Introduction to the Atomic Mass Evaluation

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CERN, March 22

Outline

1. Introduction
   - Atomic Mass
   - History of AME
2. Evaluation technique
   - Input data
   - Least-squares method
   - Input files
3. AME2016

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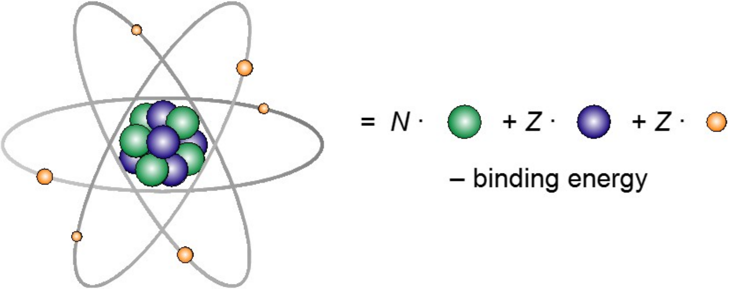
Atomic Mass

Mass $\longrightarrow$ Binding energy $\longrightarrow$ Interaction



- Nuclear physics : shells, shapes, pairing, nuclear models ...
- Nuclear astrophysics : r,rp,νp-process
- Atomic physics : QED
- Metrology : Fundamental constants
- ...

Atomic Mass

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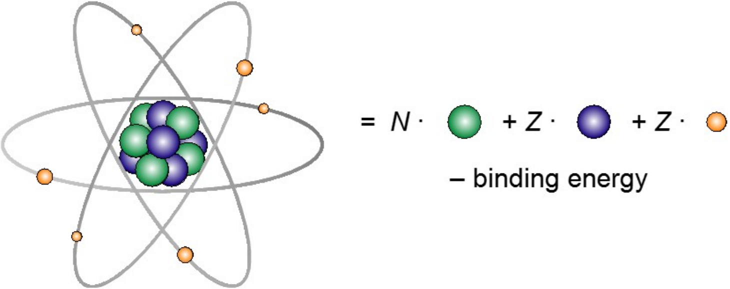

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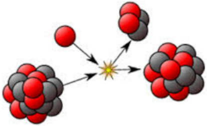
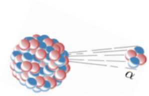
Why "Atomic" mass?

- Most measurements give the mass of the atom or of the single charged ion.
- Easy to derive Q-value...

Mass Measurements

- **Indirect methods: Energy**
  - Reaction Energies $A(a,b)B$: $Q_r = M_A + M_a - M_b - M_B$
    - ⋆ (n,γ) and (p,γ) help building the backbone
    - ⋆ close to stability
  - Decay Energies: α, β, p decays
    - ⋆ far from stability





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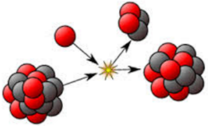
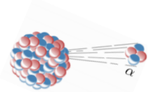
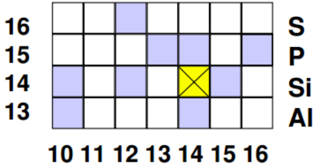




- **Direct Methods: Time of flight or frequency**
  - TOF (MSU, GANIL)
  - Penning Traps (ISOLDE, TRIUMF, . . .) also for the backbone
  - Storage Rings (GSI, IMP)
  - Multi-Reflection Time-of-flight mass spectromer (ISOLDE, GSI, RIKEN)

60 years of mass evaluation

- In the early 1950's, it was found that many relations (direct and indirect) overdetermined the mass value of many nuclides.
  e.g.



