## **De-excitation tool for neutrino experiments: GEMINI++4**

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The 23rd International Conference on Few-Body Problems in Physics (FB23), Beijing, Sep 26, 2024







- 1. Motivation
- 2. De-excitations from TALYS
- 3. De-excitations from GEMINI++
- 4. GEMINI++4v
- 5. Summary

TALYS:H. Hu, W.L. Guo, et al., Phys. Lett. B 831 (2022) 137GEMINI++/4v:Y.J. Niu, W.L. Guo, M. He, J. Su, arXiv: 2408.14955







Nuclear de-excitations in v experiments are playing an increasingly significant role associated with



- Liquid scintillator
  - neutrons
  - unstable isotopes
  - Water Cherenkov
    - $\succ$  monoenergetic  $\gamma$
    - neutrons
  - Liquid Argon TPC
    - Emitted particles



However, no universally adopted and quantitatively accurate models to describe de-excitation cascade!





#### Statistical model codes were widely used to predict de-excitations related to some topics

- **1.** TALYS  $\rightarrow p \rightarrow \bar{v} K^+$ , DSNB, Strange axial coupling constant
- **2.** ABLA  $\rightarrow$  Energy resolution of accelerator neutrinos

See arXiv:2408.14955 for relevant references

- **3. SMOKER**  $\rightarrow$  Neutron invisible decays
- 4. **CASCADE**  $\rightarrow$  Experimental data of <sup>11</sup>B<sup>\*</sup> and <sup>15</sup>N<sup>\*</sup> de-excitations

#### **Common features of theses codes:**

- Input Nucleus(N/A), Excited energy, Spin, Parity
- $\blacktriangleright$  Apply nuclear model to calculate partial decay width for evaporation of particle *i*
- De-excitations are dealt with as a sequential binary decays

In order to assess performances of de-excitation codes, it is necessary to compare their predictions with measurements for interested nuclei.

<sup>11</sup>B<sup>\*</sup> and <sup>15</sup>N<sup>\*</sup> experimental data are the best for us to validate these codes!



## Experiment 1 from Yosoi et al.





- Quasi-free (p, 2p) reaction, targets are carbon (  ${}^{12}C \rightarrow {}^{11}B^*$ ) and ice (  ${}^{16}O \rightarrow {}^{15}N^*$ )
- Different thresholds: 3.1, 4.0, 4.6 and 4.5 MeV for p, d, t and  $\alpha$
- Results shown above, darker color for '2-body' decay and lighter for '3-body' decay







- Good energy resolution, no threshold for particle identification, even residual nuclei
- Only three two-body decay channels of  ${}^{11}B^*$  were analyzed:  ${}^{10}B + n$ ,  ${}^{9}Be + d$  and  ${}^{7}Li + \alpha$



$$\frac{n+10}{10}$$
  $\frac{(d+9Be)+(\alpha+7Li)}{10}$ 



# TALYS is a nuclear reaction program, and is extensively used for both basic and applied science

#### https://nds.iaea.org/talys/

A.J. Koning, D. Rochman, Nucl. Data Sheets 113 (2012) 2841

Code	TALYS
Input	Nucleus, Excited energy table (spin, parity)
Formulism of width $\Gamma_i$	Hauser-Feshbach (HF)
Output	Statistical branching ratios and energy spectra
Convenience	Not event-by-event, Inconvenience

TALYS-1.95

A nuclear reaction program



User Manual

Arjan Koning Stephane Hilaire Stephane Goriely

## TALYS+Geant4 $\rightarrow$ NucDeEx $\rightarrow$ Event by event

See next talk or S. Abe, Phys. Rev. D 109 (2024) 036009



## the TALYS workflow



#### Inputting

#### USER INPUT FILE

#	basic
projectile	0
element b	
mass 11	
energy Ex_	10MeV

#### $E_x$ spectrum:

152	1	0
153	3	0
154	5	0
155	7	0
156	9	0
157	11	0
158	13	0
159	15	Θ
160	17	1846
161	19	1795
162	21	1858
163	23	1776
164	25	1619
165	27	1449
166	29	1166
167	31	1036
168	33	920
169	35	755
170	37	608
171	39	594
172	41	484
173	43	481
174	45	422
175	47	381
176	49	373
177	51	321
178	53	274
179	55	259

