# **LANL Light Element Evaluations**

# in Nuclear Security, Energy, Safety & Science

Mark Paris Gerry Hale LANL Theoretical Division Workshop for Applied Nuclear Data Applications

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# **Overview**

- LANL provides most of the existing ENDF light element evaluations
  - "Light elements" mean less than ~20 nucleons
  - Essential for actinide evaluations and these should be done concurrently
  - LANL R-matrix analysis code "EDA"
    - Large code-modernization effort: higher energies, charged-particle, break-up reactions
  - ALL available data is analyzed
    - Neutron & charged-particle induced
    - ALL scattering & reactions (direct, compound, transfer, break-up, ...)
    - Unpolarized & polarized
- End-user applications:

### \*Light-element data relevant for most applications\*

- Most of the state-of-the-art ENDF/B-VIII.0 light-element evaluations were done at LANL by Gerry Hale and collaborators
- Nuclear security: thermonuclear fusion; TN boost & burn; ...
- Nuclear energy: inertial & magnetic confinement fusion; plasma-nuclear interactions
- Nuclear safety: Criticality Safety Project (important elements: H, Li, C, O,...)
- Basic & applied nuclear science: nuclear & particle physics, astrophysics, cosmology

# LANL-EDA evaluation capabilities

## R-matrix formalism [Wigner(1947)]

- Unified description of many reactions
- Fully quantum-theoretic approach

# Capabilities

- Any projectile: n, p, D, T, <sup>3</sup>He,  $\alpha$ , ...
- Any target: H, He, Li, Be, B, C, N, O, F, ...
- All data fit together, at the same time
  - Elastic, inelastic, rearrangement, breakup, capture
- All observables
  - Cross sections: elastic, reaction, total
  - Angular distributions/excitation functions
  - Polarization observables
  - Break-up spectra: 2→3- & 4-body
  - Capture/electromagnetic
- Covariance/uncertainty information generated
- High-fidelity fit:
  - Typical chi-squared:  $\chi^2$ /dof ~ 1.2 1.5

$\sim$	t+ <sup>4</sup> He	4.02		5	
	n+ <sup>6</sup> Li	5.0		3	
	$n+^{6}Li^{*}$	5.5		1	
*	$d+{}^{5}\mathrm{He}$	6.0		0	
Reaction	Energy Ran	nge (MeV)	# I	Pts.	Observables
$^{4}\text{He}(t,t)^{4}\text{He}$	$E_t = 0 - 14$		16	61	$\sigma(\theta), A_y(t)$
$^{4}\text{He}(t,n)^{6}\text{Li}$	$E_t = 8.75 - 14.4$		37		$\sigma_{\text{int}}, \sigma(\theta)$
${}^{4}\text{He}(t,n){}^{6}\text{Li}^{*}$	$E_t = 12.9$			4	$\sigma(\theta)$
$^{6}\text{Li}(n,t)^{4}\text{He}$	$(a,t)^{4}$ He $E_{n} = 0 - 4$ $(a,n)^{6}$ Li $E_{n} = 0 - 4$ $(a,n)^{6}$ Li <sup>*</sup> $E_{n} = 3.35 - 4$		1406		$\sigma_{\text{int}}, \sigma(\theta)$
$^{6}\text{Li}(n,n)^{6}\text{Li}$			8	00	$\sigma_{\mathrm{T}}, \sigma_{\mathrm{int}}, \sigma(\theta), P_{y}(n)$
$^{6}\text{Li}(n,n')^{6}\text{Li}^{*}$				8	$\sigma_{int}$
$^{6}\text{Li}(n,d)^{5}\text{He}$	$E_n = 3.35$ -	4		2	$\sigma_{int}$
Total			39	18	13

 $a_c$  (fm)  $l_{max}$ 

Channel

## Unified, simultaneous fit

- describe all data together
- fit quantum mechanical amplitudes, not cross sections

## Built-in Quality Assurance

- Normalization constrained
  - Weed-out underestimated exp'l uncertainties
- Superior to single-channel or polynomial fitting