^{27}Al (p,γ) ^{28}Si	^{28}Si (d,p) ^{29}Si
^{28}Si (^{3}He,^{8}Li) ^{23}Al	^{28}Si (p,γ) ^{29}P
^{28}Si (^{4}He,^{8}He) ^{24}Si	^{28}Si (π^{+},π^{-}) ^{28}S
^{28}Si (p,t) ^{26}Si	^{31}P (p,α) ^{28}Si
^{28}Si (p,n) ^{28}P	and ^{28}Si / ^{12}C

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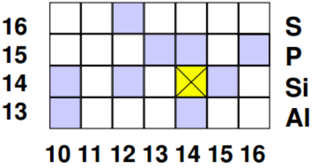

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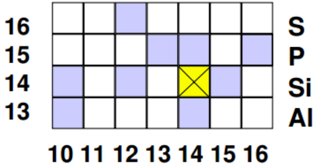

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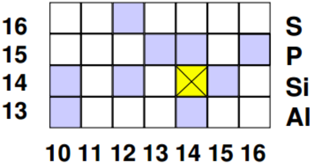

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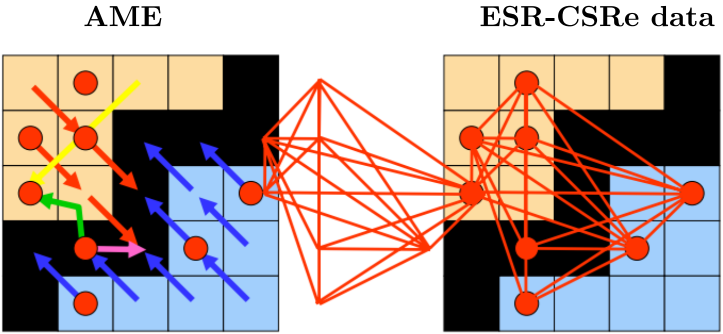
  - Best values for the atomic masses and their associated uncertainties.
  - AME1955, AME1961, AME1964, AME1971, AME1977, AME1983, AME1993, AME2003, AME2012, **AME2016.**

Evaluation of Nuclear Data

- Theoretical evaluation (= theoretical predictions)
  predict values for large sets of nuclei
  make effective calculations for : r-process - reactors - . . .
  uncertainties : just starting security <=> feasibility
- Evaluation of experimental data
  basic blocks : results from experiments
  if available : prefered to theoretical predictions
  allows also to test theoretical "evaluations"

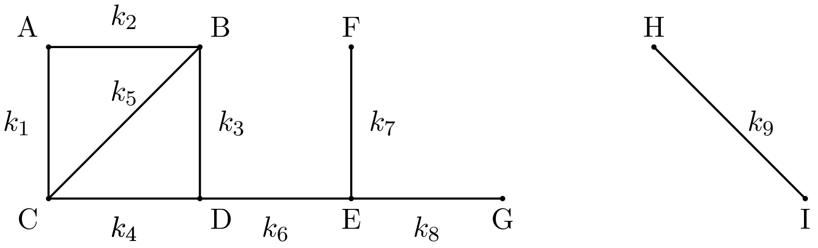
Csnsm *Georges Audi*

Input data for AME



- **Reaction Energies (eV)**
  - (**p,n**), (**n**,γ)
- **Desintegration Energies (eV)**
  - β-decay(β^-, β^+)
  - α-decay(α)
- **Mass Spectrometry (u)**
  - Penning trap: Frequency ratios between two ions (relatively simple).
  - ESR-CSRe: Frequency correlations between all known and unknown (complex).
  - MR-TOF.

Data Connections–Schematic



Connections plot with *primary*, *secondary* and unconnected items.

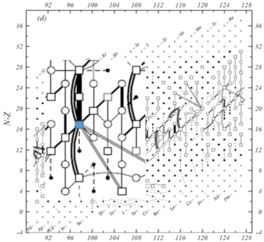
- *primary* : A, B, C, D $\Rightarrow$ used in LSM
- *secondary* : E, F, G $\Rightarrow$ deduced from primaries
- unconnected : H, I $\Rightarrow$ systematic #

Data Connections–Real

- The particularity of AME is that any mass measurement basically establishes a relation between two or more nuclides, which results in an entangled network.