## B11\* Population

0	0.000	0.000E+00	0.000E+00	0.000E+00
1	2.125	0.000E+00	0.000E+00	0.000E+00
2	4.445	0.000E+00	0.000E+00	0.000E+00
3	5.020	0.000E+00	0.000E+00	0.000E+00
4	6.742	0.000E+00	0.000E+00	0.000E+00
5	6.792	0.000E+00	0.000E+00	0.000E+00
6	7.286	0.000E+00	0.000E+00	0.000E+00
7	7.978	0.000E+00	0.000E+00	0.000E+00
8	8.560	0.000E+00	0.000E+00	0.000E+00
9	8.920	0.000E+00	0.000E+00	0.000E+00
10	9.184	0.000E+00	0.000E+00	0.000E+00
11	9.272	0.000E+00	0.000E+00	0.000E+00
12	9.820	0.000E+00	0.000E+00	0.000E+00
13	9.873	0.000E+00	0.000E+00	0.000E+00
14	10.262	0.000E+00	0.000E+00	0.000E+00
15	10.330	0.000E+00	0.000E+00	0.000E+00
16	10.602	0.000E+00	0.000E+00	0.000E+00
17	10.960	0.000E+00	0.000E+00	0.000E+00
18	11.272	0.000E+00	0.000E+00	0.000E+00
19	11.450	0.000E+00	0.000E+00	0.000E+00
20	11.600	0.000E+00	0.000E+00	0.000E+00
21	11.893	0.000E+00	0.000E+00	0.000E+00
22	12.040	0.000E+00	0.000E+00	0.000E+00
23	12.554	0.000E+00	0.000E+00	0.000E+00
24	12.917	0.000E+00	0.000E+00	0.000E+00
25	13.137	0.000E+00	0.000E+00	0.000E+00
26	13.160	0.000E+00	0.000E+00	0.000E+00
27	14.040	0.000E+00	0.000E+00	0.000E+00
28	14.340	0.000E+00	0.000E+00	0.000E+00
29	14.563	0.000E+00	0.000E+00	0.000E+00
30	15.290	0.000E+00	0.000E+00	0.000E+00
31	15.877	4.490E+02	4.490E+02	0.000E+00
32	17.096	1.168E+03	1.168E+03	0.000E+00
33	18.409	1.230E+03	1.230E+03	0.000E+00
34	19.822	1.336E+03	1.336E+03	0.000E+00
35	21.344	1.461E+03	1.461E+03	0.000E+00
36	22.983	1.511E+03	1.511E+03	0.000E+00
37	24.747	1.494E+03	1.494E+03	0.000E+00
38	26.647	1.455E+03	1.455E+03	0.000E+00
39	28.693	1.285E+03	1.285E+03	0.000E+00

L.194E+03 1.194E+03 0.000E+00

N	Multiple emissions						
	Emission particle	Residual nuclei					
	Y	<sup>11</sup> B*					
	n	<sup>10</sup> B*					
	р	<sup>10</sup> Be*	Cor				
	d	<sup>9</sup> Be*					
	t	<sup>8</sup> Be*	nu				
	h (He3)	<sup>8</sup> Li*	nı				
	α	<sup>7</sup> Li*	g				

Fractions depend on nuclear model and  $E_x$ ,Spin,Parity of B11

Continue multiple	
emissions of	
secondary	
residual	
nuclei ;until all	
nuclides are in	
ground state.	

