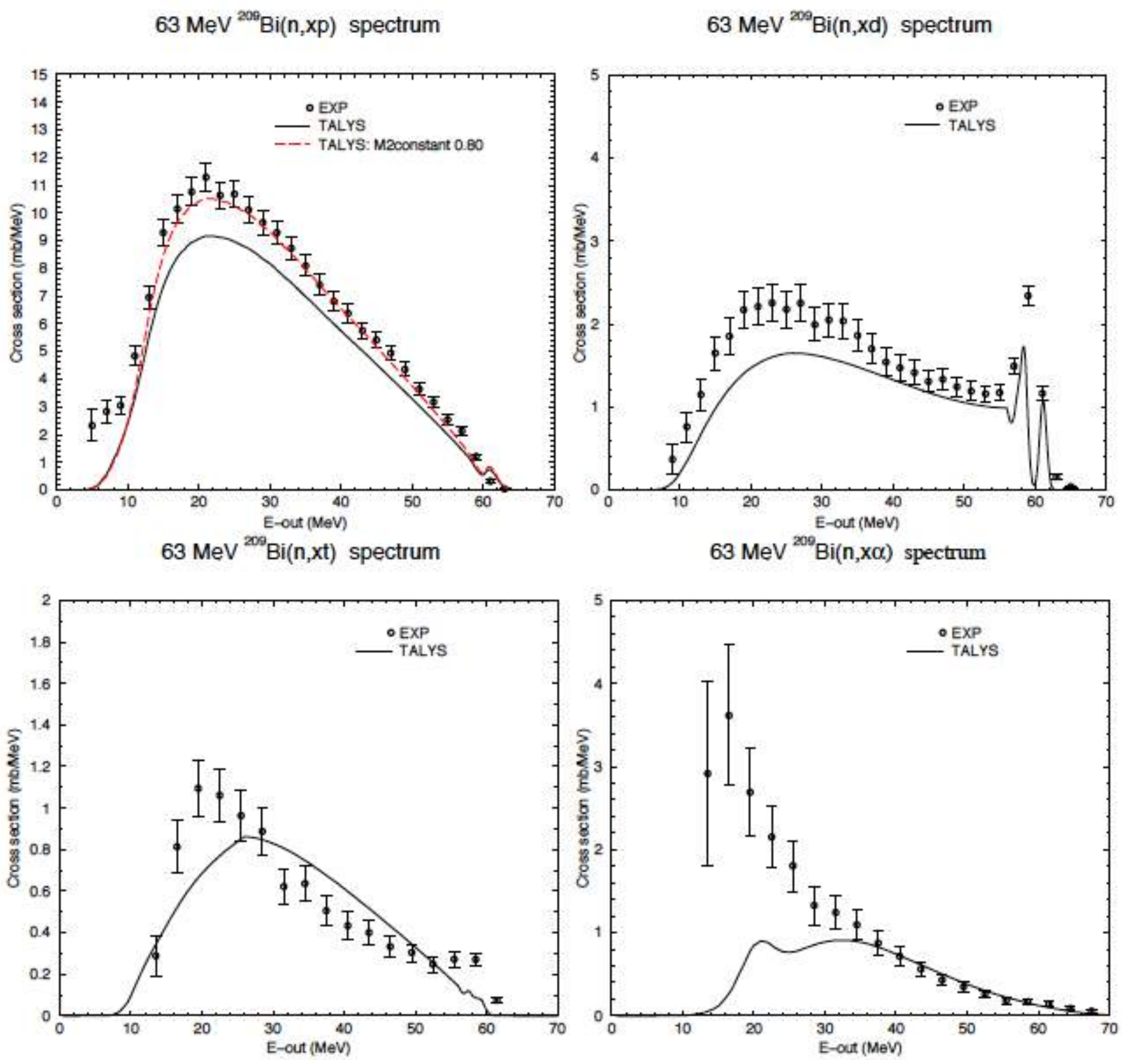


Figure 7.6: Angle-integrated proton, deuteron, triton and alpha emission spectra for 63 MeV neutrons on ^{209}Bi. The experimental data are from [417].

