Highlights of Low Energy Hadronic Physics

L.G. Sarmiento, Lund University, Sweden
with borrowed slides from various collaborators

21th Geant4 collaboration meeting
September 2016

Notes and Summaries from the Geant4 Radioactive Decay Mini-workshop

Dennis Wright
28 March 2016

Summaries from Talks

- Database Improvements (talk by L. Desorgher)
  - levels in RadioactiveDecay4.3.1, PhotoEvaporation3.2.1 and ENSDFSTATE1.1 now consistent
  - some corrections for Geant4 10.2. p01
  - Q values now taken directly from Qcalc
  - PhotonEvaporation db now has easy-to-read format
  - corrected use of BRICC to compute internal conversion coefficients

Summaries from Talks

- RDM tests (L. Desorgher)
  - single decay of different nuclei from example rdecay02 (gamma, x-rays, electrons from ^{214}Bi, alphas from ^{238}U,
  - generally good comparison to data
  - in biased mode, looked at activity in bunker walls from 45 MeV electrons (very good agreement)
  - example rdecay02: ^{137}Cs, ^{99}Mo, ^{226}Ra => generally good agreement (see plots)

Notes from Discussions

- Dealing with floating levels
  - how do we handle transitions which are
    - floating to fixed
    - fixed to floating
  - check to see if any floating levels can be made fixed by evaluating existing data
  - when any change made, document in data file header
    - also any data coming from other than ENSDF (e.g. Nuclear Wallet Cards) should be documented in header
  - user should be able to configure data reader to set X, Y, and Z
  - nuclides with X, Y, Z etc. levels should be trackable objects, unique from nuclides with fixed level

Notes from Discussions

- Atomic de-excitation
  - current model is approximate and does not handle pick-up or loss of electrons into outer shells (e.g. for alpha, beta decay)
    - results in energy non-conservation
  - RDM currently uses G4UAtomicDeexcitation
    - should use G4VAtomicDeexcitation
  - detailed model of Tibor Kibedi is available as a possible replacement
  - currently local energy deposit is not done
    - implementing this may help a bit with energy non-conservation

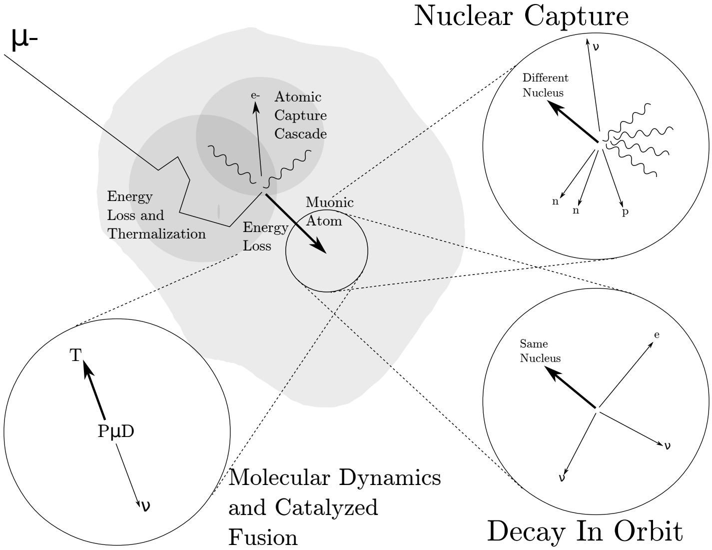
A proposal for improving muon capture in Geant4

Kevin Lynch

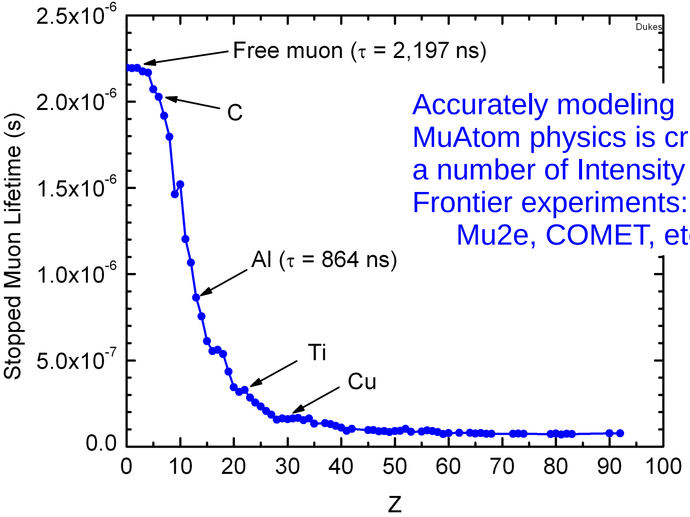
20th Geant4 Collaboration Meeting
Fermilab
September 27-October 2, 2015

YORK College
THE CITY UNIVERSITY OF NEW YORK

The atomic, nuclear, and particle physics of the μ^- in matter is quite varied



MuAtom physics varies widely with *Z*



Accurately modeling MuAtom physics is critical to a number of Intensity Frontier experiments:
Mu2e, COMET, etc

Muon Capture [update]

Kevin Lynch (CUNY) and Krzysztof Genser (Fermilab)

Working on an alternative code to G4MuonMinusCapture process
Making the muonic atom a new particle type which is

- Transportable
- Allows to special case the light atoms/molecules naturally factorizing the process model
- Separating atomic cascade, capture, and decay in orbit physics into separate processes that can be customized on a per species
- This should also allow radiative extensions (radiative muon decays)

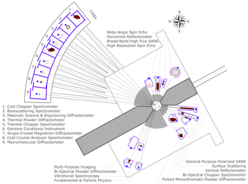
Trying to build upon the G4Ions framework to reuse the existing code where possible.