#### Not event by event

Em	itte	ed pa	artio	cles		cross	section	reaction
	р	d		h				
Θ	Θ	Θ	Θ	Θ	Θ	2.0	7032E+03	(g,g)
	Θ			0		1.69	9535E+03	(g,n)
Θ			Θ	0		5.83	3451E+02	(g,p)
						7.79	9416E+02	(g,d)
						3.75	5780E+02	(g,t)
						1.90	0771E+01	(g,h)
						4.54	4468E+02	(g,a)
	0					9.14	1239E+02	(g,2n)
		0 🗸				1.99	9535E+03	(g,np)
1 🧹	0	_1				2.26	6783E+03	(g,nd)
	1/					7.42	2452E+01	(g,pd)
	0	2/	-0			1.0	1104E+02	(g,2d)
		3	1	<u> </u>		6.9	7048E+01	(g,nt)
			<u> </u>	0		4.3	5866E+01	(g,pt)
			°1⁄	1		6.09	9453E+01	(g,dt)
			Θ	<u> /</u>	Θ	8.92	2146E+01	(g,nh)
				1	1	1.8	5022E+03	(g,na)
				0	<u>د ا</u>	2.60	0059E+01	(g,pa)
					Y	2.2	7855E+02	(g,da)
Θ	Θ	0		0	1	1.6	7928E+01	(g,ta)
3	Θ	0	Θ	0	Θ	Č 573	315E+01	(g, 3n)
2		Θ	Θ	Θ	Θ	- i -	11E+03	(g,2np)
	2	Θ	Θ	0	Θ	1.64	6482+02	(g,n2p)
2	Θ		Θ	Θ	Θ	1.5	9954F + 02	(g, 2nd)
	1	1	Θ	Θ	Θ	3.95	5761	(g,npd)
	Θ	2	Θ	Θ	Θ	2.43	3055E+0	(1, n2d)
Θ	1	2	Θ	Θ	Θ	1.02	2633E+01	(g p2d)
2	Θ	Θ		Θ	Θ	1.00	6419E+01	2011
	1	Θ	1	Θ	Θ	2.15	5312E+02	(g,opt)
Θ	1	1	1	Θ	Θ	3.05	5659E+01	(g,pdt)
						1.18	8952E+02	(g,2nh)
1	1	Θ	Θ	1	Θ	1.95	5448E+01	(g,nph)
						4.9	1123E+01	(g,2na)
						5.22	2685E+02	(g,npa)
						3.3	2887E+01	(g, 3np)
						1.46	5930E+02	(g,2n2p)
						1.16	6789E+01	(g, 3nd)
						1.34	4623E+02	(g,2npd)
						2.7	3945E+01	(g,n2pd)
						1.5	7760E+01	(g,2n2d)
						3.95	5762E+01	(g,np2d)
						6.3	3796E+01	(g,n2pt)
						1.45	5623E+01	(g,npdt)
						1.8	7126E+01	(g,n2pa)
Absorp	otion	n cro	oss s	secti	ion			: 4926.3
Sum ou	er -	exclu	siv	e cha	annel	cross	section	15: 17612 7
(n.an)	+	(n.a.	() +		n.ga	cross	section	ns: 0.0
Total					nga.			: 17612 7
Initia	al po	opula	ation	n cro	oss s	ection	1	: 22643.1
				1.	•			
	5r	'Я1	nc	'n	in	$[\mathbf{\sigma}]$	rati	OS
	-		-					