- One can change parameters to fit data; but what has one learned?
- Models obtain overall physics, but lack some details
- Error bars of the experimental data can be fairly large

Sources of model error

- Contributions to the error budget of a given model

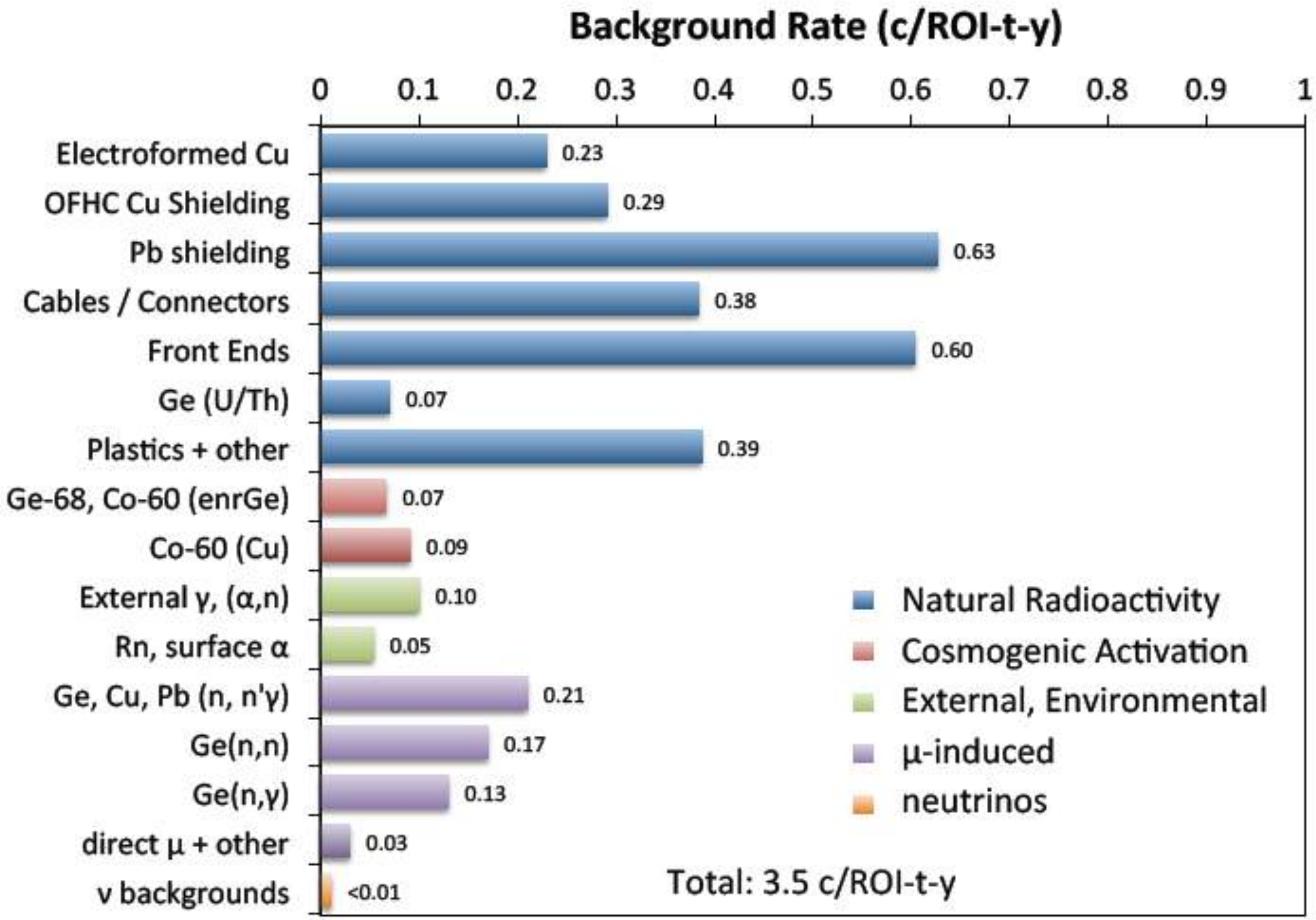
$$M^{(mod)} = M^{(par)} + M^{(num)} + M^{(def)}$$

Parameter Uncertainty	Numerical Uncertainty	Model Deficiency
• Statistically well defined • Can be taken into account in a KALMAN code system	• Numerical implementation error • Non-stastical error, usually well known, but usually small	• Non-statistical error • Strongly related to the predictive power of the model • Problem of quantitative estimation