Expect to provide the above alternative by the end of the year, possibly in 10.3, light atom physics should follow.

NCrystal: Modelling scattering of low-energy neutrons in poly- and single-crystals

See dedicated talk, Monday (Parallel 2B)

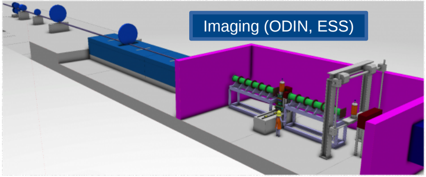
Motivation: Extend capabilities of Geant4 to allow Instrument simulations for neutron scattering facilities.



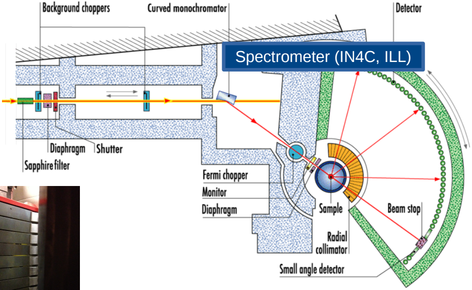
Xiao Xiao Cai, ESS & DTU (xcai@dtu.dk)
Thomas Kittelmann, ESS (thomas.kittelmann@esss.se)

EUROPEAN SPALLATION SOURCE   DTU Technical University of Denmark   brightness

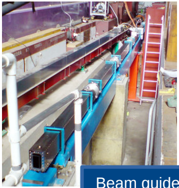
Badly needed – most neutron-instrument components rely on n+Crystal physics!



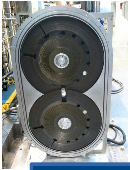
Imaging (ODIN, ESS)



Spectrometer (IN4C, ILL)

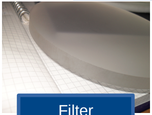


Beam guides



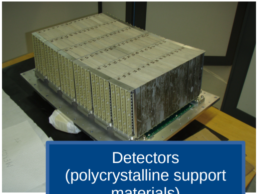
Choppers

Monochromator (single crystals)



Filter (single- or poly-crystals)

User sample (anything, like crystals)



Detectors (polycrystalline support materials)

State of instrument simulations:
- Using dedicated codes (like **McStas**) with custom models of components.
- But *only* handles lowE neutrons!
- Must augment with other (like **MCNP**) to model shielding, source, detectors.
- But usually impossible to get all aspects in single application.
- Hopefully can improve this with G4!

Disclaimer: images merely representative, not actually from the instruments abovei

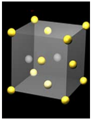
Relevant crystals handled by NCrystal

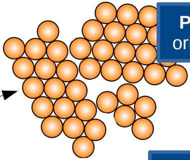
Base structure defined by unit cell
(NCrystal supports any symmetry group,
via embedded NXS/SgInfo lib)

Al.nxs

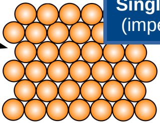
```
space_group = 225
lattice_a = 4.049
lattice_b = 4.049
lattice_c = 4.049
lattice_alpha = 90
lattice_beta = 90
lattice_gamma = 90
debye_temp = 429.0
add_atom = Al 3.449 0.008 0.23 26.98 0.0 0.0 0.0
```

example user input



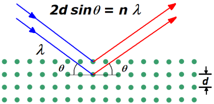


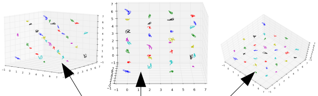
Poly-crystal : randomly oriented crystalline grains



Single-crystal : aligned grains (imperfect realistic alignment)

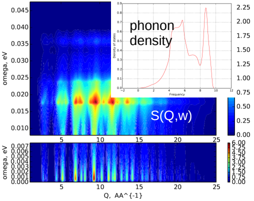
Physics provided:
Bragg diffraction (elastic)

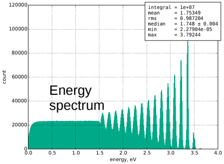




Note: many scattering planes exists in a given crystals

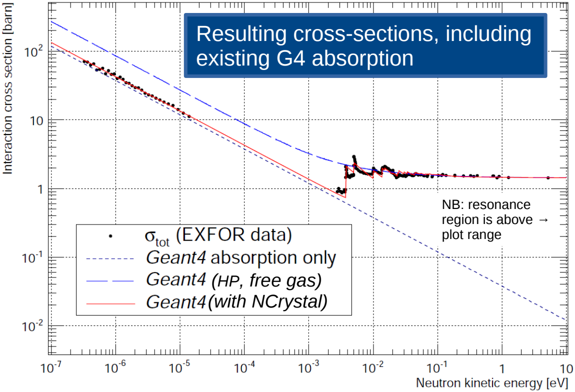
Also providing inelastic components (n+phonon).
Work ongoing to optionally increase realism.