For ^{96}Mo as an example, its mass is determined by:

JY1	2016Al03	3602.919	0.092	μu	96Zr-96Mo
MMn	1991Is02	9154.32	0.05	keV	95Mo(n,γ)96Mo
MBdn	2006Fi.A	6821.5	0.4	keV	96Mo(n,γ)97Mo
JY1	2016Al03	3426.80	0.17	μu	96Nb-96Mo
......					



Its mass cannot be calculated by simple average but by the AME method!

Treatment of Data–LSM-1

Q equations to N parameters ($Q > N$)

$$\sum_{j=1}^{N} k_{ij} m_j = q_i \pm dq_i \quad i = 1, \ldots, Q \quad \Rightarrow \quad K\left|m\right\rangle = \left|q\right\rangle$$

Simple construction

$$\begin{aligned} {}^{t}KWK\left|m\right\rangle &= {}^{t}KW\left|q\right\rangle \\ A\left|m\right\rangle &= {}^{t}KW\left|q\right\rangle \end{aligned}$$

A: normal matrix, W: error matrix $\omega_i = 1/(dq_i dq_i)$

Parameters–Masses

$$\left|\bar{m}\right\rangle = A^{-1\,t}KW\left|q\right\rangle \quad \Rightarrow \quad \left|\bar{m}\right\rangle = R\left|q\right\rangle$$

Treatment of Data–LSM-2

Flow-of-information matrix

$$F = {}^tR \otimes K$$

G. Audi et al, NIMA 249 (1986) 443

- The(i, j) element of F represents the influence of datum i on mass m_j
- A column of F represents all the contributions brought by all data to a given mass m_j
- A row of F represents the influences given by a single piece of data to each nuclide, their sum is the significance of the data

Adjusted input data

$$|\bar{q}\rangle = KR\,|q\rangle$$

What are the values of : $A=?$ $B=?$ $A+B=?$ $A\text{-}B=?$

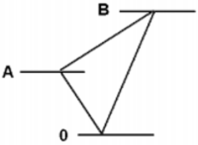
Measured quantities are :

$A = 1 \pm 1$

$B = 2 \pm 1$ $\quad \mathbf{K} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \\ 1 & 1 \end{pmatrix} \quad |\mathbf{m}\rangle = \begin{pmatrix} A \\ B \end{pmatrix} \quad |\mathbf{q}\rangle = \begin{pmatrix} 1 \\ 2 \\ 4 \end{pmatrix}$

$A+B = 4 \pm 1$

And the weight matrix is : $\mathbf{W} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$



Thus : In matrix notation :

$\mathbf{K}|\mathbf{m}\rangle = |\mathbf{q}\rangle \pm |\mathbf{dq}\rangle$ or $\begin{pmatrix} 1 & 0 \\ 0 & 1 \\ 1 & 1 \end{pmatrix} \begin{pmatrix} A \\ B \end{pmatrix} = \begin{pmatrix} 1 \\ 2 \\ 4 \end{pmatrix} \pm \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}$

$\mathbf{A} = {}^{\mathbf{t}}\mathbf{KWK} = {}^{\mathbf{t}}\begin{pmatrix} 1 & 0 \\ 0 & 1 \\ 1 & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & 1 \\ 1 & 1 \end{pmatrix}$ is the Normal Matrix

$$A^{-1} = \left[\begin{pmatrix} 1 & 0 \\ 0 & 1 \\ 1 & 1 \end{pmatrix}^{t} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}^{-1} \begin{pmatrix} 1 & 0 \\ 0 & 1 \\ 1 & 1 \end{pmatrix} \right]^{-1} = \begin{pmatrix} 2/3 & -1/3 \\ -1/3 & 2/3 \end{pmatrix}$$ Covariance Matrix