## Change discrete level number of nuclides



8

#### In TALYS, all discrete states of all nuclides only emit *γ*, finally decay into their ground state

	Emit	ted flux	<pre>c per excitat</pre>	ion energy l	oin of Z= 4	N= 6 ( 10Be	e):			
	bin	Ex	gamma	neutron	proton	deuteron	triton	helium-3	alpha	Total
	0	0.000	0.00000E+00							
	1 2	3.368	4.27753E+02 5.99935E+01	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	4.27753E+02 5.99935E+01
Discrete	3 4	5.960 6.179	1.01168E+02 1.77084E+02	9.00000E+00 9.00000E+00	0.00000E+00 0.00000E+00	0.00000E+00 0.00000E+00	0.00000E+00 0.00000E+00	0.00000E+00 0.00000E+00	0.00000E+00 0.00000E+00	1.01168E+02 1.77084E+02
states	5 6	6.263 7.371	6.35393E+01 5.62423E+00	9.00000E+00 9.00000E+00	0.00000E+00 0.00000E+00	0.00000E+00 0.00000E+00	0.00000E+00 0.00000E+00	0.00000E+00 0.00000E+00	0.00000E+00 0.00000E+00	6.35393E+01 5.62423E+00
States	7	7.542 9.270	3.40607E+01	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	3.40607E+01
	9	9.560	1.80959E+01	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	1.80959E+01
	10	10.150	3.47120E-04	3.1/3/6E+01	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	3.58///E+00	3.53257E+00
Continuous	12 13	11.510 12.509	4.39/4/E-04 5.78110E-04	3.52/65E+01 4.03321E+01	0.00000E+00 0.00000E+00	0.00000E+00 0.00000E+00	0.00000E+00 0.00000E+00	0.00000E+00 0.00000E+00	5.88183E+00 6.45328E+00	4.1158/E+01 4.67860E+01
ototoo	14 15	13.595 14.775	9.19605E-04 1.56067E-03	4.66271E+01 5.44424E+01	0.00000E+00 0.00000E+00	0.00000E+00 0.00000E+00	0.00000E+00 0.00000E+00	0.00000E+00 0.00000E+00	6.44623E+00 8.37811E+00	5.30742E+01 6.28221E+01
states	16 17	16.058 17.452	2.77599E-03 5.81825E-03	6.05345E+01 7.05929E+01	0.00000E+00 0.00000E+00	0.00000E+00 0.00000E+00	0.00000E+00 1.36527E-01	0.00000E+00 0.00000E+00	8.54838E+00 7.87023E+00	6.90857E+01 7.86055E+01
	18	18.967	9.47813E-03	7.62352E+01	0.00000E+00	0.00000E+00	5.76376E+00	0.00000E+00	6.36011E+00	8.83686E+01

#### To accurately give B11\* de-excitation results:

- 1. Should know population of every discrete state **OK**
- 2. Should know decay BRs of every discrete state

#### To reduce uncertainty, we change discrete level number:

<sup>9</sup>B <sup>8</sup>B <sup>9</sup>Be Nuclide  $^{10}\mathbf{B}$ <sup>10</sup>Be <sup>8</sup>Be <sup>7</sup>Be <sup>9</sup>Li <sup>8</sup>Li <sup>7</sup>Li <sup>6</sup>Li others Default 10 5 5 8 7 5 10 10 4 10 9 10 5 5 3 5 5 5 3 3 3 3 New 5 1

X

Lead to a wrong result, for example

<sup>11</sup> $B^* \rightarrow p + {}^{10}Be^* \implies {}^{11}B^* \rightarrow p + {}^{10}Be + \gamma$ 

#### If Be10\* is in 7th discrete state

E(level) (keV)	$J^{\Pi}$ (level)	T <sub>1/2</sub> (level)	<mark>Ε(γ)</mark> (keV)	Ι(γ)	м(ү)	Final Levels
0.0	0+	$\begin{array}{rrrr} 1.51{\times}10^{+6} \ y \ 4 \\ & 8 \ \beta^- = 100 \end{array}$	B	e10 i	n١	NDC
3368.03 <i>3</i>	2+	125 fs <i>12</i> % IT = 100	3367.415 <i>30</i>	100	E2	0.0 0+
5958.39 <i>5</i>	2+	< 55 fs % IT = 100	2589.999 <i>60</i> 5955.9 5	>90 <10	M1 E2	3368.03 2+ 0.0 0+
5959.9 <i>6</i>	1-	% IT = 100	2591.5 6 5958.0 6	17 <i>8</i> 83 <i>8</i>	E1 E1	3368.03 2+ 0.0 0+
6179.3 7	0+	0.8 ps +3-2 % IT ≈ 100	219.4 3 2811 7 6178	24 <i>2</i> 76 <i>2</i>	E1 E2 E0	5959.9 1- 3368.03 2+ 0.0 0+
6263.3 <i>50</i>	2-	% IT = 100	303.4 50 2894.9 50 6261.2 50	≤1 99 1 1 1	E1 M2	5959.9 1- 3368.03 2+ 0.0 0+
7371 1	3-	15.7 keV 5 % IT > 0 % n > 0	1412 4002	15 <i>11</i> 85 <i>8</i>	E1 E1	5958.39 2+ 3368.03 2+
7542 1	2+	6.3 keV 8 % α = 3.5 12 % n > 0	11 <b>D</b> *		1 2	9 <b>D</b> o
9270	(4-)	150 keV 20 % n > 0	D	$\rightarrow p$ -		l + be
9560 <i>20</i>	2+	141 keV 10 % α = 0.16 4 % n > 0	<sup>11</sup> B*	ightarrow p ·	+ 0	α + <sup>6</sup> He
10150 <i>20</i>	3-	296 keV 15 % α > 0				



## **TALYS** predictions







TALYS can partially account for experiment data, bad for t mode!





