OAK RIDGE National Laboratory

Status Report on Nuclear Data Activities at Oak Ridge National Laboratory

USNDP 2021

Michael Smith, Caroline Nesaraja, Murray Martin, Larry Zhang

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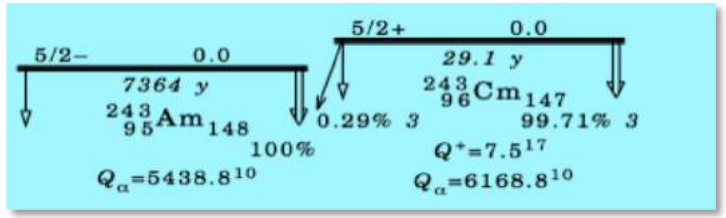
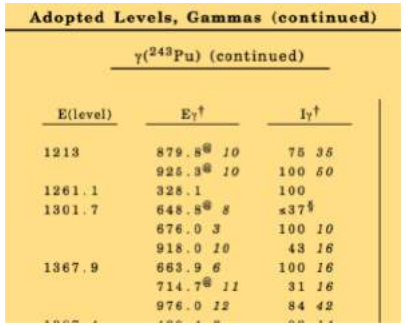
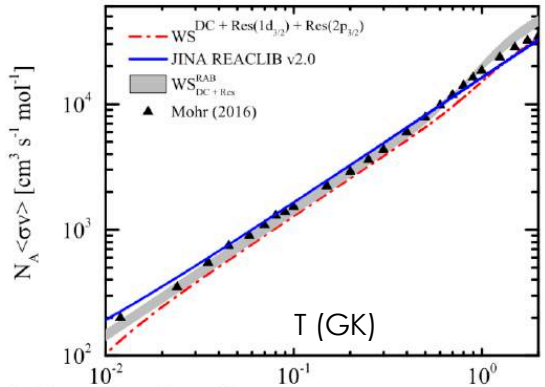
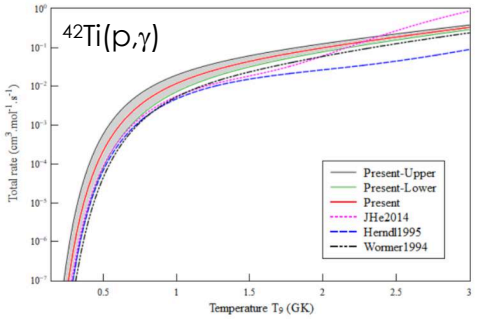
U.S. DEPARTMENT OF ENERGY

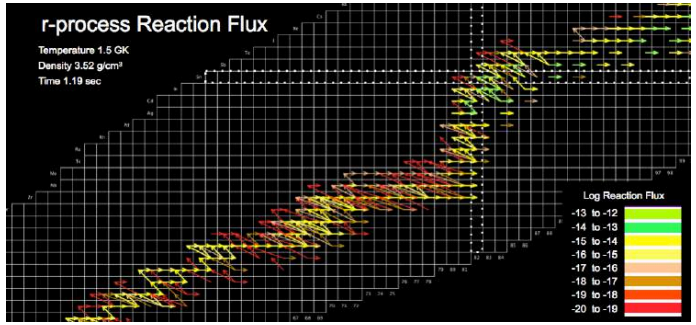
Members and Scope of Activities

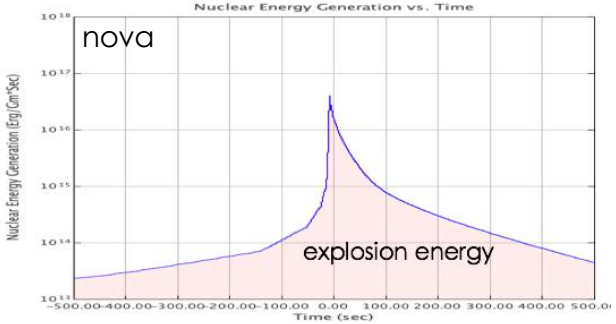












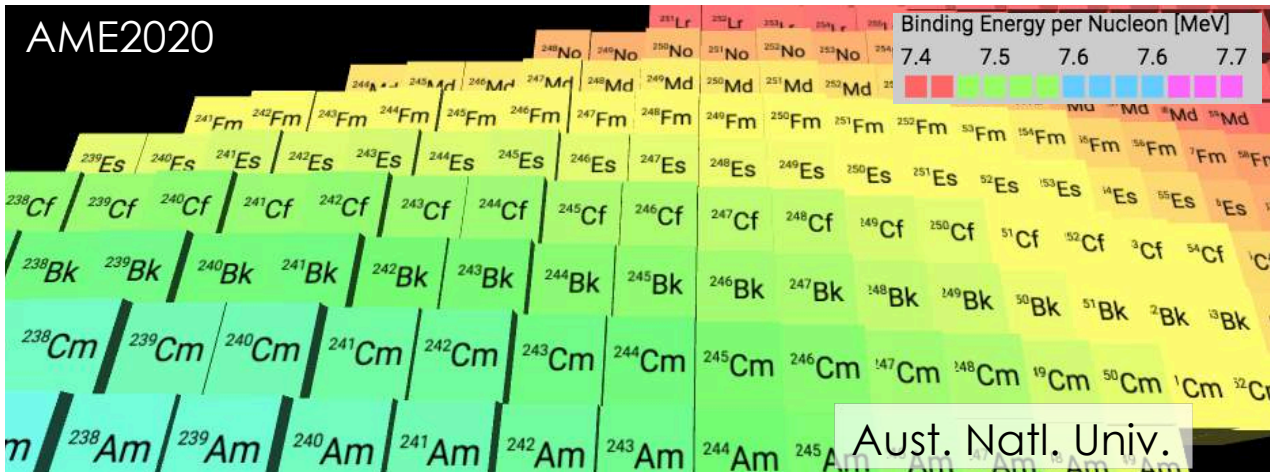
nucastrodata.org

- Members and Activities:
  - Caroline Nesaraja: Research Staff Member - ENSDF evaluator
  - Murray Martin: Subcontractor - ENSDF evaluator and consultant
  - Michael Smith: Research Staff Member - nuclear astro data, software systems
  - Larry Zhang : Student - nuclear astrophysics data

Nuclear Structure Data ENSDF Evaluations

Caroline Nesaraja
Murray Martin

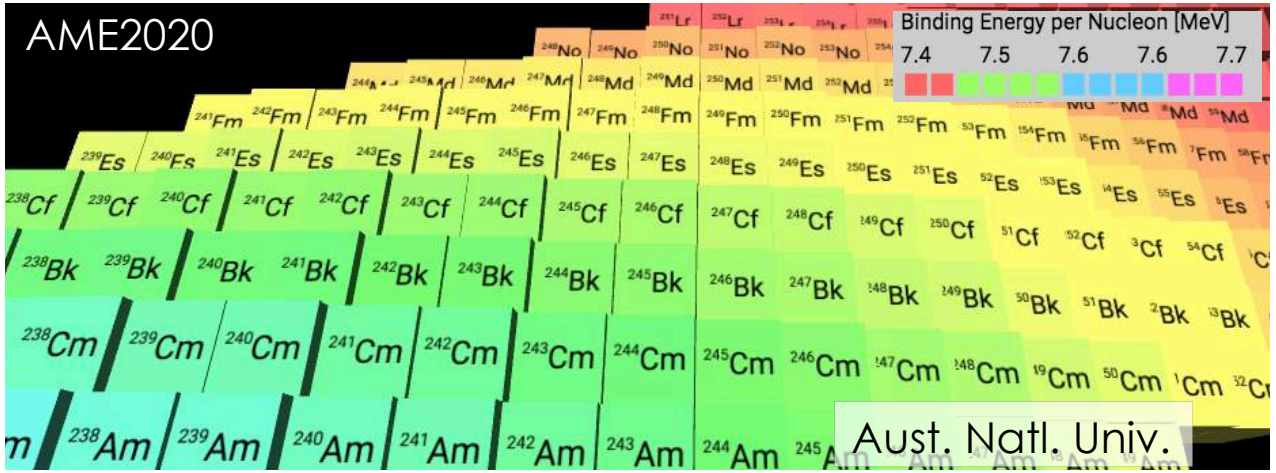
- **ORNL responsibility: A=241-249**



A	Current Lit Cut Off Date	Current Publication Year	Authors	Reference	New Lit Cut Off Date	Latest Status	New Evaluator
241	Sep-15	2015	C.D. Nesaraja	NDS 130 (2015) 183			
242	Sep-01	2002	Y. Akovali	NDS 96 (2002) 177		Post Rev- Submitted	M. Martin
243	Sep-13	2014	C.D. Nesaraja & E.A. McCutchan	NDS 121 (2014) 695			
244	Aug-17	2017	C.D. Nesaraja	NDS 146 (2017) 387			
245	Jun-10	2011	E. Browne & J.K. Tuli	NDS 112 (2011) 447		Post Rev	C.D. Nesaraja
246	Jan-11	2011	E. Browne & J.K. Tuli	NDS 112 (2011) 1833			
247	Mar-14	2015	C. D. Nesaraja	NDS 125 (2015) 395			
248	Sep-14	2014	M.J. Martin	NDS 122 (2014) 377			
249	Dec-10	2011	K. Abusaleem	NDS 112 (2011) 2129		Submitted	C.D. Nesaraja