The errors on A and B are : $\sigma_A = \sigma_B = \sqrt{\frac{2}{3}} = 0.82$

and the correlation coefficient of A&B is : $\frac{-\frac{1}{3}}{\sigma_A \sigma_B} = -\frac{1}{2} = -0.5;$

$$|m\rangle = A^{-1}\, {}^{t}KW|q\rangle$$

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$$A = 1.33 \pm 0.82 \qquad B = 2.33 \pm 0.82$$

$$\sigma^2(A \pm B) = \sigma_A^2 + \sigma_B^2 \pm 2\,\mathrm{cov}(A,B).$$

$$A+B = \frac{11}{3} \pm \frac{\sqrt{6}}{3} \qquad A\text{-}B = -1 \pm \sqrt{2}$$

$$A+B = 3.67 \pm 0.82 \qquad A\text{-}B = -1 \pm 1.41$$

$$\mathbf{A}^{-1} = \left[\begin{pmatrix} 1 & 0 \\ 0 & 1 \\ 1 & 1 \end{pmatrix}^{t} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}^{-1} \begin{pmatrix} 1 & 0 \\ 0 & 1 \\ 1 & 1 \end{pmatrix} \right]^{-1} = \begin{pmatrix} 2/3 & -1/3 \\ -1/3 & 2/3 \end{pmatrix}$$ Covariance Matrix

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$A = 1.33 \pm 0.82$ $\qquad$ $B = 2.33 \pm 0.82$

$$F = \begin{bmatrix} 0.67 & 0 \\ 0 & 0.67 \\ 0.33 & 0.33 \end{bmatrix}$$

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Covariance Matrix

Variance and Covariance (in nano-amu**2)

n	H	D	4He	13C	14N	15N	16O	28Si
0.24139								
-0.00617	0.00879							
0.01218	0.00262	0.01480						
0.00000	0.00000	0.00000	0.00401					
0.00469	-0.00620	-0.00151	0.00000	0.05315				
-0.00130	0.00236	0.00106	0.00000	0.03908	0.04299			
-0.00118	0.01397	0.01279	0.00000	-0.00323	0.00942	0.41639		
-0.00084	0.00231	0.00147	0.00000	0.01184	0.01429	0.00705	0.03007	
-0.00509	0.00950	0.00442	0.00000	0.04140	0.04353	0.05130	0.02433	0.27456

Covariance matrix provided to Codata group as requested

The covariance matrix is available on AMDC website

http://amdc.impcas.ac.cn/

Input files

Q-file

```
000 00000000001 Data-file  (Q-file)   input/qflfu       G.Audi     v 24 feb 2017
000 00000001000
000 00000001010       File of input data for atomic mass calculation
000 00000001020
000 00000001030       DDDDDDD       FFFFFFFF  II   LL       EEEEEEEE
000 00000001040       DDDDDDDD      FFFFFFFF  II   LL       EEEEEEEE
000 00000001050       DD    DD      FF        II   LL       EE
000 00000001060       DD    DD      FF        II   LL       EE
000 00000001070       DD    DD  XX  FFFFF     II   LL       EEEEE
000 00000001080       DD    DD  XX  FFFFF     II   LL       EEEEE
000 00000001090       DD    DD      FF        II   LL       EE
000 00000001100       DD    DD      FF        II   LL       EE
163 090666000a1 UKTG1 15Sc13        2.72      0.77     163Ho O-163Dy O              -71112.8      1.9  m
163 090666000b1  KSH2 15El03        3.042     0.037    163Ho-163Dy                  -66378.27     0.80 m
163 180665000a1 UhR04 64De15     -5069        42       162Dy 37Cl-163Dy 35Cl
163 180665000b1 UhR04 64De15      2164        35       163Dy-162Dy
163 180665000b2 UhR04 64De15      1985        38       163Dy-162Dy
163 180665000b3 UhR04 64De15      2174        40       163Dy-162Dy
163 800665000a1  KTG1 15Sc13   -76349.06      0.86     163Dy O-C15                  -71118.69     0.80 m
163 800675000a1  KTG1 15Sc13   -76346.61      0.97     163Ho O-C15                  -71116.41     0.91 m
163 850733000a1  M    83Sc18,*   4741.5      15.       163Ta(a)159Lu                  4625       15    A
```