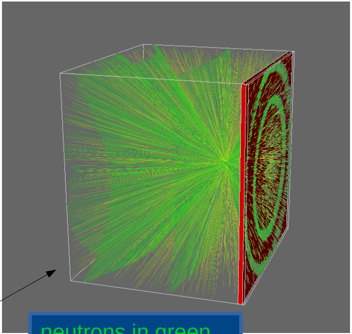


Poly-crystal in Geant4 with NCrystal

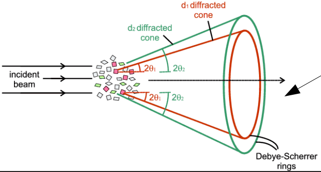
Resulting cross-sections, including existing G4 absorption



G4 simulation of monochro-matic neutron on polycrystal giving Debye-Scherrer cones

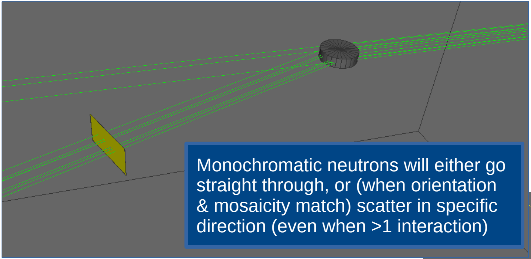


neutrons in green, gammas in yellow

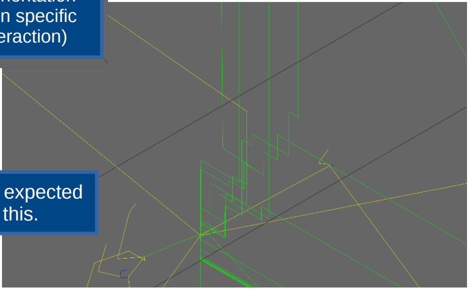


Single-crystal in Geant4 with NCrystal

Describes imperfections in crystallite alignment with mosaicity parameter



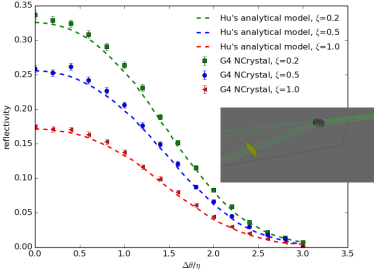
Monochromatic neutrons will either go straight through, or (when orientation & mosaicity match) scatter in specific direction (even when >1 interaction)

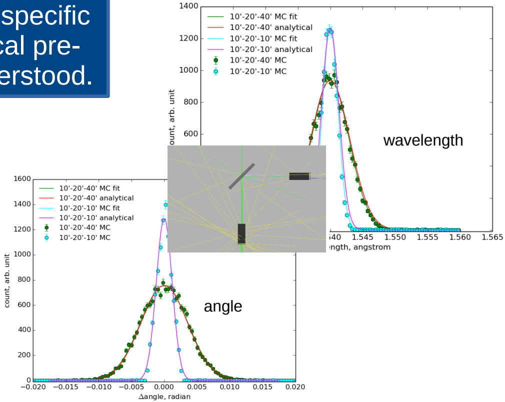


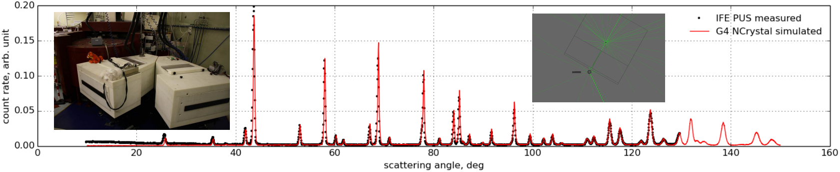
Closeup reveals the expected zig-zag walk behind this.

Validation of Geant4 with NCrystal

Validated against data or using specific simple setups for which analytical predictions exists. Differences understood.