Nuclear Structure Data ENSDF Evaluations

Caroline Nesaraja
Murray Martin



- **ORNL responsibility: A=241-249**

sorted by cut-off date

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Aug-17	244	2017	C.D. Nesaraja	NDS 146 (2017) 387			
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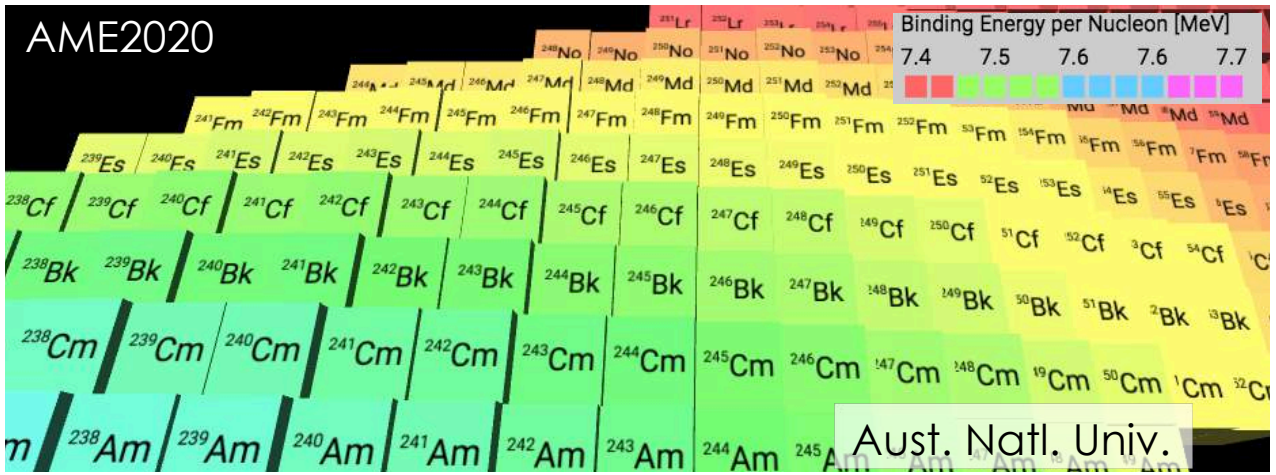
Nuclear Structure Data ENSDF Evaluations



- **Mass chains we evaluated that are outside ORNL's responsibility:**

A= 41 – Published

A= 58 – Published

A= 66 – Post Review

A= 69 – Published

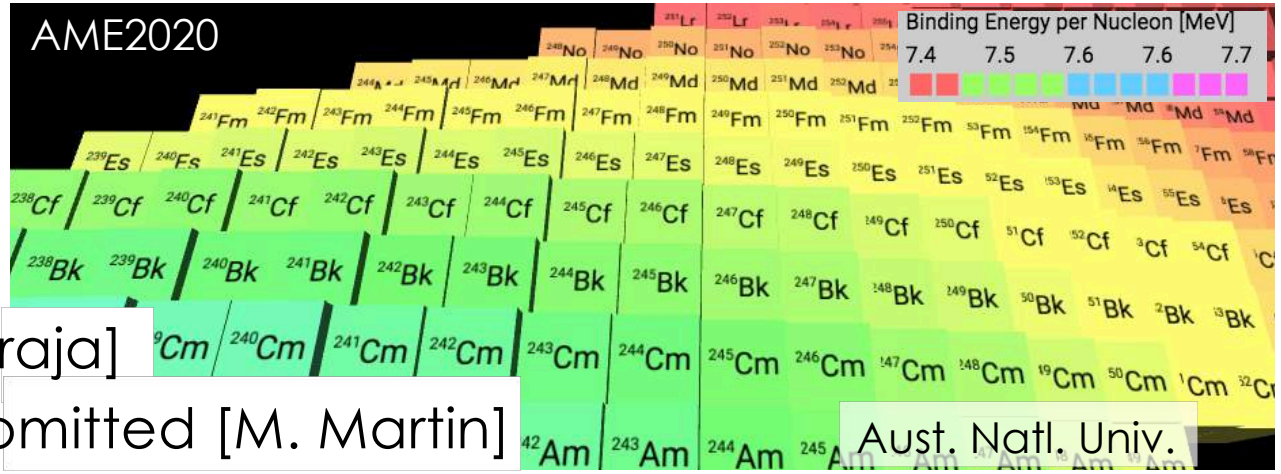
A=137 - Post Review

A= 208 - Published

A= 216 - Underway

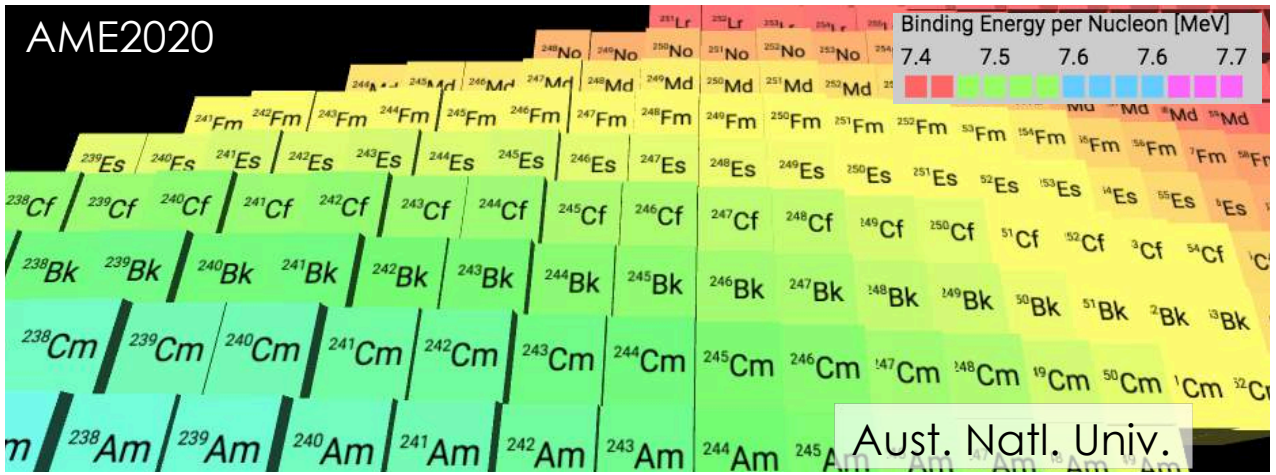
A= 63 – Next in line for evaluation

Nuclear Structure Data
ENSDF Evaluations



- **FY21 Evaluations**
  - A=249 8 Nuclides [C. Nesaraja]
  - A= 242 post review edits submitted [M. Martin]
- **FY21 Edits *in Progress***
  - A=137 16 nuclides [C. Nesaraja]
  - Very lengthy and challenging mass chain
  - post review editing and addition of new work in progress
- **FY21 Review**
  - A=48 [C. Nesaraja]
- **Others**
  - Guidelines for Evaluators [M. Martin]- complete

Nuclear Structure Data
ENSDF Evaluations



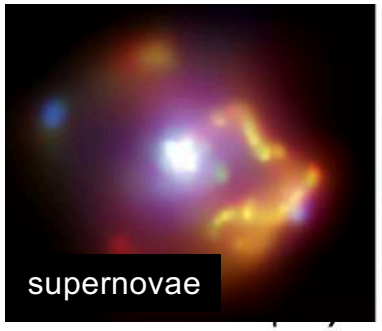
- **FY22 Post Review Edits**
  [C. Nesaraja]

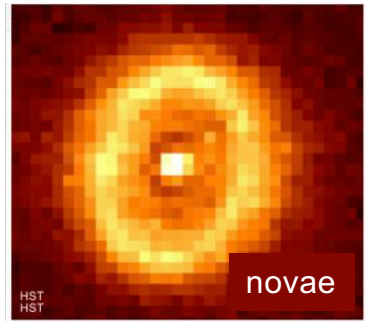
  A=137, A=66 A=245

- **FY22 Evaluation**

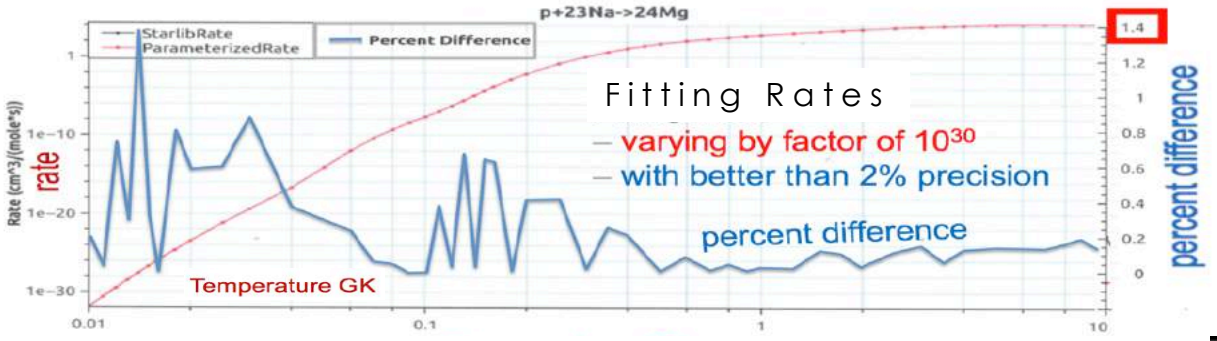
  A=216 [M. Martin]