M-file

```
163 0660   163Dy  -66381.2      0.8                          stbl            5/2-        10          34.IS=24.896 42
163 0670  *163Ho  -66378.3      0.8                        4.570 ky 0.025  7/2-        10          57.EC=100
163 0670 * 163Ho    T : other: 92Ju01=47(+5-4) d for q=66+ (bare ion)                     92Ju01t
163 0671W  163Hom -66080.4      0.8      297.88     0.07        1.09    s 0.03  1/2+        10          57.IT=100
163 0672W  163Hon -64268.9      0.9     2109.4      0.4       800      ns 150   (23/2+)        12Sw01etj12.IT=100
163 0680   163Er  -65168        5                             75.0     m 0.4   5/2-        10          53.B+=100
163 0681W  163Erm -64723        5        445.5      0.6       580      ns 100   (11/2-)     10          74.IT=100
```

R-file

```
2015El03 .* PRLTA 115, 062501 [SH1-163Ho] S.Eliseev, K.Blaum, M.Block, S.Chenmarev, H.Dorrer, Ch.E.D\"ullmann, C.Enss, P.E.Filianin, L.Gasta
r, F.Lautenschl\"ager, Yu.N.Novikov, A.Rischka, R.X.Sch\"ussler, L.Schweikhard, A.T\"urler
2015Et01*  .PRVCA  91, 064317 A.\'Etil\'e, D.Verney, N.N.Arsenyev, J.Bettane, I.N.Borzov, M.C.Mhamed, P.V.Cuong, C.Delafosse, F.Didierjean,
asduff, F.Ibrahim, K.Kolos, C.Lau, M.Niikura, S.Roccia, A.P.Severyukhin, D.Testov, S.Tusseau-Nenez, V.V.Voronov
2015Fe02* * PRVCA  91, 024307 B.Fernandez-Dominguez, X.Pereira-Lopez, N.K.Timofeyuk, P.Descouvement, W.N.Catford, F.Delaunay