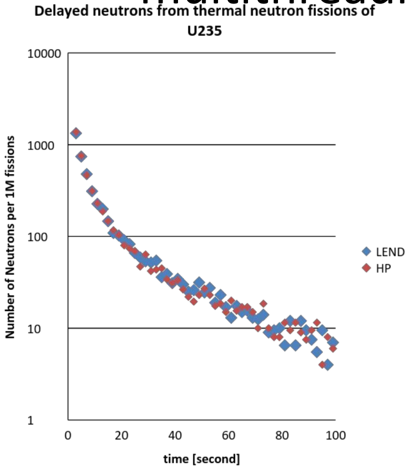


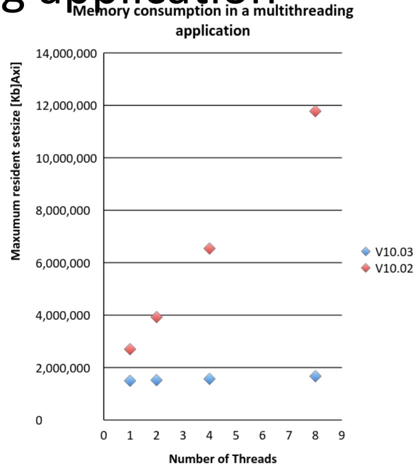


Updates of data library based models

- G4TENDL
  - Data files for ParticleHP
  - Inelastic reactions of light ions (p, d, t, He3 and a) are supported
    - G4NDL provides neutrons data for ParticleHP
  - Compressed by zlib (http://www.zlib.net)
    - 2.5Gb (v10.02) -> 561Mb (v10.03)
  - Adding information of based evaluation in each file
    - “TENDL-2014” or “ENDFVII.r1”
- G4LEND (Low Energy Nuclear Data)
  - Geant4 interface for GIDI/GND format
  - Neutron and photon projectiles are supported
  - Adding delayed neutron emission after fissions
  - Reducing memory consumption in multithreading application
  - Data for charged particles will be available.

Delayed neutron emissions and memory consumption in multithreading application





New developments

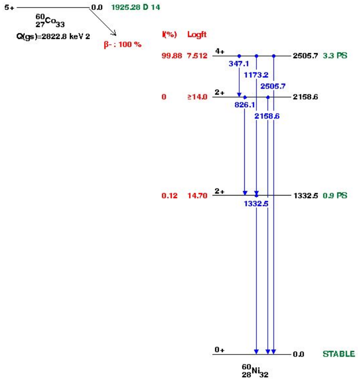
- Neutron capture model based on PGAA data base
  - In some isotope (for example Cd113), we have poor agreement in spectra of gammas after capture of neutrons.
  - This causes a trouble to adapt our result in non-destructive inspection
  - Neutron-capture prompt-gamma activation analysis (PGAA) data base is provided by IAEA
  - Plan to provide a model based on the data base.
  - The model also can be used as a sub model of HP and LEND package.
- Handling self-shielding effects in unresolved resonances rejoin(URR).
  - Currently we use cross sections which NJOY99 RECONR module provides
  - This implies the effect of self-shielding in URR is underestimated.
  - We begin to investigate applying "Probability Table Method" for proper handling of self-shielding effects in the region.

New photon evaporation model

- There are 3 use cases:
  - Hadron inelastic interaction
    - no atomic shells, single de-excitation or full deexcitation chain to be simulated
    - atomic de-excitation is disenabled
  - Neutron capture
    - atomic shell exist, full chain gamma cascade to be simulated
    - atomic de-excitation may be enabled
  - Radioactive decay
    - atomic shell exist, single gamma transition to be simualted
    - Atomic de-excitation may be enabled
- Normally the same instance or few different instances of the photon evaporation per thread may be used
  - To distingwish the case the consumer model should set flags for the photon evaporation model

Jason Detwiler: motivation for correlated gamma emission for ^{60}Co Decay

- An important source of background in my experiment (MAJORANA neutrinoless double beta decay search)
- Background rate depends on both gammas hitting one detector: angle between the gammas matter
- Well-known angular dependence, used for thermometry (“nuclear orientation thermometry”)



Jason Detwiler: IT Multipole Expansion for correlated gamma emission

- For a particular value of M_1, consider the transition:

$$|J_1^{\pi}, M_1\rangle \rightarrow |J_2^{\pi'}, M_2\rangle + |L, M\rangle$$

- In this transition, the amplitude for photon emission in direction ***k*** is

$$\text{Amplitude}(\mathbf{k}) = \sum_{M_2,L,M} A_{J_1,M_1,\pi,J_2,M_2,\pi',L,M} \, T_{J_1,J_2,L} \, D_{L,M}(\mathbf{k})$$

Clebsch-Gordannery

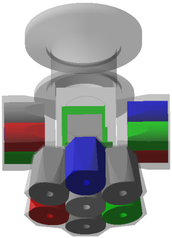
Nuclear Data

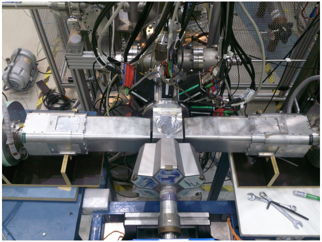
Spherical Harmonics

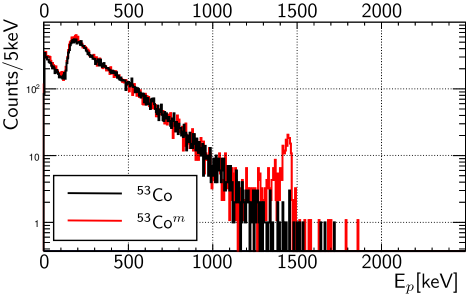
Jason Detwiler: new code required for correlated gamma simulations