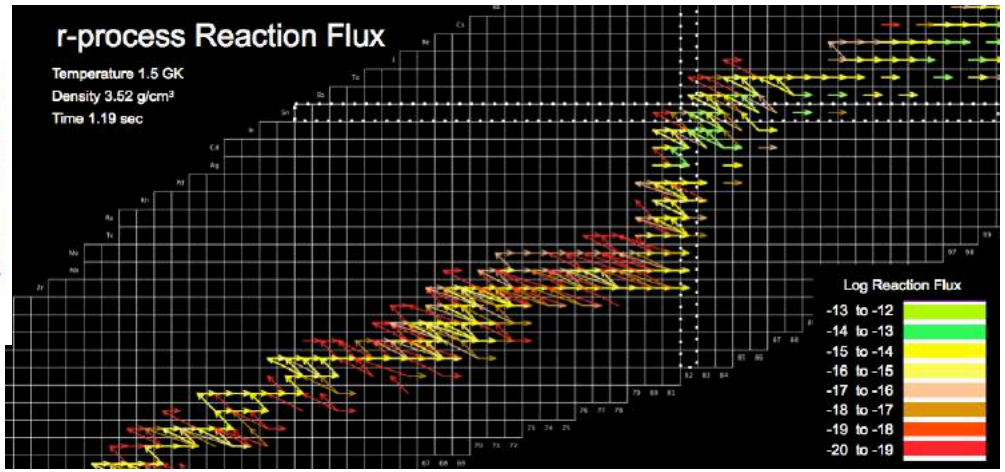
Nuclear Astrophysics Data





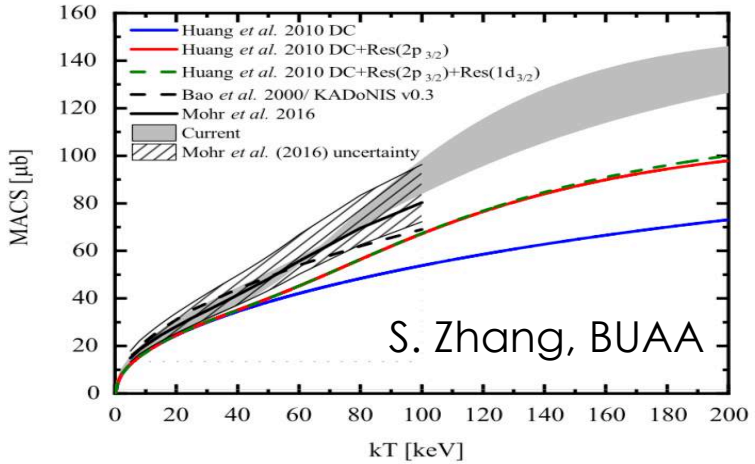
FRIB

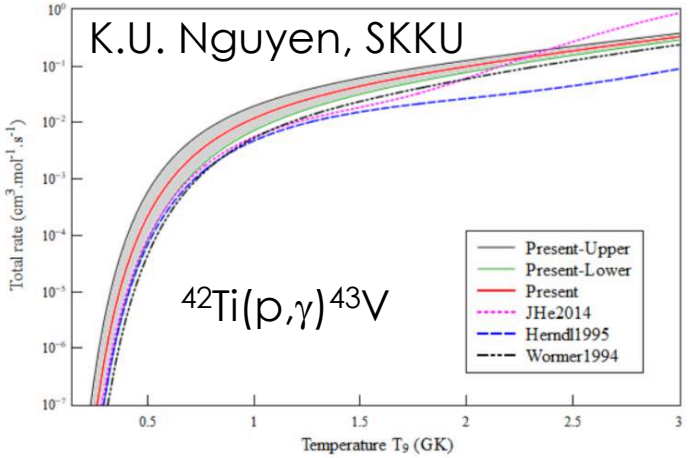




- focus on Stellar Explosions
- we **closely couple data activities to measurements** on unstable nuclei as recommended in NSAC LRP and listed as DOE NP milestones
- Personnel
  - *Michael Smith – Staff*
  - *Larry Zhang – Student*

Collaborators





- Beihang Univ. (BUAA) in Beijing, China
  - **Shisheng Zhang** (Professor) – theoretical nuclear physics, cross section predictions
  - **B. Shao**, **S. Y. Zhong, Sizhe Xu** (BUAA grad students) – theoretical nuclear physics
- SungKyunKwon Univ. (SKKU) in Korea
  - **Kyungyuk Chae** (Professor) – reaction assessments for astrophysics
  - **C. Kim, K.U. Nguyen** (SKKU grad students) – reaction assessments for astrophysics
- Emory Univ. (Atlanta)
  - **Eric Zhang** (undergrad) – uncertainty quantification in nuclear astrophysics

Reaction Assessments

with BUAA

Eur. Phys. J. A (2021) 57:114
https://doi.org/10.1140/epja/s10050-021-00434-7

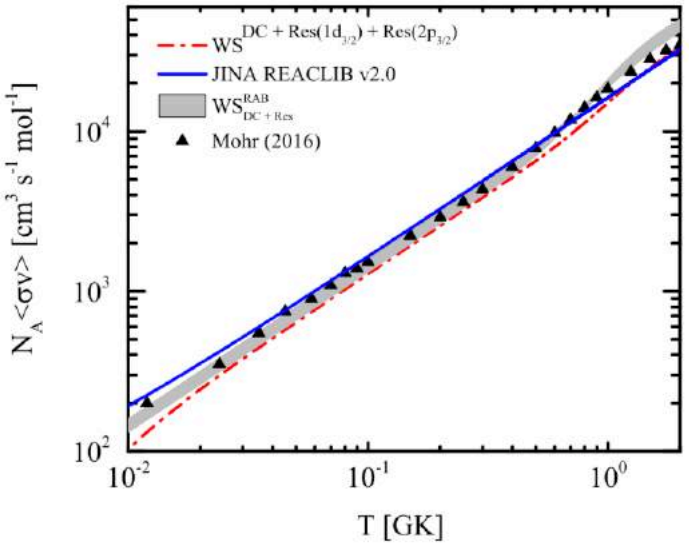
THE EUROPEAN PHYSICAL JOURNAL A

Regular Article -Theoretical Physics

Neutron capture on ^{16}O within the framework of RMF + ACCC + BCS for astrophysical simulations

Shisheng Zhang[1,a] , Sizhe Xu[1] , Meng He[1] , Michael S. Smith[2,b]

[1] School of Physics, Beihang University, Beijing 100191, China
[2] Phy



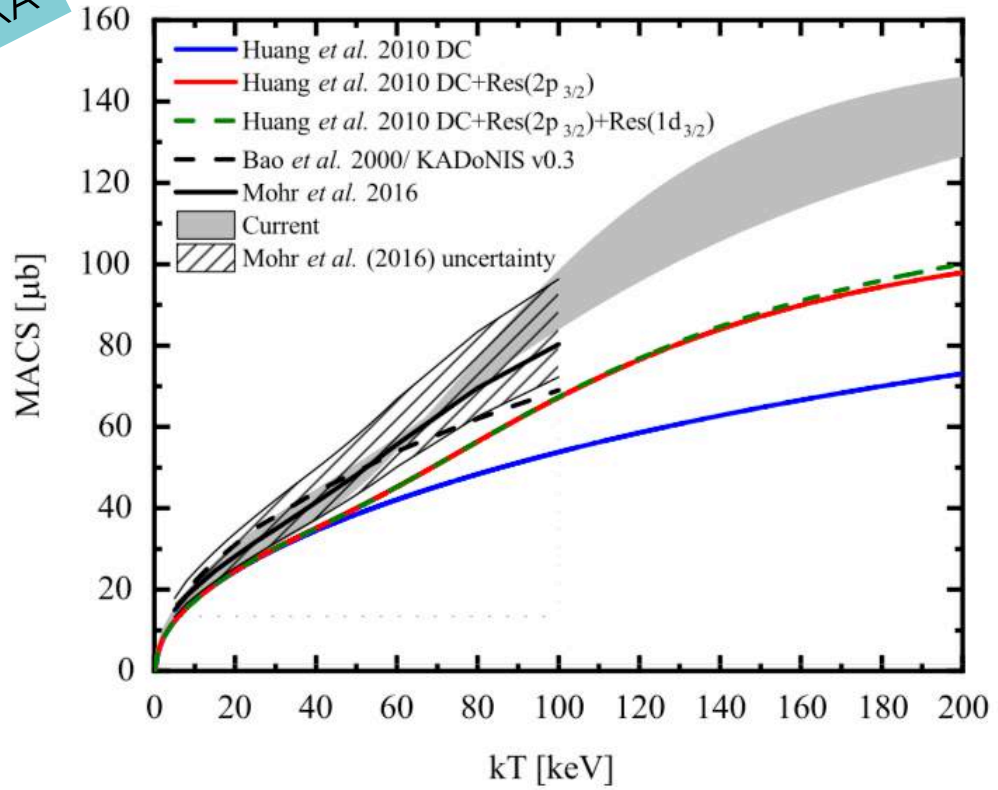


Fig. 3 The ^{16}O(n, γ)^{17}O Maxwellian averaged cross sections (MACS) from four effective interactions using the RAB approach are shown spanning the gray region. Also shown are the MACS from the KaDoNIS database of neutron capture reactions [51], from Mohr et al. [4] with uncertainty, and the direct capture only from Huang et al. [27] along with the resonant contributions added in for the $2p_{3/2}$