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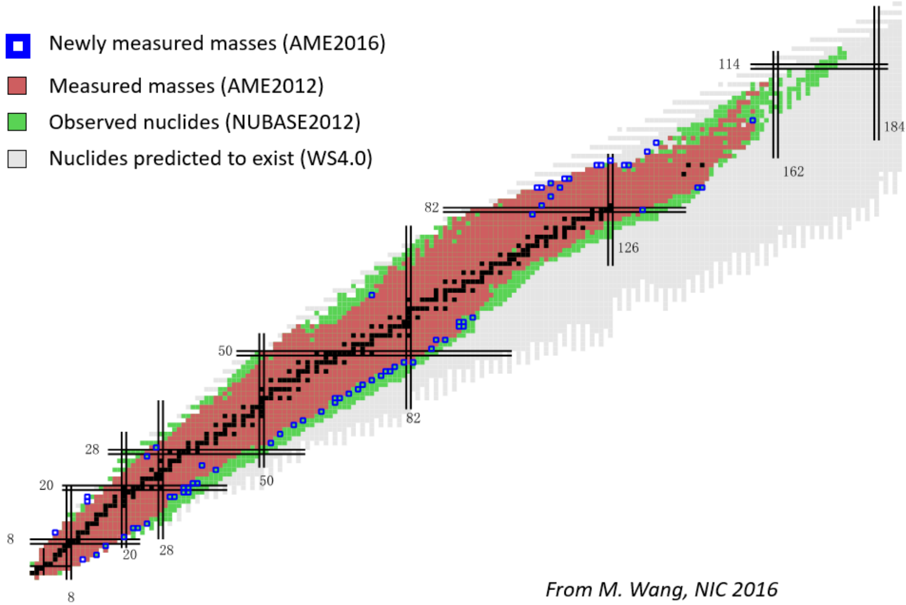
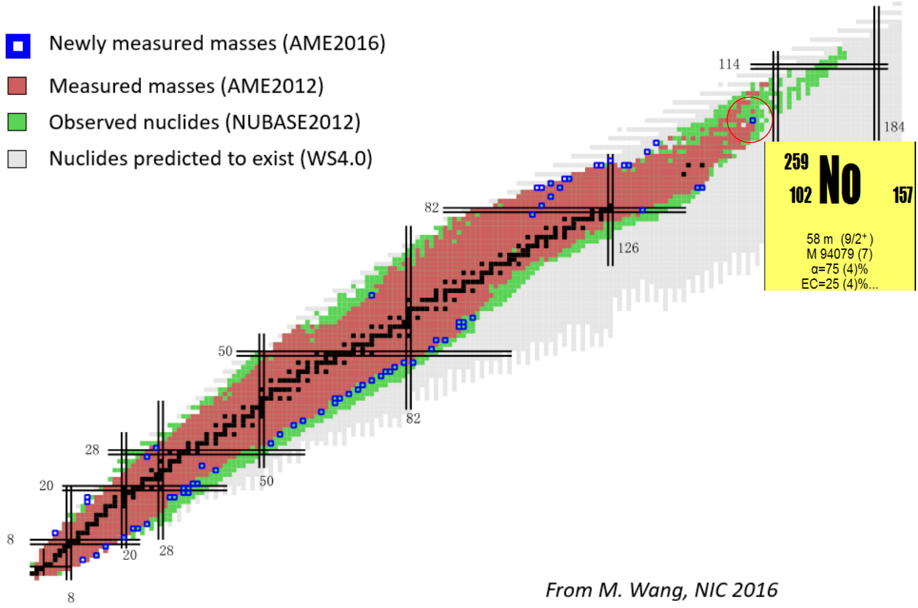
AME2016



Newly measured masses (AME2016)
Measured masses (AME2012)
Observed nuclides (NUBASE2012)
Nuclides predicted to exist (WS4.0)
114
184
162
82
126
50
82
28
50
20
8
20
28
8
From M. Wang, NIC 2016

AME2016



From M. Wang, NIC 2016

Some numbers of AME2016

Typical Size

- **13035** experimental data
  5663 'U', **844** 'O', **853** not accepted ('B', 'C', 'D' and 'F')
- **5675** valid input, compressed to **3884** in the pre-average procedure
  - **2023** primary data (Q)
  - **1207** primary nuclide (N)

Least-squares procedure

- Total $\chi = 825$ (expected 816 ± 20)

3923 masses (96 more)

- **2497** experimental G.S + ^{12}C (59 more)
- **369** experimental ISO (23 more)
- **938** systematical G.S (23 more)
- **119** systematical ISO (9 less)

Summarise

- *Credible and reliable*–identifies and resolves contradictory results, not just compiles.
- *Complete*–includes all measured quantities and their uncertainties.
- *up to date*–results from most recent publications are included.

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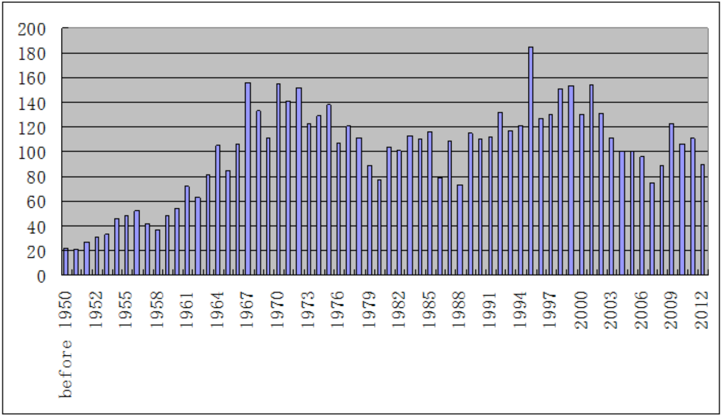

International cooperation

Collaborators

CSNSM	IMP	Argonne National Laboratory	RIKEN
G. Audi W.J. Huang	M. Wang (coordinator) X. Xu	F.G. Kondev	S. Naimi