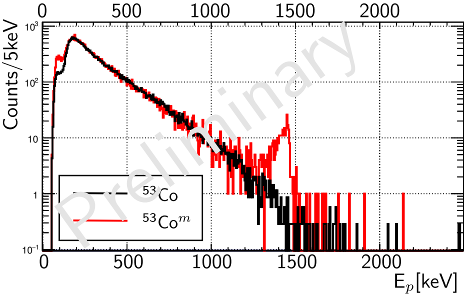
- Utility classes added to Geant4
  - G4Clebsch (Wigner6J() and Wigner9J() functions, etc.)
  - G4LegendrePolynomial
    - N-th coefficient, associated Legendre polynomial evaluation
  - G4PolynomialPDF
    - set coefficients, randomly sample
  - G4NuclearPolarization: the "statistical tensor"
    - data object attached to G4Fragment
  - G4PolarizationTransition
    - samples angles and modifies the G4NuclearPolarization after decay
- Extended gamma level data
  - To be added L, L', δ to each gamma level
  - Laurent Desorgher has prepared a new data extended data set for 10.3
    - To be validated
- This new feature may be released but extra efforts required

Proton emission

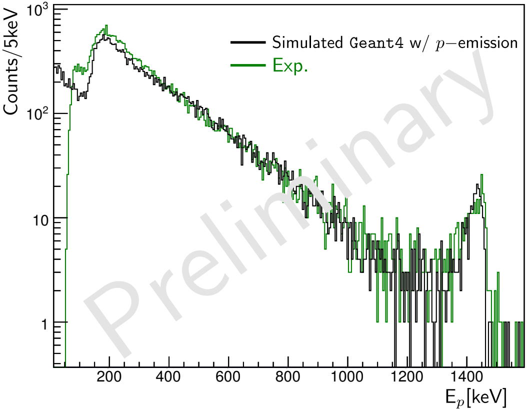








Proton emission



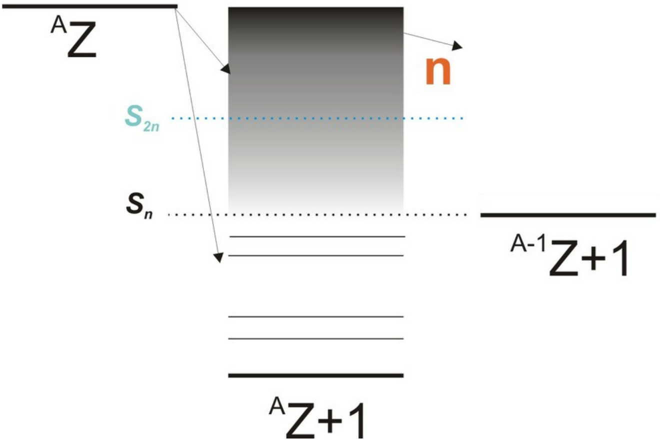
The match is fantastic[ly boring]

The branching ratio $b_p \lesssim 1.5$

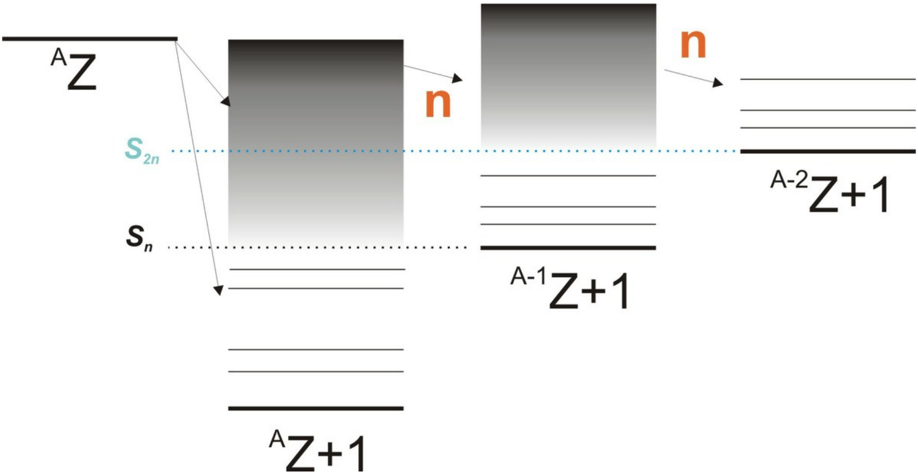
Improved ($\sim \times 20$) $E_p = 1558.8(17)$ keV

... it was measured for the very first time(!)
with the help of the quantum-state selectivity of the JYFLTRAP