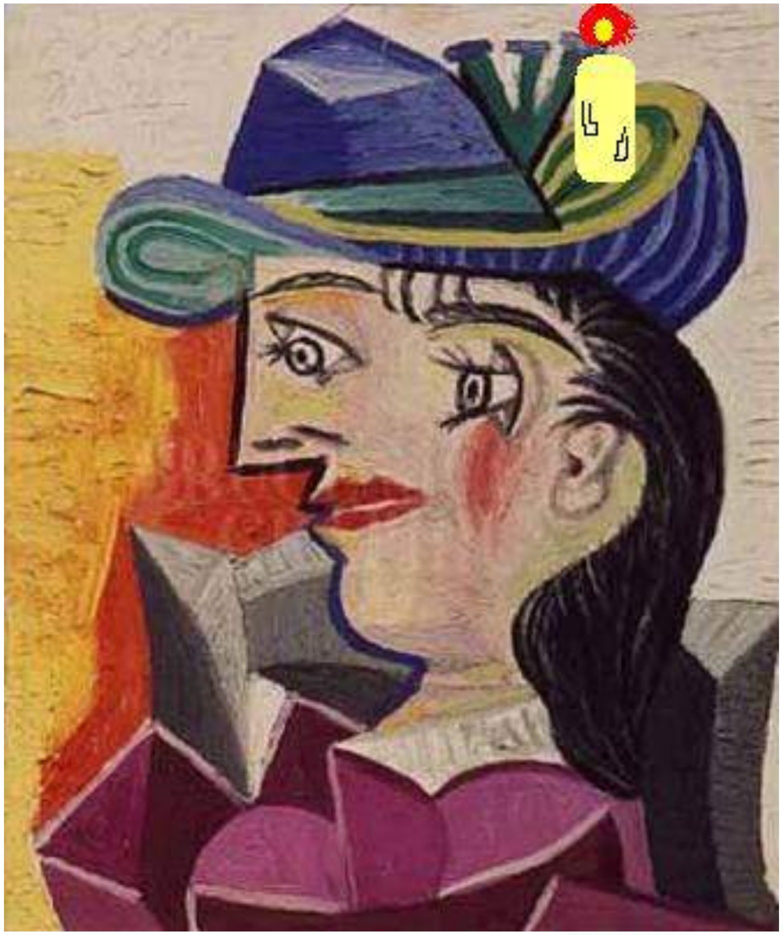
Error analysis that takes into account all three error sources could point to important measurements that would improve models and nuclear data applications

Nuclear data for nuclear physics example

Majorana Demonstrator background budget. Note neutron reactions in purple

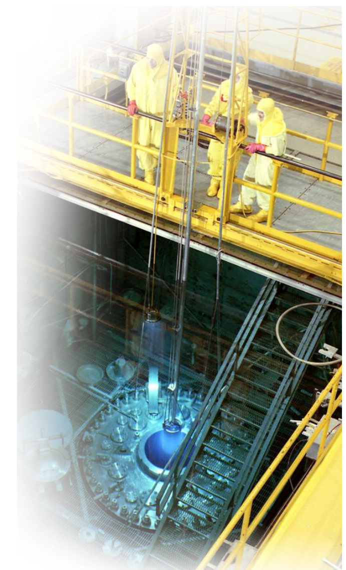


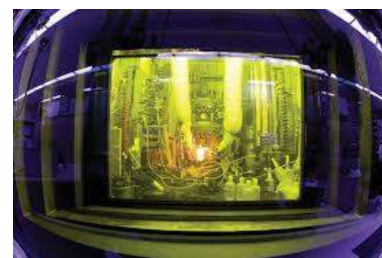
How much fidelity does one need?