#### **GEMINI++: a Monte Carlo code, is an improved C++ version based on GEMINI**



https://lise.frib.msu.edu/gemini.html

Code	TALYS	GEMINI++
Input	Nucleus, Excited energy table (spin, parity)	Nucleus, Excited energy, Spin
Formulism of width Γ <sub>i</sub>	Formulism Hauser-Feshbach (HF) HF or Weissko of width $\Gamma_i$ (WE)	
Output	Statistical branching ratios and energy spectra	Complete de-excitation cascade
Convenience	Not event-by-event, Inconvenience	Event-by-event, Convenience

This code has been extensively used in nuclear physics and got cheerful achievements

GEMINI++, like other codes, is designed for handling complex fragment formation in heavy-ion fusion reactions, light nuclei?





#### For <sup>11</sup>B<sup>\*</sup> and <sup>15</sup>N<sup>\*</sup>, the Weisskopf-Ewing formalism is used in GEMINI++

$$\Gamma_i^{WE} = \frac{2S_i + 1}{2\pi\rho^0(E_x)} \int \sum_{l=0}^{\infty} (2l+1)T_l(\varepsilon)\rho(U)d\varepsilon,$$

 $\Gamma_i^{WE}$ : the partial decay width for evaporation of particle *i* 

- $S_i$ , l: the spin and orbital angular momenta
- $T_l(\varepsilon)$ : the transmission coefficient,  $\varepsilon$ : the kinetic energy of i

$$U$$
 :  $E_x - B_i - E_{rot} - \varepsilon_i$ 

 $\rho^{\,0}$  ,  $\rho\colon$  the SI level densities of the parent and daughter nuclei

#### **Back-shifted term** *E*<sub>1</sub>**:**

$$\rho(U) \propto \frac{\exp[2\sqrt{a(U - E_1)}]}{a^{1/4}(U - E_1)^{5/4}},$$

Pairing/Shell corrections = modify excited energy

#### Suppression factors F<sub>s</sub>:

$$\Gamma_i = \Gamma_i^{WE} \times F_s$$

Adjust its predictions Final results based on  $\Gamma_i$ 



### **GEMINI++** predictions





GEMINI++ can't describe de-excitations of both <sup>11</sup>B<sup>\*</sup> and <sup>15</sup>N<sup>\*</sup> well



## (4) GEMINI++4v



# **GINIMI++4v** is developed for **neutrino** experiments to handle de-excitations of residual nuclei associated with v interaction and nucleon decay based on **GEMINI++** code

#### **Open source:**

https://github.com/NiuYJ1999/GEMINI\_4nu

#### Making three reasonable modifications:

- ✓ Remove back-shifted term
- ✓ Add discrete states
- ✓ Remove/adjust suppression factors

	If + code designed for de-	excitation	
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### The back-shifted term $E_1$ is equivalent to reducing $E_x$ of the compound nucleus

Suppress emissions of massive particles compared with  $\boldsymbol{\gamma}$  emission

Massive particles will require a higher  $E_x$  to begin their evaporation

#### **Threshold values:**

We simulate 5000 events for every interval of 0.1 MeV in the range of 0 MeV  $\leq$  Ex  $\leq$  50 MeV.