# Status of existing LANL evaluations ENDF/B-VIII.0

### <u>Highlights</u>

- 1. p+t, p+<sup>3</sup>He, p+<sup>6,7</sup>Li
- 2. d+d, d+t, d+<sup>3</sup>He
- 3. t+t, t+<sup>6</sup>Li
- 4. n+<sup>6</sup>Li, n+<sup>12</sup>C, n+<sup>13</sup>C
- 5. <sup>9</sup>Be system
- 6. <sup>15</sup>N system
- 7. n+<sup>16</sup>O

# Ongoing work:

- Code modernization
- Interface EDA evaluation NJOY, MCNP, weapons application codes, ...
- Toward global evaluations
  Allow concurrent evaluations of light/heavy/benchmarking

#### **Existing LANL evaluations** Energy Range (MeV) System Channels p+p; n+p, 0-40 N-N 2 γ+d 0-40 N-d p+d: n+d 0-4 3 <sup>4</sup>H: <sup>4</sup>Li n+t: p+<sup>3</sup>He 0-20 p+t; n+<sup>3</sup>He; d+d 0-11; 0-10; 0-10 4 <sup>4</sup>He $n+\alpha$ ; d+t; <sup>5</sup>He+y 0-28; 0-10 <sup>5</sup>He 5 p+ $\alpha$ : d+<sup>3</sup>He 0-24: 0-1.4 <sup>5</sup>L i System (Channels) Α <sup>6</sup>He (<sup>5</sup>He+n, t+t); <sup>6</sup>Li (d+<sup>4</sup>He, t+<sup>3</sup>He); <sup>6</sup>Be (<sup>5</sup>Li+p, <sup>3</sup>He+<sup>3</sup>He) 6 <sup>7</sup>Li (t+<sup>4</sup>He, n+<sup>6</sup>Li); <sup>7</sup>Be (γ+<sup>7</sup>Be, <sup>3</sup>He+<sup>4</sup>He, p+<sup>6</sup>Li) <sup>8</sup>Be (<sup>4</sup>He+<sup>4</sup>He, p+<sup>7</sup>Li, n+<sup>7</sup>Be, p+<sup>7</sup>Li<sup>\*</sup>, n+<sup>7</sup>Be<sup>\*</sup>, d+<sup>6</sup>Li) 8 <sup>9</sup>Be (<sup>8</sup>Be+n, d+<sup>7</sup>Li, t+<sup>6</sup>Li); <sup>9</sup>B (γ+<sup>9</sup>B, <sup>8</sup>Be+p, d+<sup>7</sup>Be, <sup>3</sup>He+<sup>6</sup>Li) 9 10 <sup>10</sup>Be (n+<sup>9</sup>Be, <sup>6</sup>He+α, <sup>8</sup>Be+nn, t+<sup>7</sup>Li); <sup>10</sup>B (α+<sup>6</sup>Li, p+<sup>9</sup>Be, <sup>3</sup>He+<sup>7</sup>Li) 11 <sup>11</sup>B (α+<sup>7</sup>Li, α+<sup>7</sup>Li<sup>\*</sup>, <sup>8</sup>Be+t, n+<sup>10</sup>B); <sup>11</sup>C (α+<sup>7</sup>Be, p+<sup>10</sup>B) $^{12}C$ (<sup>8</sup>Be+ $\alpha$ , p+<sup>11</sup>B) 12 13 $^{13}C(n+^{12}C, n+^{12}C^*)$ 14 $^{14}C(n+^{13}C)$ 15 <sup>15</sup>N (p+<sup>14</sup>C, n+<sup>14</sup>N, $\alpha$ +<sup>11</sup>B) 16 <sup>16</sup>O ( $\gamma$ +<sup>16</sup>O, $\alpha$ +<sup>12</sup>C) <sup>17</sup>O (n+<sup>16</sup>O, $\alpha$ +<sup>13</sup>C) 17

<sup>18</sup>Ne (p+<sup>17</sup>F, p+<sup>17</sup>F<sup>\*</sup>, α+<sup>14</sup>O)

18



**Follow-on material** 

# T(d,n)α evaluation (I)

### Simultaneously fits all known low-E data

- neutron & charged-particle channels
- polarization (distinguishes partial waves, etc.)
- High-fidelity X<sup>2</sup> ~ 1.5 below 10 MeV
- All resonances/partial waves included