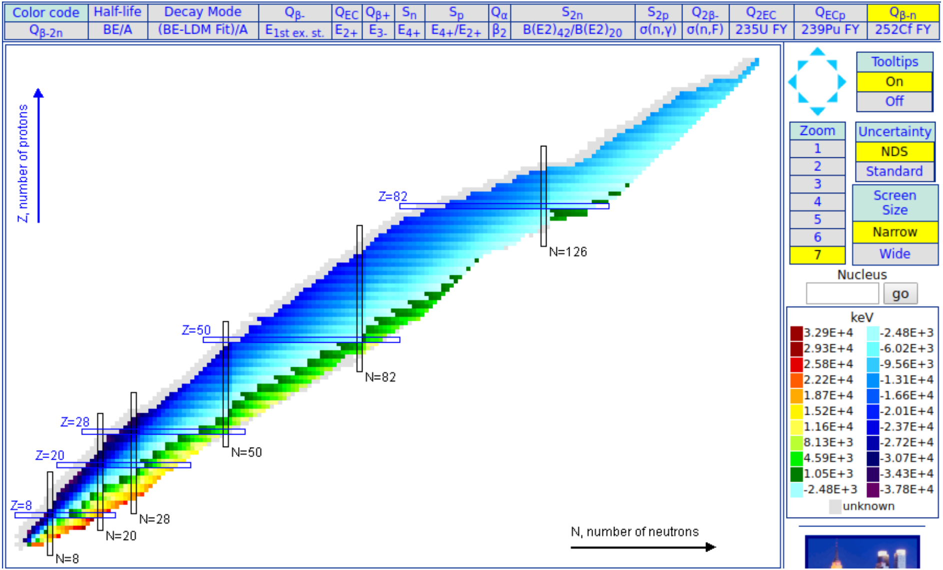
β-delayed neutron emission



β-delayed neutron emission



β-delayed neutron emission



β-delayed neutron emission

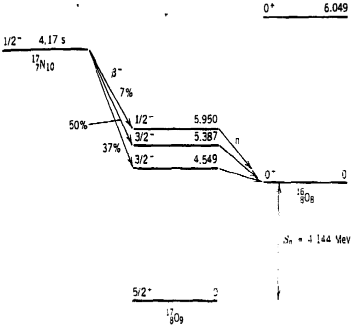
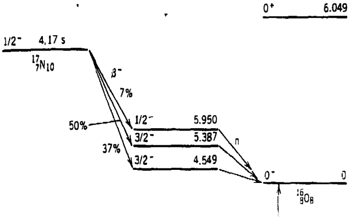


Figure 9.15 The β-delayed neutron decay of ^{17}N.

β-delayed neutron emission



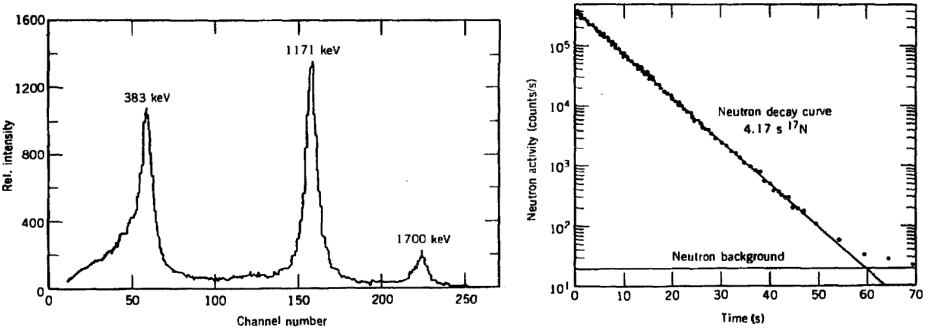


Figure 9.14 Beta-delayed neutrons following the decay of ^{17}N. The neutron energy spectrum is shown at the left; the decay of the neutron activity with time is at the right. From H. Ohm et al., *Nucl. Phys. A* **274**, 45 (1976).

β-delayed neutron emission

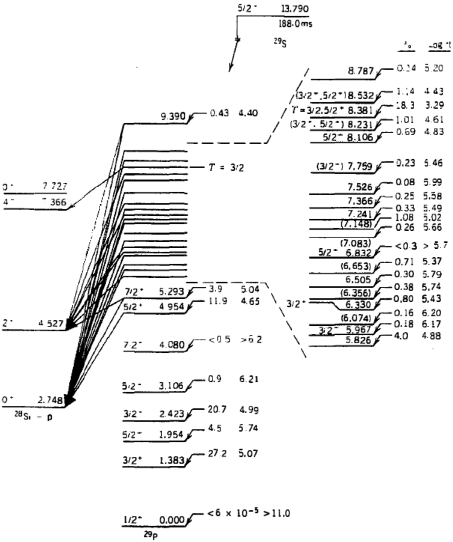


Figure 9.17 Excited states of ^{29}P deduced from the β-delayed proton decay of ^{29}S. The *ft* values are deduced from the intensity of the observed protons. Note the strong decay branch (small *ft* value) in the decay to the state at 8.381 MeV, which is the analog state of the ^{29}S ground state.