Modes	Theory	GEMINI++	$\operatorname{GEMINI}_{++4\nu}$
$n + {}^{10}\mathrm{B}$	11.5	12.2	12.2
$p + {}^{10}\mathrm{Be}$	11.2	17.1	12.2
$d + {}^{9}\mathrm{Be}$	15.8	16.6	16.6
$t + {}^{8}\text{Be}$	11.2	20.5	12.1
$\alpha + {^7{\rm Li}}$	8.7	10.1	10.1
		/	

the back-shifted term  $E_1$  is not used properly for the case of light nuclei

No available  $E_1$ 

Remove  $E_1$ 



## Impact of Modification 1 on de-excitations





#### **Only Removing back-shifted term:**

- Increase p and t BRs versus GEMINI++
- <sup>11</sup>B\*: basically agree with Exps 1 and 2
- <sup>15</sup>N\*: become worse for *n* and *p* BRs

Modes	Theory	GEMINI++	$\operatorname{GEMINI}_{++4\nu}$
$n + {}^{10}\mathrm{B}$	11.5	12.2	12.2
$p + {}^{10}\mathrm{Be}$	11.2	17.1	12.2
$d + {}^{9}\mathrm{Be}$	15.8	16.6	16.6
$t + {}^{8}\text{Be}$	11.2	20.5	12.1
$\alpha + {}^{7}\mathrm{Li}$	8.7	10.1	10.1





#### **GEMINI++ only considers continuous levels**

Daughter nuclei of de-excitations are usually left in discrete levels when its  $E_x$  is low

## Add discrete states :

Due to the unclear boundary between discrete and continuum states, we only consider the discrete levels:

✓  $E_x$  < 6 MeV ✓ Decay known

#### **Implement: modify outputs**

- If the excited energy of parent nucleus in the last binary decay is higher than the highest discrete level considered obviously, this GEMINI++ event will be kept;
- If it is lower than all of the discrete levels, this state will be set as the ground state and the kinematics of the previous decay will be recalculated;
- If it lies between two discrete levels, we shall reset this state to the lower level and recalculate the kinematics of the previous decay.



## Impact of Modifications 1 and 2 on de-excitations





#### Both Removing BS and Add discrete states:

- Increase all BRs of Exp. 1 versus Modification 1
- <sup>11</sup>B\*: basically agree with Exps 1 and 2
- ${}^{15}N^*$ : become worse for *p* and *alpha*

Including discrete levels can increase the kinetic energy of the finally emitted particles  $\rightarrow$  over thresholds





#### Default $F_s$ settings originate from the de-excitations of heavy nuclei

Settings	n	p	d	t	<sup>3</sup> He	α
Default	1.0	1.0	0.5	0.5	0.5	1.0
$F_s = 1.0$	1.0	1.0	1.0	1.0	1.0	1.0
$F_s = 0.5$	1.0	0.5	0.5	0.5	0.5	0.5

### Are default settings reasonable for light nuclei?



 $F_s = 0.5$  for all charged particles. Compared with default, only two changes



### **GEMINI++4v** predictions



#### Including all 3 modifications, present both $F_s = 1.0$ and $F_s = 0.5$ results:



**GEMINI++4v** with  $F_s = 1.0$ :

- > Good agreement with  $^{11}B^*$  data
- > Can't account for  ${}^{15}N^*$  data well

**GEMINI++4v** with  $F_s = 0.5$ :

#### **Recommend!**

- > Good agreement with  $^{11}B^*$  data
- > Partially account for  ${}^{15}N^*$  data, include *n*

This is the first time that a code can basically reproduce both  ${}^{11}B^*$  and  ${}^{15}N^*$  data 19





#### Fixed energy ranges of $16 \le Ex \le 35$ MeV for ${}^{11}B^*$ and $20 \le Ex \le 40$ MeV for ${}^{15}N^*$

Compare the ratio of each type of charged particle emission among four types for every energy bin



 $\succ$   $F_s = 1.0$  and  $F_s = 0.5$  differences

are relatively small

- Predicted shapes are basically consistent with data except α
- Discrepancy maybe come from

 $^{11}\text{B}^* \rightarrow t + \alpha + \alpha$ 

#### Not coincidental!







- De-excitations are playing an increasingly significant role in v experiments
- De-excitation codes were widely used, should be compared with experimental data
- TALYS can partially account for experimental data, not event-by-event
- GEMINI++4v give the best predictions for both <sup>11</sup>B\* and <sup>15</sup>N\* de-excitations, event-by-event

## Thanks for your attention!