- Theoretical neutron capture study – benchmark study

Reaction Assessments

with SKKU

Assessment of the reaction rates of ^{42}Ti(p,γ)^{43}V in type I X-ray burst

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M. S. Smith

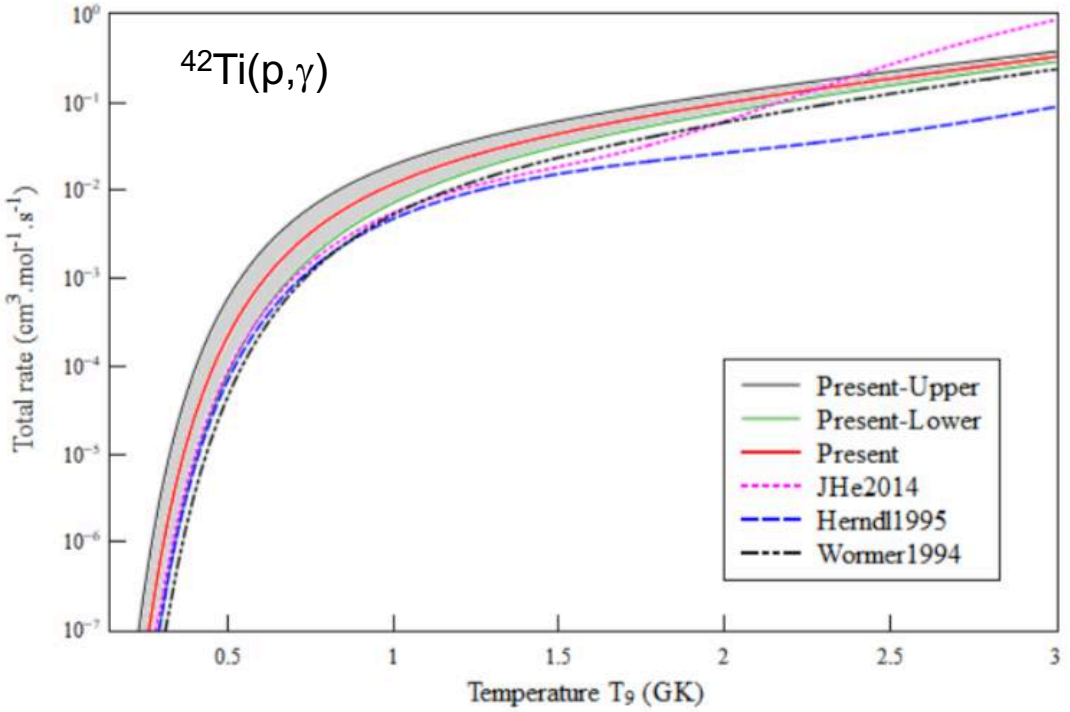
Physics Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA

L. Xayavong

Department of Physics, National University of Laos, 7322, Dongdok, Vientiane, Lao PDR

Table 2. The presently parameters for the ^{42}Ti(γ,p)^{43}V resonant reaction rates. The adopted proton separation energy $S_p = 100 \pm 43$ keV regarding to the AME16 relied on Ref. [16].

E_x (MeV)	E_i (MeV)	τ (ps)	J^π	l	C^2S_p	Γ_γ (eV)	Γ_p (eV)	$\omega\gamma$ (MeV)
0.436	0.336	22.00	$(\frac{5}{2})^-$	3	0.150	2.99×10^{-05}	1.73×10^{-08}	5.18×10^{-14}
0.537	0.437	117.00	$(\frac{3}{2})^-$	1	0.046	5.63×10^{-06}	1.09×10^{-04}	1.07×10^{-11}
1.014	0.914	9.14	$(\frac{3}{2})^-$	1	0.002	7.20×10^{-05}	6.07×10^{-02}	1.44×10^{-10}
1.844	1.744	0.61	$(\frac{3}{2})^-$	1	0.905	1.09×10^{-03}	$6.74 \times 10^{+03}$	2.17×10^{-09}



- Assessment of the ^{42}Ti(p,γ) rate for X-ray burst nucleosynthesis studies

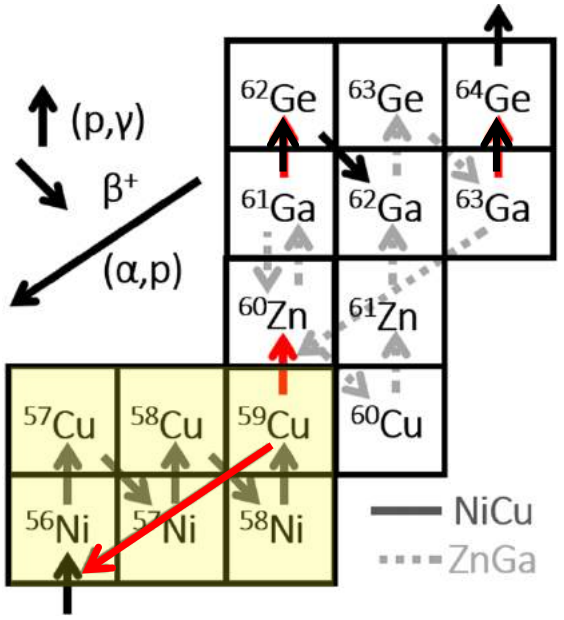
Reaction Assessments

with SKKU

Nuclear Evaluation on 60Zn:

59Cu(p,g) vs 59Cu(p,a) reaction rates based on Monte Carlo method

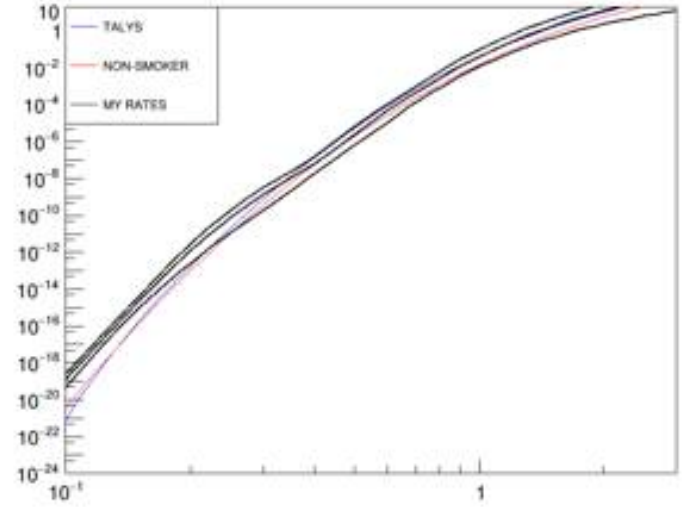
Chanhee Kim, K.Y. Chae et al. SKKU
M.S. Smith, ORNL



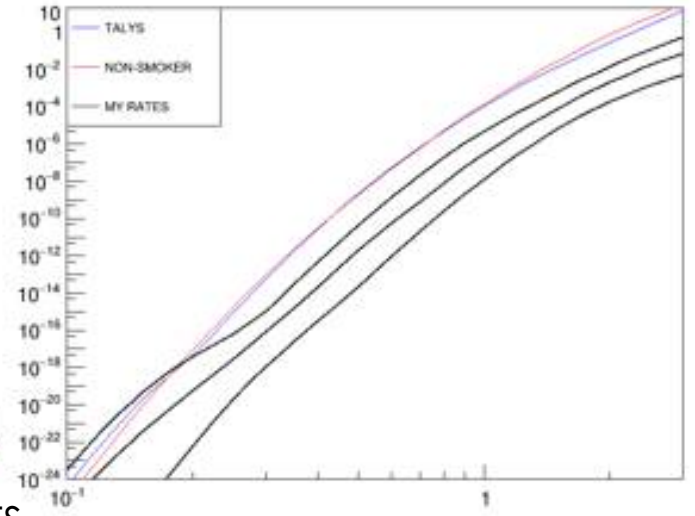
Level energies

Weighted Avg		Uncertain
5.183097		0.06
5.2918		8.94E-04
5.336		0.004
5.369		0.002
5.501858		2.00E-03
5.729		0.003
5.954825		0.07
6.344086		0.07
6.637687		0.002984
6.920409		0.048507
7.112626		0.07
7.31784058		0.05
7.3704		0.003947
7.469003		0.003999
7.641622		0.07
7.940262		0.05

59Cu(p,g)



59Cu(p,a)