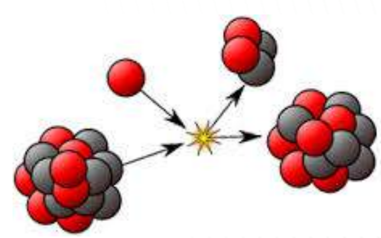


ORNL Isotope Program: Applications matter

How to make isotopes



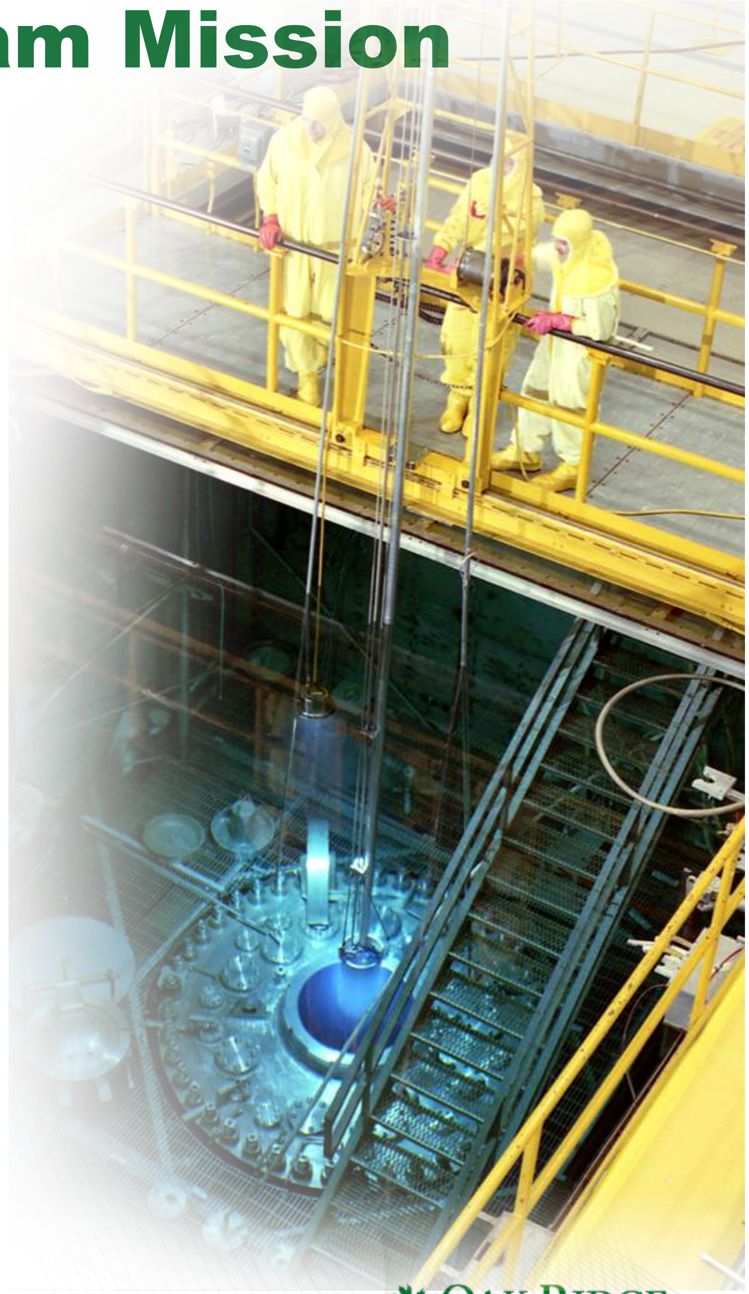




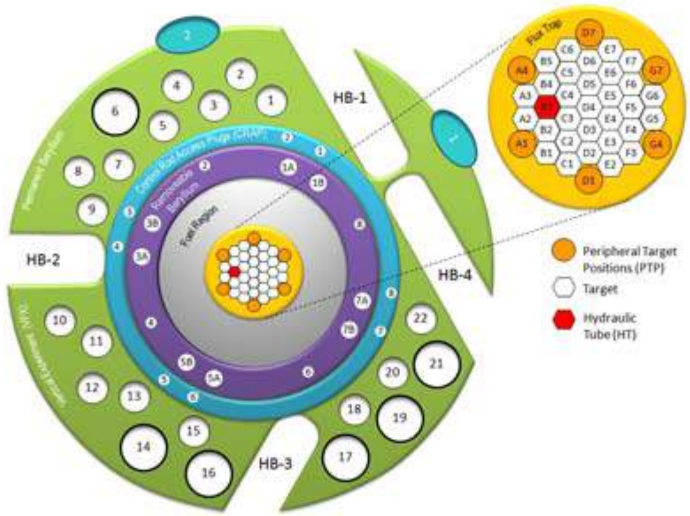
- Blow things up (not a good idea)
- Irradiate existing isotopes
  - Neutron capture in a reactor (ORNL, INL, MURR)
  - Proton or light-ion reactions in an accelerator (LANL, BNL)
- Chemical separations (nuclear chemistry)
  - Almost every production method relies on chemical separations
  - Harvest isotopes from Cold War surplus material
- Mechanical separations
  - Stable isotope production with electromagnetic or centrifuge technology (or diffusion)
- Import (Russian)
  - But…