EDA also provides covariance matrices



		channel		a <sub>c</sub> (fm)		I <sub>max</sub>	
		n+4He		3.0		5	
		γ+⁵He		60		1	
			d+ <sup>3</sup> H 5.		1	5	
		n+ <sup>4</sup> He* 5		5.	0	1	
Reaction	En (N	ergies ⁄IeV)	# p	data oint s	# ty	data /pes	
<sup>4</sup> He(n,n) <sup>4</sup> He	E <sub>n</sub> = (	0 – 40		817		2	
<sup>3</sup> H(d,d) <sup>3</sup> H	E <sub>d</sub> = 0	0 – 8.6		700		6	
<sup>3</sup> H(d,n) <sup>4</sup> He	E <sub>d</sub> = 0	0 – 30	1	185		14	
<sup>3</sup> H(d,γ) <sup>5</sup> He	E <sub>d</sub> = (	0 – 8.6		17		2	
<sup>3</sup> H(d,n) <sup>4</sup> He <sup>*</sup>	E <sub>d</sub> = 4	4.8 – 8.3		10		1	
total			2	729		25	

### T(d,n)α evaluation (II) Angular distributions T(d,el)



### T(d,n)α evaluation (II) σ<sub>NI</sub> T(d,el) nuclear plus interference



### Nuclear + interference cross section

- requires multichannel fit
- strong energy dependence
- not necessarily > 0

# Status of existing LANL evaluations ENDF/B-VIII.0

==> neutrons-VIII_0_owners.txt <==						
0 – N – 1	LANL	EVAL-APR16	HALE, PARIS	25	1451	
1-H - 1	LANL	EVAL-JUL16	G.M.Hale	125	1451	
1-н - 2	LANL	EVAL-FEB97	P.G.Young,G.M.Hale,M.B.Chadwick	128	1451	
1-H - 3	LANL	EVAL-NOV01	G.M.Hale	131	1451	
2-Не- 3	LANL	EVAL-MAY90	G.Hale,D.Dodder,P.Young	225	1451	
2-Не- 4	LANL	EVAL-SEP10	Hale	228	1451	
3-Li- 6	LANL	EVAL-JAN17	G.M. Hale	325	1451	
3-Li- 7	LANL	EVAL-AUG88	P.G.Young	328	1451	
4-Be- 7	LANL	EVAL-JUN16	I.Thompson, P.R.Page	419	1451	
4-Be- 9	LLNL,LANL	EVAL-OCT09	G.HALE, PERKINS ET AL, FRANKLE	425	1451	
5-B - 10	LANL	EVAL-FEB17	G.M.Hale	525	1451	
5-B - 11	LANL	EVAL-MAY89	P.G.Young	528	1451	
6-C - 12	LANL, ORNL	EVAL-AUG15	G.M. Hale, P.G. Young, C.Y. Fu	625	1451	
6-C - 13	LANL,	EVAL-AUG15	G.M. Hale, M.W. Paris	628	1451	
7 - N - 14	LANL	EVAL-JUN97	M.B.Chadwick, P.G.Young	725	1451	
7-N - 15	LANL	EVAL-SEP83	E.Arthur, P.Young, G.Hale	728	1451	
8-0 - 16	LANL	EVAL-DEC16	Hale,Paris,Young,Chadwick	825	1451	