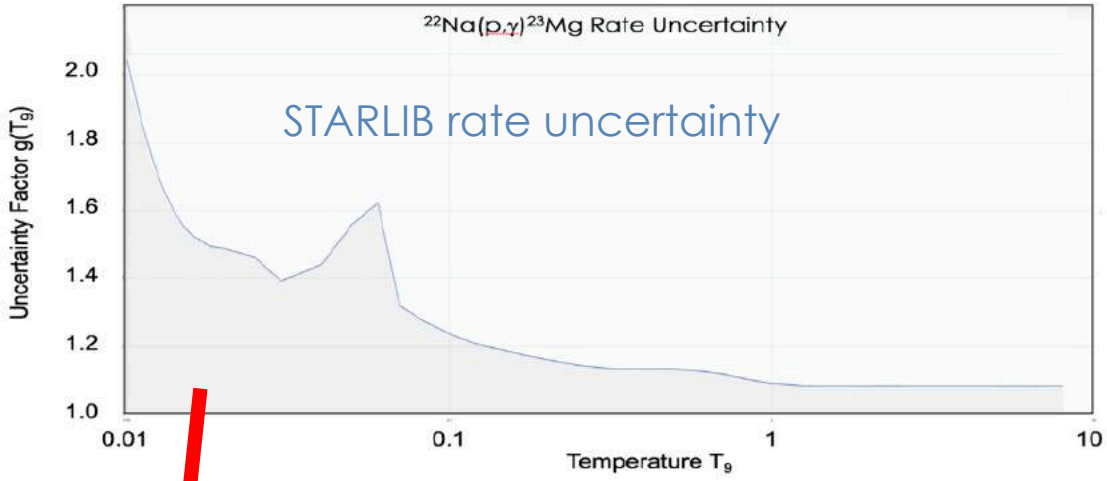


- Assessment of the $^{59}Cu(p,\gamma)$ and $^{59}Cu(p,\alpha)$ rates for X-ray bursts

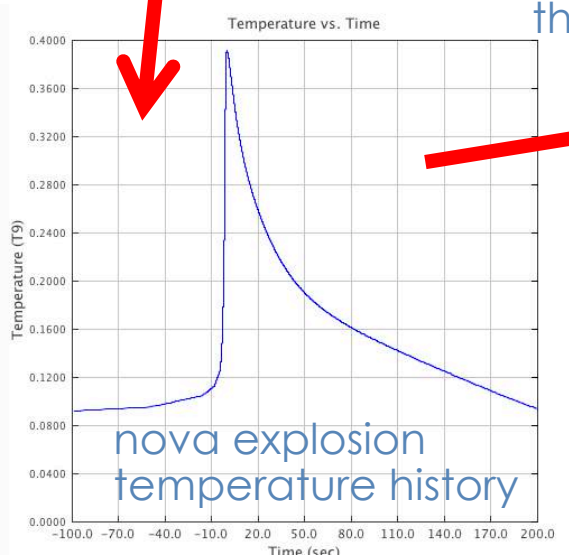
Nuclear Astrophysics Data

STARLIB rates

14C(a,g)18O	25Al(p,g)26Si	18O(p,g)19F	31P(p,a)28Si
14C(p,g)15N	25Mg(p,g)26Al	19Ne(p,g)20Na	31P(p,a)28Si
14N(a,g)18F	26Al(p,g)27Si	20Ne(a,g)24Mg	31P(p,g)32S
15N(a,g)19F	26Mg(p,g)27Al	20Ne(p,g)21Na	31S(p,g)32Cl
15O(a,g)19Ne	26Si(p,g)27P	21Na(p,g)22Mg	32Cl(p,g)33Ar
16O(a,g)20Ne	27Al(p,a)24Mg	21Ne(p,g)22Na	32S(p,g)33Cl
16O(p,g)17F	27Al(p,g)28Si	22Mg(p,g)23Al	34Ar(p,g)35K
17F(p,g)18Ne	27P(p,g)28S	22Na(p,g)23Mg	35Ar(p,g)36K
17O(p,a)14N	27Si(p,g)28P	22Ne(p,g)23Na	35Cl(p,a)32S
17O(p,g)18F	28Si(p,g)29P	23Al(p,g)24Si	35Cl(p,g)36Ar
18F(p,a)15O	29P(p,g)30S	23Mg(p,g)24Al	35K(p,g)36Ca
18F(p,a)15O	29Si(p,g)30P	23Na(p,a)20Ne	36Ar(p,g)37K
18F(p,g)19Ne	30S(p,g)31Cl	23Na(p,g)24Mg	38Ar(p,g)39K
18O(a,g)22Ne	30Si(p,g)31P	24Al(p,g)25Si	39Ca(p,g)40Sc
18O(p,a)15N	31Cl(p,g)32Ar	24Mg(a,g)28Si	40Ca(p,g)41Sc
		24Mg(p,g)25Al	



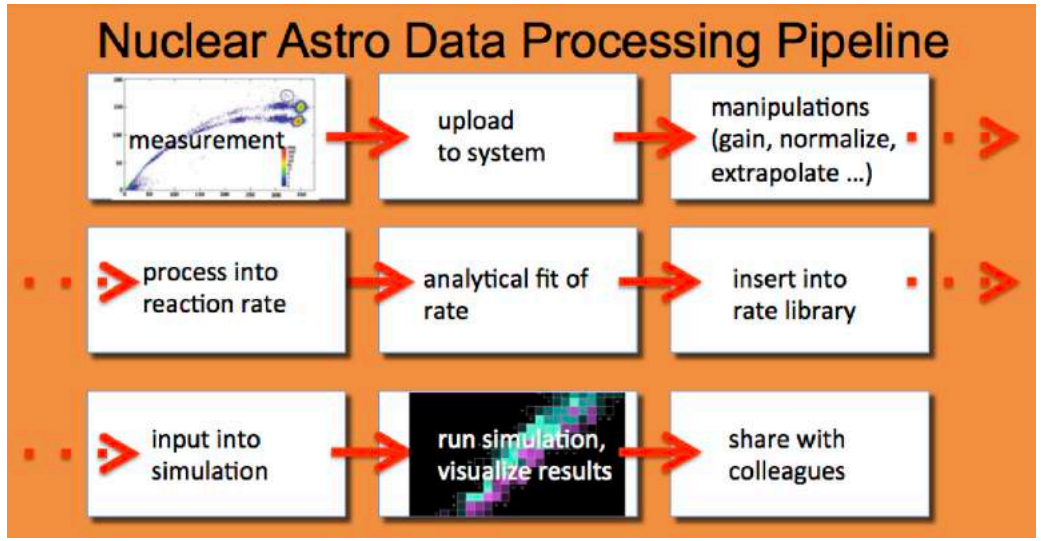
thermally avg uncertainty



Rate	Uncertainty Factor
n13 (p,g) o14	1.41
n14 (p,g) o15	1.08
n14 (a,g) f18	1.14
n15 (p,g) o16	1.42
n15 (a,g) f19	1.76
o15 (a,g) ne19	2.88
o16 (p,g) f17	1.07
o16 (a,g) ne20	1.41
o17 (p,g) f18	1.05
o18 (p,g) f19	1.34
o18 (a,g) ne22	2.08
...	...

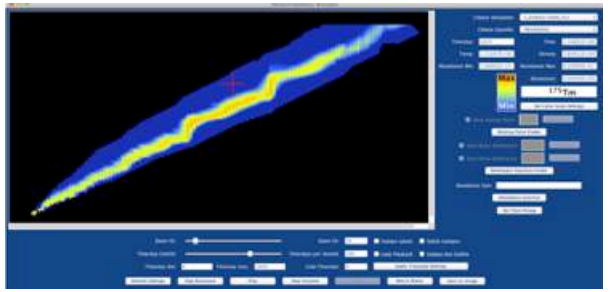
- improving thermonuclear reactions
  - processing & thermally averaging rate uncertainties