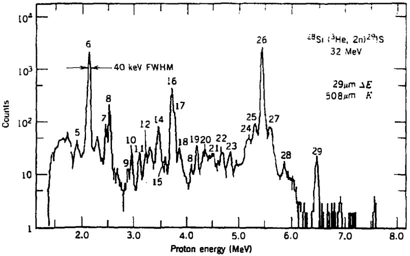
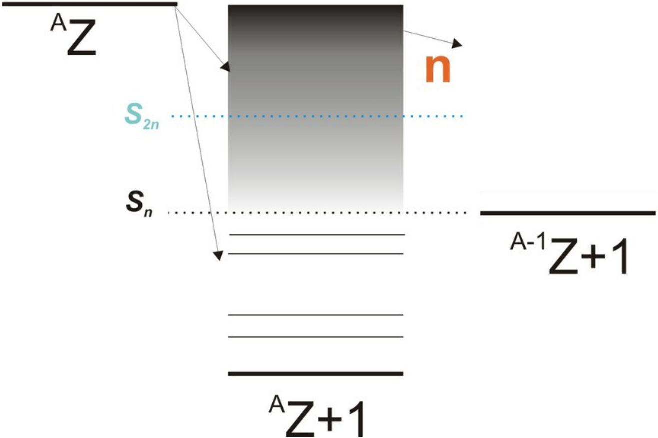


Figure 9.16 Protons emitted following the β decay of ^{29}S. The protons were observed using a $\Delta E \cdot E$ telescope of Si detectors. The numbers refer to specific proton decays of excited state of ^{29}P. Data from D. J. Vielra et al., *Phys. Rev. C* **19**, 177 (1979).

β-delayed neutron emission



β-delayed neutron emission

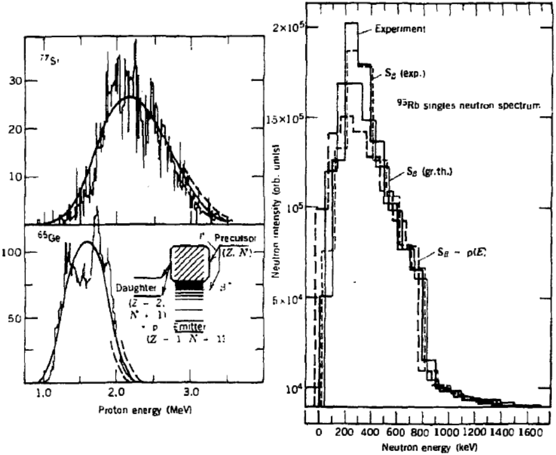


Figure 9.18 Proton (left) and neutron (right) emission following β decay in heavy nuclei. The spacing between excited states in the emitter is so small that we observe only a broad distribution, rather than the individual peaks of Figures 9.14 and 9.16. Attempts to fit the experimental data are based on statistical models, rather than on detailed calculations of individual nuclear states. Proton data from J. C. Hardy et al., *Phys. Lett. B* **63**, 27 (1976); neutron data from K.-L. Kratz et al., *Z. Phys. A* **306**, 239 (1982).

Superheavy Elements News

IUPAC

International Union of Pure and Applied Chemistry

Highlights

- The IUPAC Network
- Periodic Table of the Elements
- Color Books

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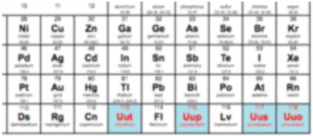
Category: Press Releases

Discovery and Assignment of Elements with Atomic Numbers 113, 115, 117 and 118

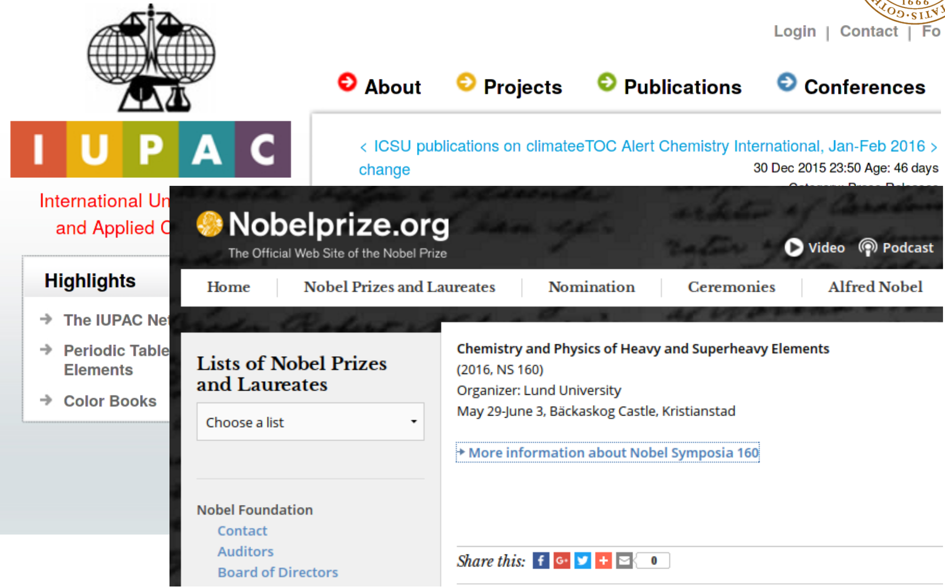
IUPAC announces the verification of the discoveries of four new chemical elements: The 7th period of the periodic table of elements is complete.