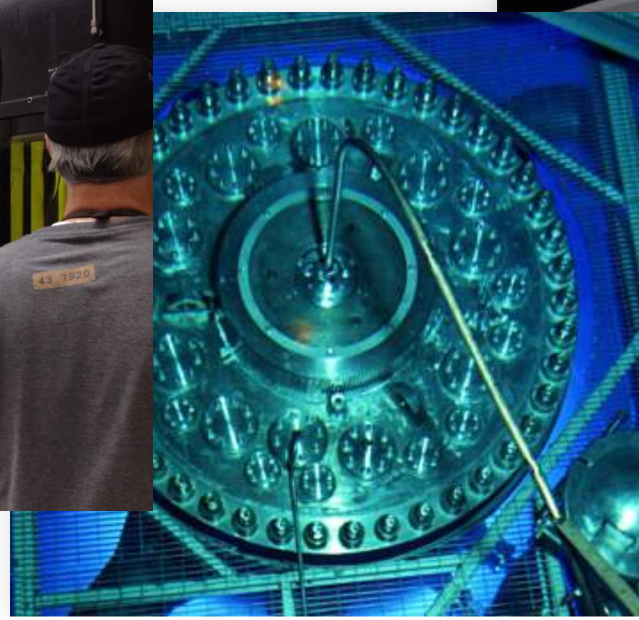
The ORNL Isotope Program Mission

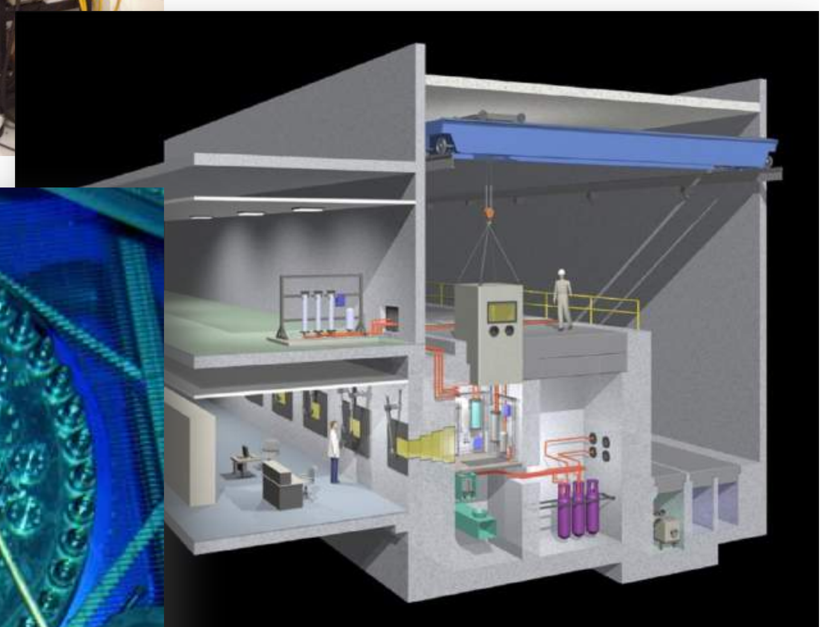
"We utilize the unique resources at ORNL to meet DOE needs for isotope products and services which are beyond the means of commercial enterprise"