Online Software Systems



Computational Infrastructure for Nuclear Astrophysics

since 2004



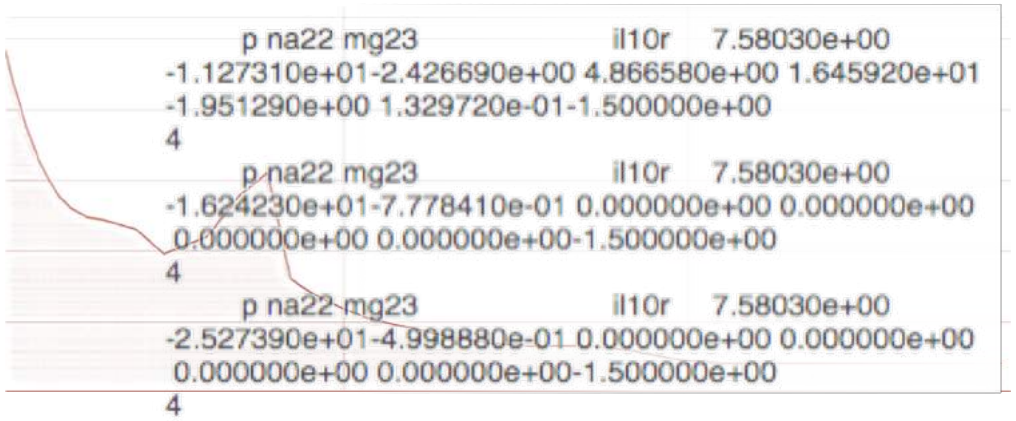
nucastrodata.org

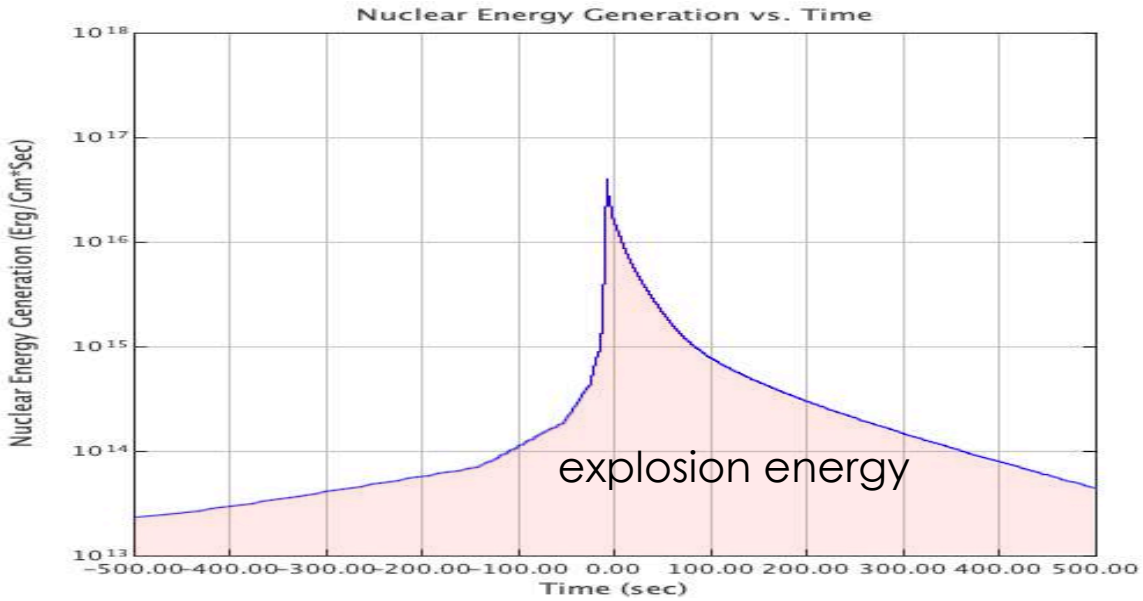
nuclearmasses.org

BIG BANG ONLINE

- ***unique*** set of online software systems that **serve** the community carrying out DOE NP-supported research programs and endorsed by NSAC LRP
- systems used by researchers in over **180 institutions** in **42 countries**
- systems improve return on investment of **nuclear data for research projects**
- many ideas for expanding and improving these services
- *budget crisis in FY21 prevented any work on these important systems*

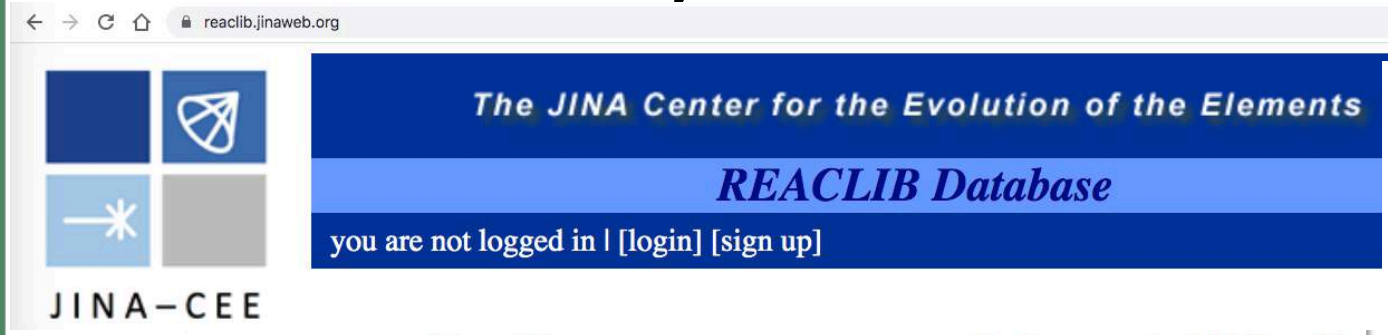
Future Possible Projects





- add **uncertainties** to REACLIB thermonuclear rate library
- update REACLIB **content** !
- develop benchmark simulations and integral parameters (*e.g.*, k_{eff} equivalents) to help validate nuclear astrophysics rate libraries
- explore processing (some) TALYS cross sections into REACLIB rate format

Future Possible Projects




```
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 1.286780e+01 0.000000e+00 0.000000e+00 1.021480e+00
-3.346380e-01 2.587080e-02 0.000000e+00
         p na22 mg23                          il10r     7.58030e+00
-1.127310e+01-2.426690e+00 4.866580e+00 1.645920e+01
-1.951290e+00 1.329720e-01-1.500000e+00
         p na22 mg23                          il10r     7.58030e+00
-1.624230e+01-7.778410e-01 0.000000e+00 0.000000e+00
 0.000000e+00 0.000000e+00-1.500000e+00
         p na22 mg23                          il10r     7.58030e+00
-2.527390e+01-4.998880e-01 0.000000e+00 0.000000e+00
 0.000000e+00 0.000000e+00-1.500000e+00
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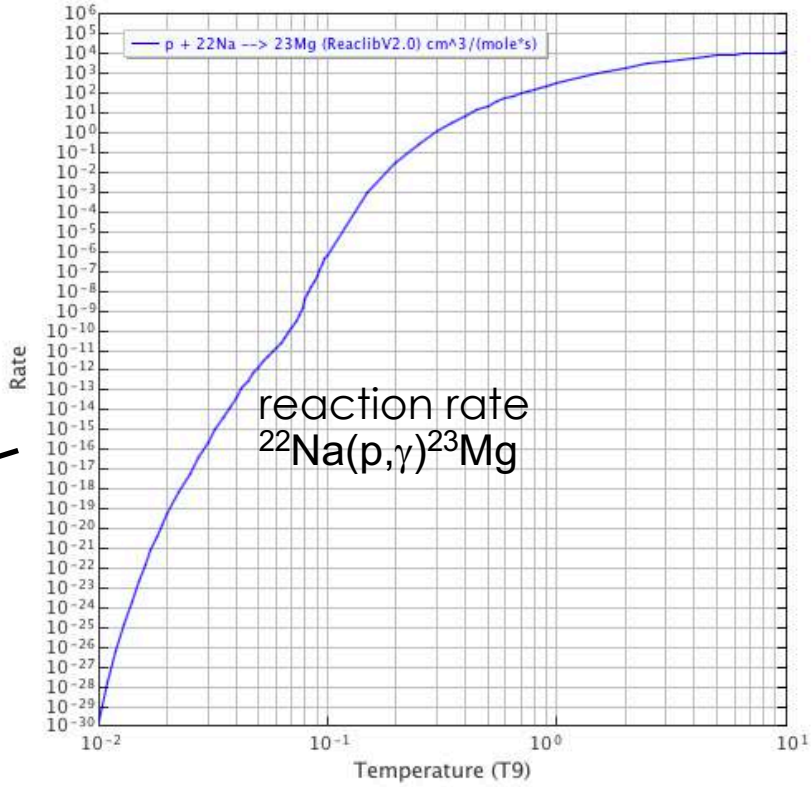
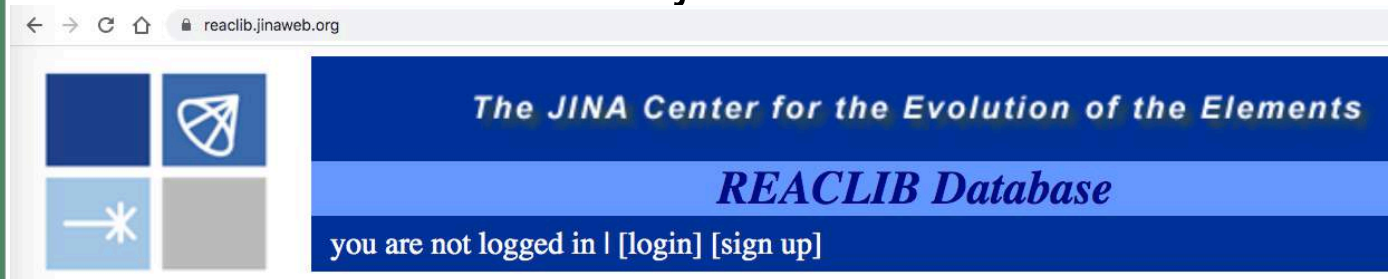


- *REACLIB thermonuclear rate library*
  - *premier library of 160K thermonuclear rates for astrophysics studies*

Future Possible Projects

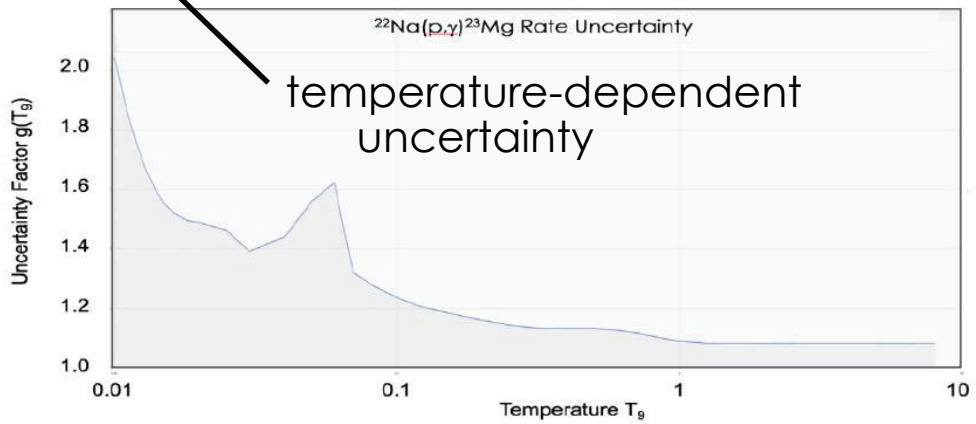