Update 21 Jan 2016: Technical Reports available

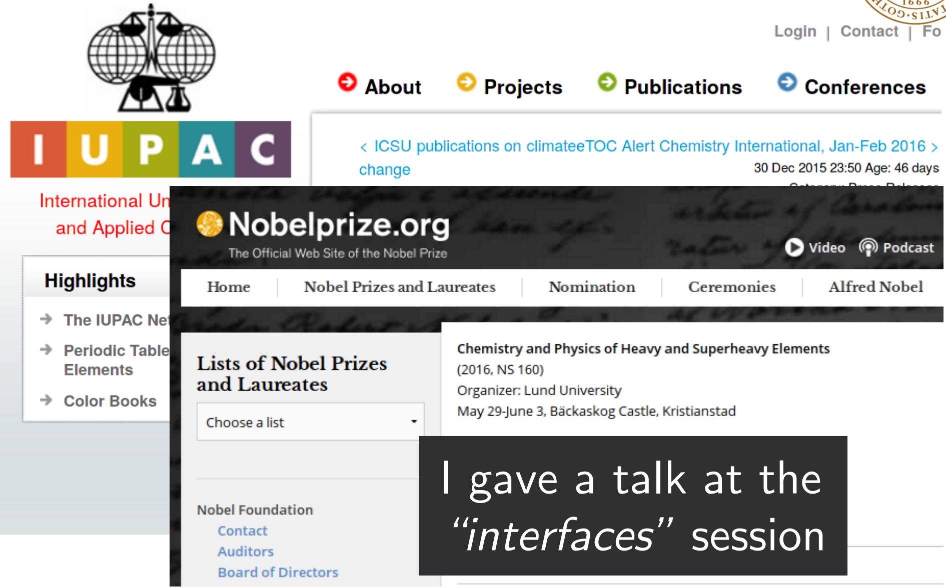
The fourth IUPAC/IUPAP Joint Working Party (JWP) on the priority of claims to the discovery of new



Superheavy Elements News



Superheavy Elements News



I gave a talk at the *"interfaces"* session

G4AtomicShells_EADL and fluorSHE

ELSEVIER

Available online at www.sciencedirect.com

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Nuclear Instruments and Methods in Physics Research A 589 (2008) 202–229

NUCLEAR INSTRUMENTS & METHODS IN PHYSICS RESEARCH Section A

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up to $Z = 110$

Evaluation of theoretical conversion coefficients using *BrIcc*

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Conversion coefficients for superheavy elements

for $110 < Z \leq 120$

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G4AtomicShells_EADL and fluorSHE

BrIcc v2.3S

Conversion Coefficient Calculator

Z (atomic number or symbol)

115

γ-energy (in keV)

200 Uncertainty

Enter (optional) uncertainty in energy as **x** or **+x-y**

Multipolarity

m1 δ Uncertainty

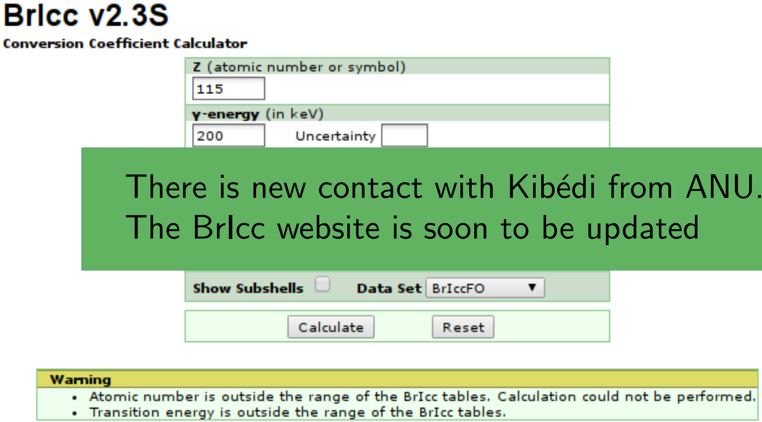
Enter (optional) uncertainty in δ as **x** or **+x-y**

Show Subshells **Data Set** BrIccFO

Calculate Reset

Warning

- Atomic number is outside the range of the BrIcc tables. Calculation could not be performed.
- Transition energy is outside the range of the BrIcc tables.



There is new contact with Kibédi from ANU.
The BrIcc website is soon to be updated

G4AtomicShells_EADL and fluorSHE

Moving away from Carlson's in G4AtomicShells_EADL is a good starting point.

The second step is to include a new database with SHE, fluorSHE:

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The second step is to include a new database with SHE, fluorSHE:

- G4EmParameters
- G4EmParametersMessenger
- G4AtomicTransitionManager
- G4UAtomicDeexcitation
- G4ECDecay
- G4ITDecay
- G4NuclearDecayChannel

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Unfortunately Kibédi's not only contains more Z values but also different occupancies

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- G4NuclearDecayChannel

... Auger database needs to be compatible

- The environment variable `G4ENSDFSTATEDATA` is mandatory
- The NeutronHP module has been replaced by ParticleHP: no change in the user code is required.
- In order to use ParticleHP for charged particles (protons, deuterons, tritons, He3 and alphas), an optional data set G4TENDL-1/0 is required, and should be downloaded in addition from the Geant4 web site.

THANK YOU
for your attention