ORNL Physical Assets



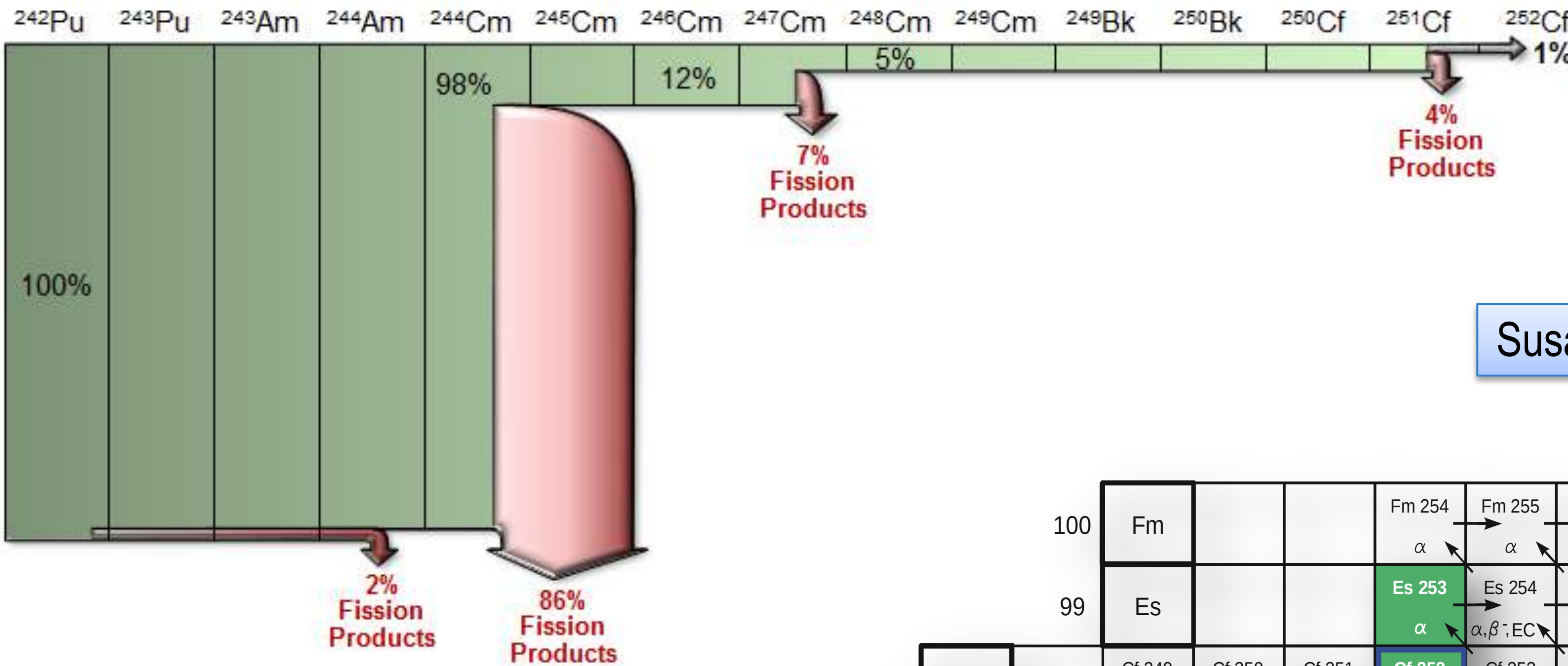




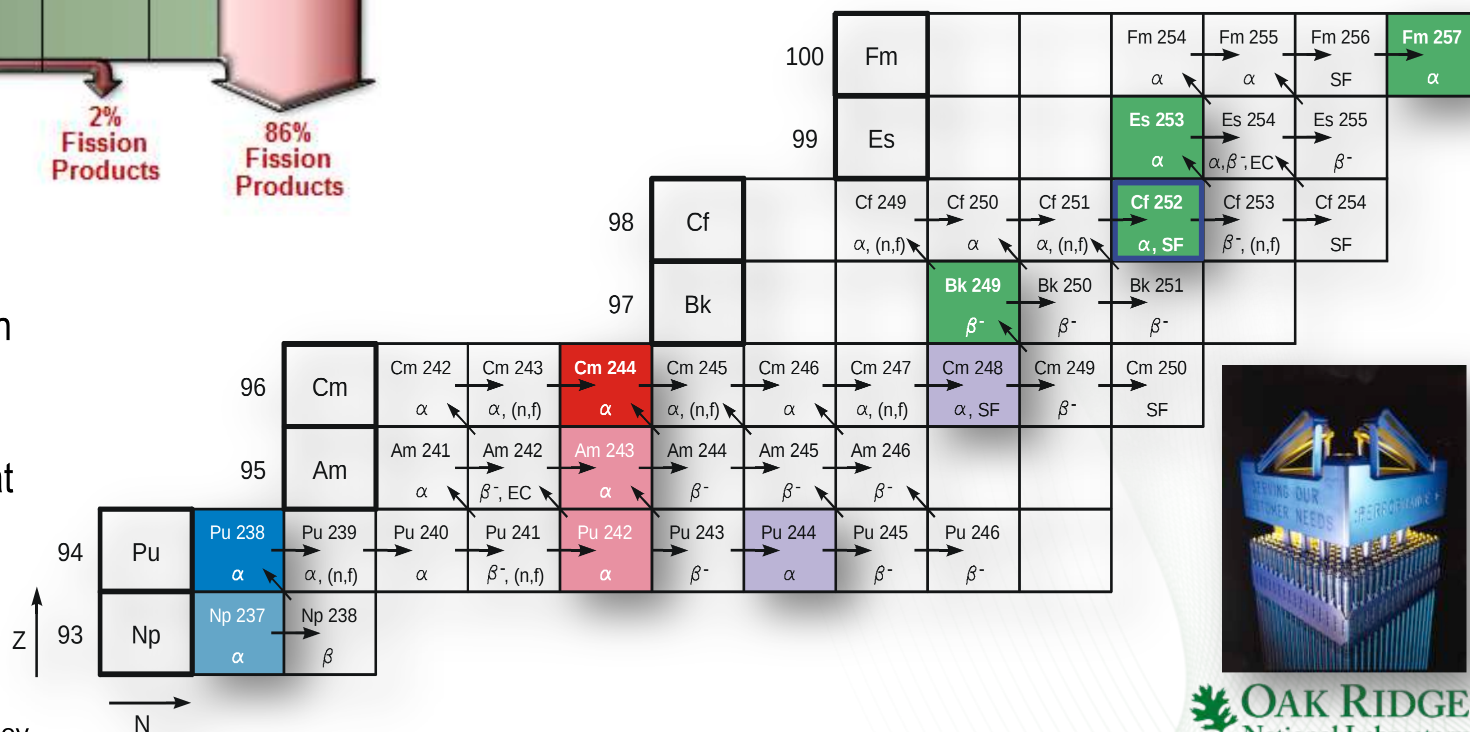
Radioisotope Production at ORNL

- ^{252}Cf
- ^{63}Ni
- ^{75}Se
- ^{225}Ac
- ^{227}Ac
- ^{212}Pb
- ^{188}W

Example: Cf-252, many industrial apps



Susan Hogel



- Feedstock (heavy curium) in place for 15+ years
- DOE produces at ORNL for a consortium
- Variety of uses

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^{252}Cf Uses

Energy	Industrial	Security
• Nuclear fuel quality control • Reactor start-up sources • Coal analyzers • Oil exploration	• Mineral analyzers • Cement analyzers • FHA measurements for corrosion (bridges, highway infrastructure)	• Handheld contraband detectors (CINDI) • Standard for all neutron fission measurements • Monitoring downblending of HEU • Identifying unexploded chemical ordnance and detecting land mines

^{63}Ni Production

Irradiation | **Radiochemistry** | **Application**

Enriched Ni-62 target material from enriched stable isotope inventory