```
      p na22 mg23                              or19u     7.58030e+00
0.217482E+01-0.473654E-01 0.305791E+01-0.544033E+01
0.376213E+00-0.246853E-01 0.242742E+01
      p na22 mg23                              or19u     7.58030e+00
0.762099E+05-0.136089E+02 0.662628E+04-0.129827E+06
0.120678E+06-0.130081E+06 0.171071E+05
```

uncertainty

thermally avg uncertainty

Rate	Uncertainty Factor
n13 (p,g) o14	1.41
n14 (p,g) o15	1.08
n14 (a,g) f18	1.14
n15 (p,g) o16	1.42
n15 (a,g) f19	1.76
o15 (a,g) ne19	2.88
o16 (p,g) f17	1.07
o16 (a,g) ne20	1.41
o17 (p,g) f18	1.05
o18 (p,g) f19	1.34
o18 (a,g) ne22	2.08
...	...



temperature-dependent uncertainty

added value: improved return on investment of nuclear data **uncertainties** for DOE NP supported research

- *REACLIB thermonuclear rate library*
  - *research community needs rate uncertainties for UQ studies*
  - *needs updated rates to keep the data base current and relevant !*

Synergistic Activities – WANDA2021

Workshop for Applied Nuclear Data Activities (WANDA 2021)

Session Three: Advanced Computing for Nuclear Data

State of computational nuclear data and future prospects

Speaker: Nicolas Schunck (LLNL)

Higher-fidelity simulations with HPC

- Predictive theory for light-ion reactions, Kostas Kravvaris (LLNL)
- HPC for fission modeling in support of nuclear data, Ionel Stetcu (LANL)
- Propagation of nuclear model uncertainties in science applications, Trevor Sprouse (LANL)
- Perspectives from the ExaSMR Project: Nuclear Data Needs and Opportunities, Paul Romano (ANL)

Speakers: Ionel Stetcu, Kostas Kravvaris, Paul Romano, Trevor Sprouse

AI/ML as Enabling Technologies

- Containerization and microservices for nuclear data, Georg Schnabel (IAEA)
- Selected topics from physics aware ML, Mateusz Ploskon (LBNL)
- Natural Language Processing for Nuclear Science Scholarship, Walid Younes (LBNL Consu
- Surrogate Modeling for Fission Cross Sections and Criticality - Studies using Artificial Neu Christian Brazell (TAMU)

Speakers: Christian Brazell, Georg Schnabel, Mateusz Ploskon, Walid Younes

Quantum Computing

Speaker: Kyle Wendt

- Advanced Computing **Session Organizer**
  - Nicolas Schunck, MSS, Bethany Goldblum, Matthew Mumpower, Ben Loer, David Brown

Synergistic Activities – WANDA2021

Current Nuclear Data Needs for Applications

Karolina Kolos[1], Vladimir Sobes[2], Ramona Vogt[1,3], Catherine E. Romano[4], Michael S. Smith[5], Lee A. Bernstein[6,7], David A. Brown[8], Mary T. Burkey[9], Yaron Danon[10], Mohamed A. Elsawi[11], Bethany L. Goldblum[6,7], Lawrence H. Heilbronn[2], Susan L. Hogle[12], Jesson Hutchinson[13], Ben Loer[14], Elizabeth A. McCutchan[7], Matthew R. Mumpower[15], Ellen M. O'Brien[16], Catherine Percher[17], Patrick N. Peplowski[18], Jennifer J. Ressler[9], Nicolas Schunck[1], Nicholas W. Thompson[13], Andrew S. Voyles[6,7], William Wieselquist[19], Michael Zerkle[20]

[317] R. Arcilla *et al.*, Continuous Integration and Deployment Software to Automate Nuclear Data Verification and Validation, Nucl. Data Sheets **118**, 422 (2014).
[318] D. Neudecker *et al.*, Enhancing Nuclear Data Validation Analysis by Using Machine Learning, Nucl. Data Sheets **167**, pp. 36-60 (2020).
[319] B. Whewell *et al.*, Evaluating ^{239}Pu(n,f) Cross Sections via Machine Learning using Experimental Data, Covariances and Measurement Features, Nucl. Instr. Meth. A **978**,164305 (2020).

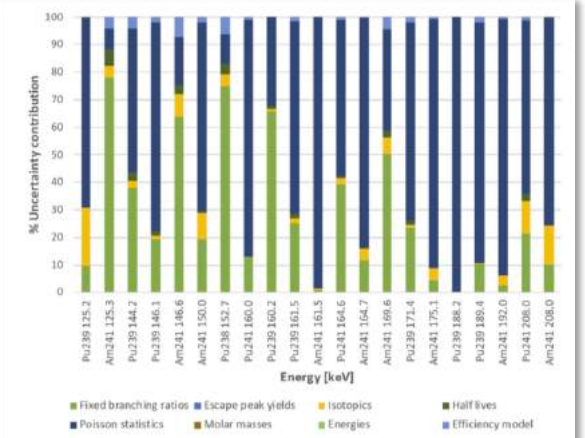


FIG. 14: Uncertainty analysis for signatures used in non-destructive assay of MSRs [261].

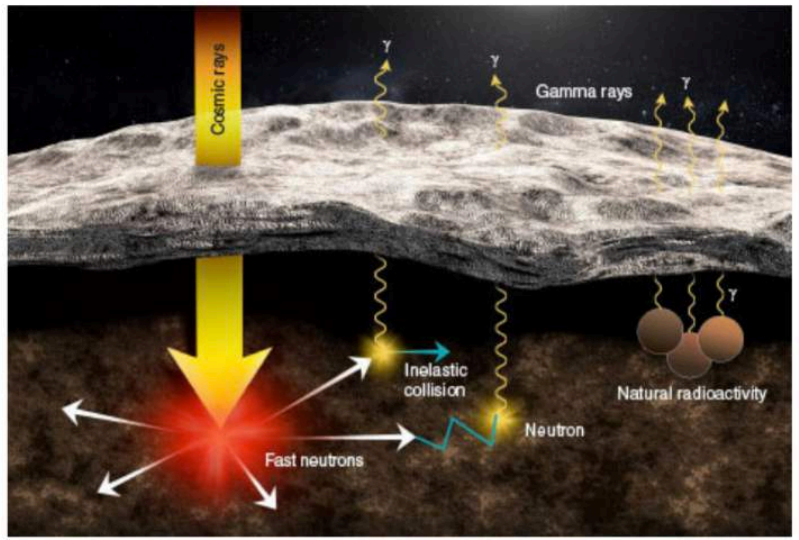


FIG. 9: Schematic of cosmic ray interactions with planetary surfaces. Rendering by Veronica Chen [231].

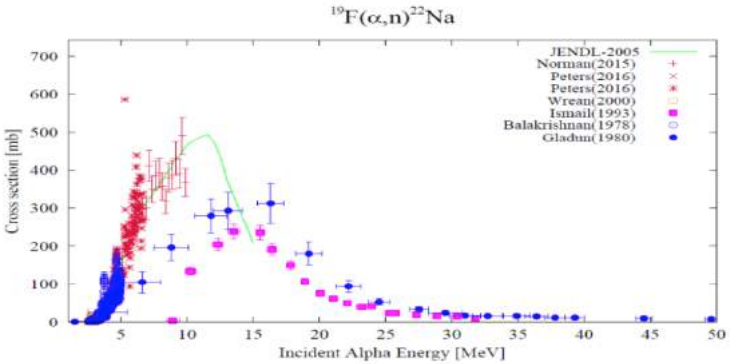
- WANDA 2021 **Proceedings Editor**
  - Ramona Vogt (Chief Editor), MSS, Kay Kolos, Vlad Sobes, Cathy Romano
  - to be published in **Phys. Rev. R**
  - 26 authors, 8 sections, 41 pages, 319 references, 14 figures