# **ENDF/B-VIII.0** evaluation custodians

==> alphas-VIII_0_owners.txt <==							
2-He- 4 LLNL E	VAL-DEC99	R.M.White,D.A.Resler,S.I.Warshaw	228	1451			
==> deuterons-VIII_0_owners.txt <==							
1-H - 2 LANL E	VAL-SEP01	G.M.HALE	128	1451			
1-H - 3 LANL E	VAL-JAN95	G.M.HALE AND M.DROSG	131	1451			
2-He- 3 LANL E	VAL-FEB01	G.M.HALE	225	1451			
3-Li- 6 LANL E	VAL-JUN04	P.R.PAGE	325	1451			
<u> 3-Li- 7 LLNL E</u>	VAL-NOV10	P. Navratil, D. A. Brown	328	1451			
==> helium3s-VIII_0_own	ers.txt <=	=					
2-He- 3 LLNL E	VAL-NOV10	P.Navratil, D.Brown, G.Hale	225	1451			
2-He- 4 LLNL E	VAL-DEC99	R.M.White,D.A.Resler,S.I.Warshaw	228	1451			
3-Li- 6 LANL E	VAL-NOV02	G.M.HALE	325	1451			
==> neutrons-VIII_0_own	ers.txt <=	=					
0 - N - 1 LANL E	VAL-APR16	HALE, PARIS	25	1451			
1-H - 1 LANL E	VAL-JUL16	G.M.Hale	125	1451			
1-H - 2 LANL E	VAL-FEB97	P.G.Young,G.M.Hale,M.B.Chadwick	128	1451			
1-H - 3 LANL E	VAL-NOV01	G.M.Hale	131	1451			
2-He- 3 LANL E	VAL-MAY90	G.Hale,D.Dodder,P.Young	225	1451			
2-He- 4 LANL E	VAL-SEP10	Hale	228	1451			
3-Li- 6 LANL E	VAL-JAN17	G.M. Hale	325	1451			
3-Li- 7 LANL E	VAL-AUG88	P.G.Young	328	1451			
4-Be- 7 LANL E	VAL-JUN16	I.Thompson, P.R.Page	419	1451			
4-Be- 9 LLNL, LANL E	VAL-OCT09	G.HALE, PERKINS ET AL, FRANKLE	425	1451			
5-B - 10 LANL E	VAL-FEB17	G.M.Hale	525	1451			
5-B - 11 LANL E	VAL-MAY89	P.G.Young	528	1451			
6-C - 12 LANL, ORNL E	VAL-AUG15	G.M. Hale, P.G. Young, C.Y. Fu	625	1451			
6-C - 13 LANL, E	VAL-AUG15	G.M. Hale, M.W. Paris	628	1451			
7-N - 14 LANL E	VAL-JUN97	M.B.Chadwick, P.G.Young	725	1451			
7-N - 15 LANL E	VAL-SEP83	E.Arthur, P.Young, G.Hale	728	1451			
8-0 - 16 LANL E	VAL-DEC16	Hale, Paris, Young, Chadwick	825	1451			

# **ENDF/B-VIII.0** evaluation custodians (cont.)

==> protons-VIII 0 owners.txt <==								
1-H - 1 LANL	EVAL-FEB98	G.HALE	125	1451				
1-H - 2 LANL	EVAL-FEB97	P.G.YOUNG,G.M.HALE,M.B.CHADWICK	128	1451				
1-H - 3 LANL	EVAL-SEP01	G. M. HALE	131	1451				
2-He- 3 LANL	EVAL-OCT83	G.HALE	225	1451				
2-He- 4 LLNL	EVAL-DEC99	R.M.White, D.A.Resler, S.I.Warshaw	228	1451				
3-Li- 6 LANL	EVAL-AUG01	G.M.HALE	325	1451				
<u>3-Li- 7 LLNL</u>	EVAL-SEP10	P. Navratil, D.A. Brown	328	1451				
4-Be- 9 LANL	EVAL-NOV88	P.G.Young, E.D.Arthur	425	1451				
5-B - 10 LANL	EVAL-AUG05	P.R.PAGE	525	1451				
6-C - 12 LANL	EVAL-JUN96	M.B.CHADWICK AND P.G.YOUNG	625	1451				
6-C - 13 LANL	EVAL-DEC04	P.R.PAGE	628	1451				
7-N - 14 LANL	EVAL-AUG97	M.B.CHADWICK & P.G.YOUNG	725	1451				
8-0 - 16 LANL	EVAL-JUN96	M.B.CHADWICK AND P.G.YOUNG	825	1451				
==> tritons-VIII_0_owners.txt <==								
1-H - 3 LANL	EVAL-FEB01	G.M.HALE	131	1451				
2-He- 3 LANL	EVAL-AUG01	G.M.HALE	225	1451				
<u>2-He- 4 LLNL</u>	EVAL-DEC99	R.M.White, D.A.Resler, S.I.Warshaw	228	1451				
3-Li- 6 LANL	EVAL-SEP01	G.M.HALE	325	1451				
3-Li- 7 LLNL	EVAL-JUN16	I.Thompson, P.Navratil, D.Brown	328	1451				

### <sup>6</sup>Li deuterons, neutrons