Ni-62 targets irradiated for 2 years in HFIR to produce high specific activity Ni-63

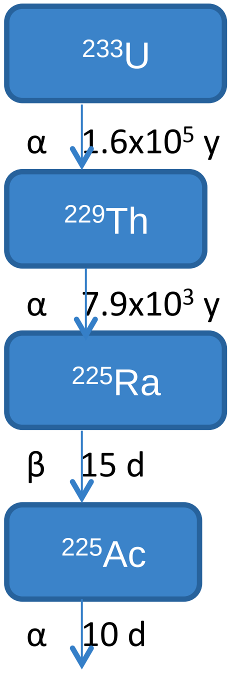
Targets processed at Radiochemical Engineering Development Center to produce purified Ni-63

Purified Ni-63 chloride

Explosives and narcotics detectors based on electron capture technology for airports and other sensitive locations

- Contract in place through 2018; Total of 800 Ci (150 Ci/yr average)
- ^{63}Ni chloride salt currently being dispensed from Building 4501 (recently moved from REDC)
- Second target using a new design based on our Se target will be processed in 2016
  - Allows easier removal of pellets

^{225}Ac Production



- Current Program
  - Production based on milking a ^{229}Th cow derived from ^{233}U
  - Producing about 700 mCi/yr

- Accelerator production in research phase
- Irradiation at LANL and BNL, ^{232}Th(p,x)^{225}Ac spallation
- Separation at ORNL
  - Product shipped for evaluation

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The DOE Isotope Program today