Synergistic Activities – Non-Proliferation

(α,n) Nuclear Data Scoping Study

Isotope	Current state of data	Reaction threshold	Applications	
			Highest priority	
^{13}C	Recent data (4–6.5 MeV) to be published, new evaluation needed.	450–800 keV	NDA/ER, safeguards, advanced reactors, background simulations	Low-energy mea… Dame measurem… data are being ev… are resolved.
^{17}O	Recent evaluation available for next ENDF release—discrepancies in neutron spectrum remain	800 keV–1.2 MeV	Safeguards, reactors, NDA/ER, background simulations	Recent Notre Da… to 7 MeV will pr… spectrum. Updat…
^{18}O	Recent evaluation available for next ENDF release—discrepancies in neutron spectrum remain	850 keV–1.4 MeV	Safeguards, reactors, NDA/ER, Background simulations	Notre Dame mea… 8 MeV will prov… spectrum. Updat…
^{19}F	No evaluation of recent data— benchmark and neutron spectrum data needed	2.3 MeV	Safeguards UF_6, FLiBe reactors, fuel cycle and waste management applications	2016 measurem… alphas.[b] Still nee… emission with lo… total cross section, angular distributions, neutron energy spectra, activation, and thick target integral measurements are needed to reduce uncertainties.
			High priority	
^{7}Li	Adjusted evaluation based on JENDL data available for next ENDF release, large discrepancies in data	3–4 MeV	FLiBe reactors, NDA/ER, safeguards Important for characterization of actinide-Li neutron sources	New experiments with ability to resolve excitation states and reaction channels and new evaluations are needed to accurately model neutron sources.
^{9}Be	Neutron spectrum has been validated and new evaluation available for next ENDF	200 KeV	FLiBe reactors, NDA/ER, safeguards Important for characterization of actinide-	New data are required specifically above 5 MeV to address the multiple breakup channels in the cross section and to collect neutron energy and angular distributions. Evaluations based on

Catherine Romano
David Brown
Stephen Croft
Andrea Favalli
Les Nakae
Marco Pigni
Steve Skutnik
Michael S. Smith
William Wieselquist
Michael Zerkle



- Non-Proliferation efforts for NNSA
  - co-authored scoping study that made recommendations for a multi-year program of evaluations & experiments of (alpha,n) for applications

Synergistic Activities – Machine Learning

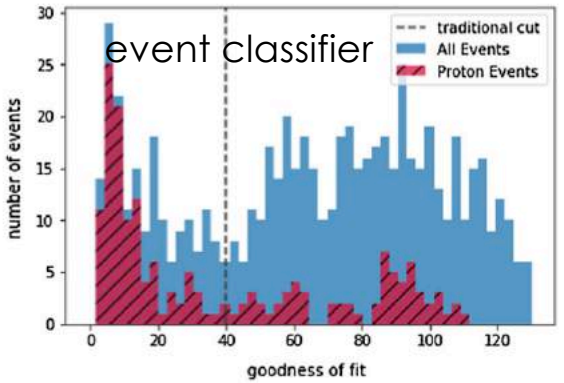
Eur. Phys. J. A (2021) 57:100
https://doi.org/10.1140/epja/s10050-020-00290-x

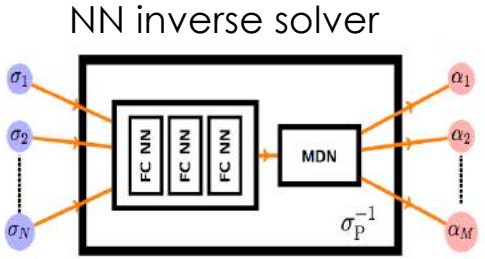
THE EUROPEAN PHYSICAL JOURNAL A

Review

A.I. for nuclear physics

Paulo Bedaque[1], Amber Boehnlein[2,a], Mario Cromaz[3], Markus Diefenthaler[2], Latifa Elouadrhiri[2], Tanja Horn[4], Michelle Kuchera[5], David Lawrence[2], Dean Lee[6], Steven Lidia[6], Robert McKeown[2], Wally Melnitchouk[2], Witold Nazarewicz[6], Kostas Orginos[2,7], Yves Roblin[2], Michael Scott Smith[8], Malachi Schram[9], Xin-Nian Wang[3]





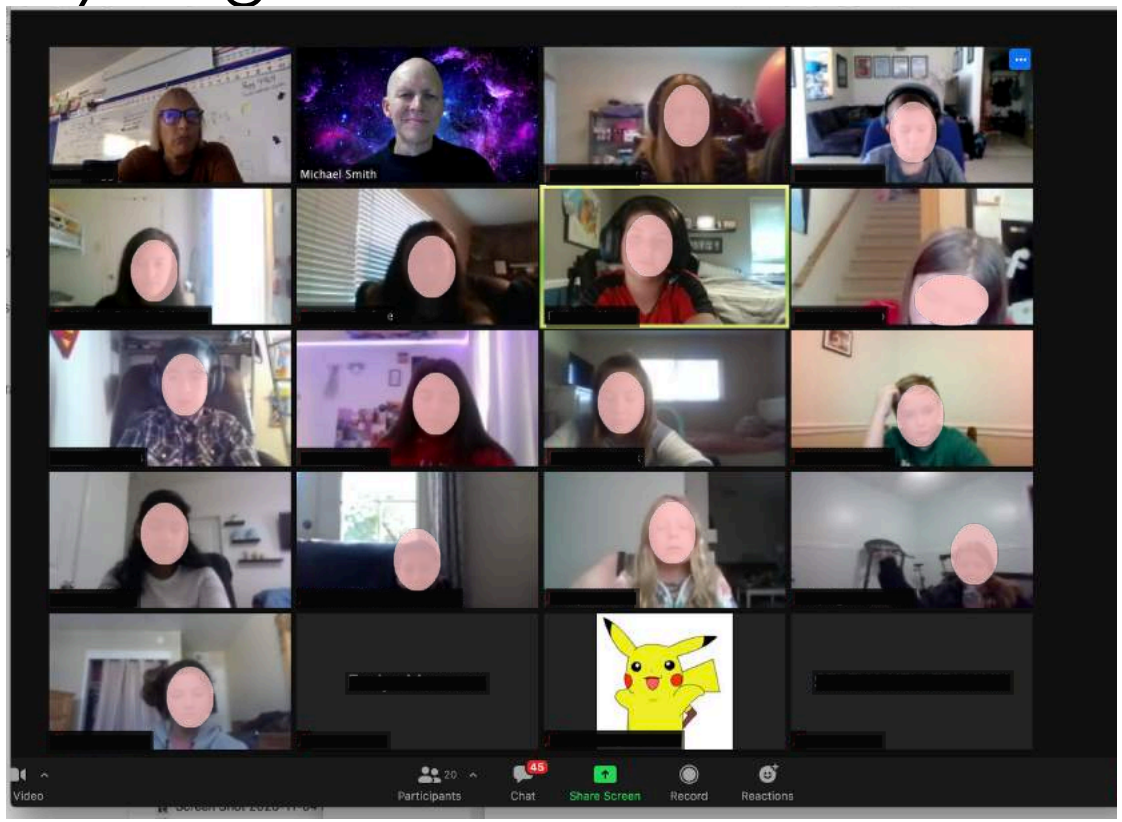
Machine learning and artificial intelligence in nuclear physics

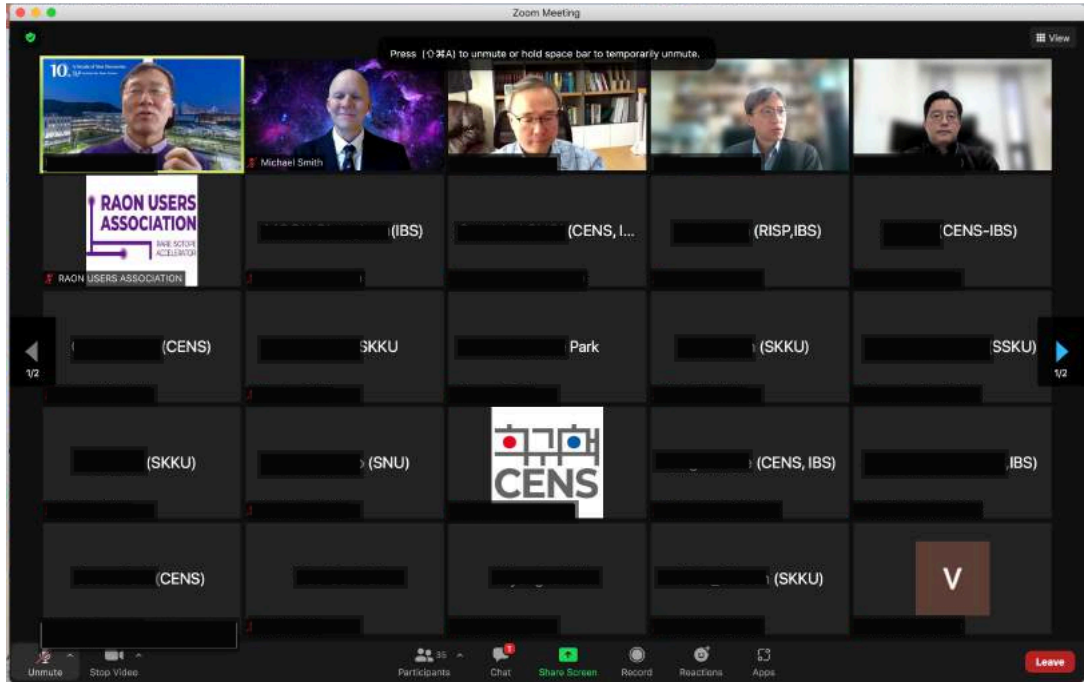
Editors
Amber Boehnlein[1], Markus Diefenthaler[1], Morten Hjorth-Jensen[4] Tanja Horn[3], Michelle Kuchera[3], Dean Lee[4], Witold Nazarewicz[4], Kostas Orginos[1,5], Alan Poon[7], Michael S. Smith[6], Xin-Nian Wang[7], Long-Gang Pang[8] Veronique Ziegler[n],

[1] *Thomas Jefferson National Accelerator Facility*
[2] *Catholic University*
[3] *Davidson College*
[4] *Michigan State University*
[5] *College of William & Mary*
[6] *Oak Ridge National Laboratory*
[7] *Lawrence Berkeley National Laboratory*
[8] *Central China Normal University*

- co-author of two articles on **ML in NP**
  - EPJA article (2021) and RMP article (to be published in 2022)
  - wrote the "ML in nuclear data" sections

Synergistic Activities – Outreach





- Remote **outreach presentations** on nuclear astrophysics & nuclear data given to middle schools, high schools, undergrads, grads, postdocs … in USA, China, Korea
- **Chair** of APS Committee to Inform the Public (CIP)