Continues to provide stable and radio isotopes in short supply

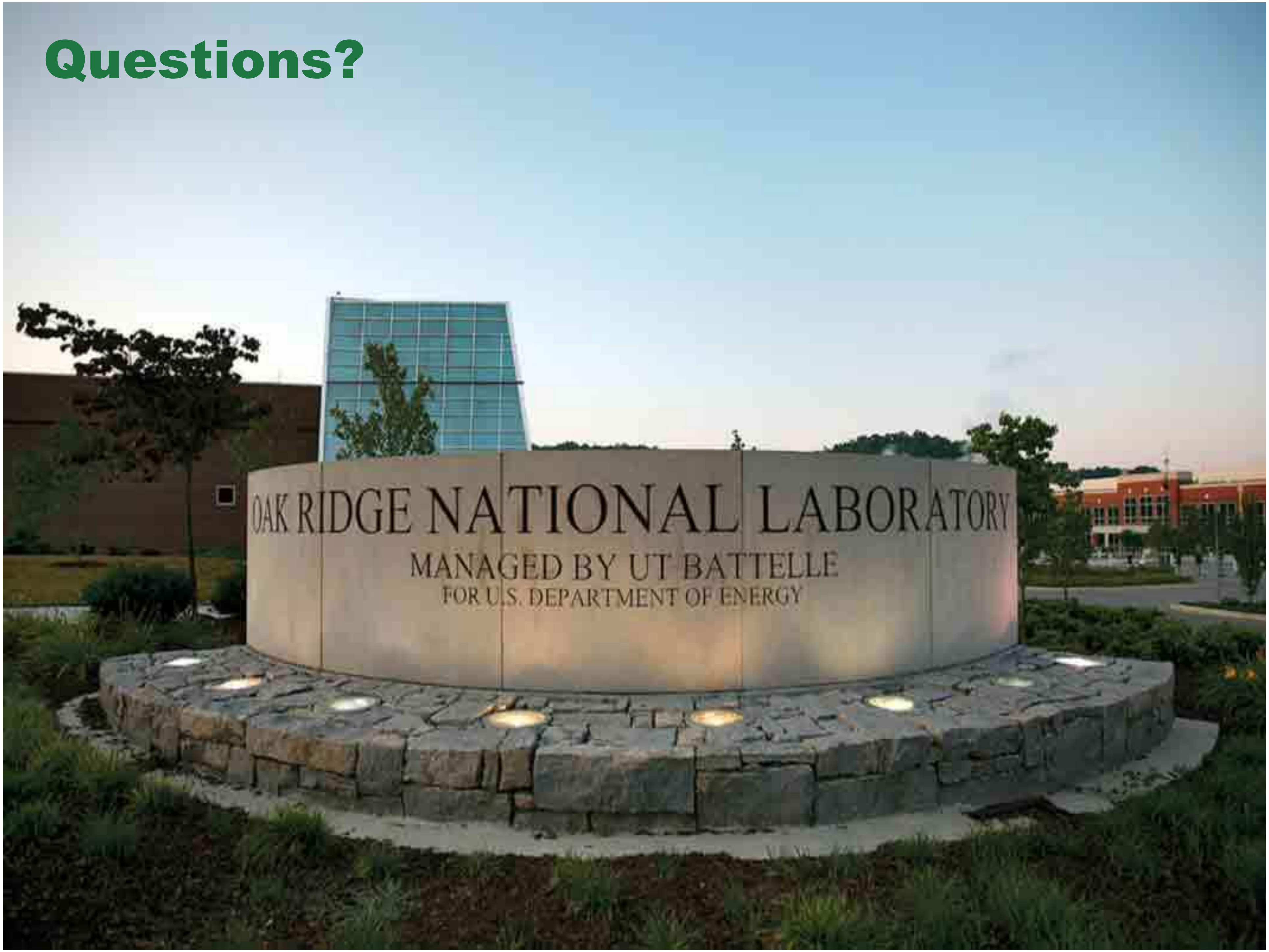
Some key isotopes and radioisotopes and the companies that use them

Strontium-82, Rubidium-82	Imaging / Diagnostic cardiology
Germanium-68, Gallium-68	Calibration / PET scan imaging
Californium-252	Oil and gas exploration and manufacturingcontrols
Selenium-75	Radiography / Quality control
Actinium-225, Yttrium-90, Rhenium 188	Cancer / Infectious disease treatment
Nickel-63	Explosives detection at airports
Gadolinium-160, Neodymium-160	Tracers and contrast agents for biological agents
Iron-57, Barium-135	Standard sources for mass spectroscopy
Sulfur-34	Environmental monitoring
Rubidium-87	Atomic frequency / GPS applications
Lithium-6, Helium-3	Detection of Special Nuclear Materials
Samarium-154	Solar energy /transportation applications

Conclusions

- For isotope production, much more going on than just cross sections
  - Medical Isotopes: FDA approval, chemical purity, toxicity
  - Appropriate assay
  - Requires a robust radio chemical effort
- Precise data can lead to a better physics understanding
  - Decay heat for neutrino reactor anomaly
  - Quantification of background in 0nubb decay efforts
- No dedicated facility for this purpose
  - Data proposals do not compete well with discovery proposals on PACs
  - Need for a dedicated facility should be demonstrated
- Identifying ‘needed’ data requires a stronger coupling between applied R&D and the ND program
- Data codes need to include error estimates

Questions?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