

### $LISE_{cute}^{++}$ , Reaction Mechanisms for Exotic Nuclei Production



Oleg Tarasov

8th International Expert Meeting on challenging issues of next-generation high-intensity in-flight separators

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- Introduction
- Porting to Qt
- Assistance team

- Reaction Mechanisms for Exotic Nuclei Production
  - $\circ \quad \textbf{Abrasion-Fission}$ 
    - ✓ Initial Fissioning nucleus
  - Abrasion-Ablation
  - Multistep reaction contribution study *(tomorrow)*
  - Isotope production with High Z beams (tomorrow)

- LISE site statistics
- LISE development plans
- Summary
- Acknowledgements



# **Introduction**





### Introduction



"Cu 🐺 ↔ Ţe



LISE<sup>++</sup> : Rare Isotope Beam Production with Fragment Separators

2°Cu ₩ ΦΦ Te



- The program is constantly expanding and evolving from the feedback of its users around the world
- Many "satellite" tools have been incorporated into the LISE<sup>++</sup> framework
- It can be freely downloaded from the following internet addresses: <u>http://lise.nscl.msu.edu</u>





#### Squeezed for the experts meeting



predict the <u>fragment separator settings</u> necessary to obtain a specific RIB predict the <u>intensity and purity</u> of the chosen RIB

simulate identification plots for on-line comparison

provide a highly user-friendly graphical environment







Reaction Utilities (Characteristics, Converters, Plots),

" «BI»- the automatized search of two-dimensional peaks in spectra

Italy India 0.0 5% 9%

15%

Germany

Japan

640 South Shaw Lane · East Lans

# LISE++ porting

This time is better known as the time of Covid...





## LISE<sup>++</sup> transportation $\rightarrow$ LISE $_{cute}^{++}$



- The LISE<sup>++</sup> code (v.6-13) was developing at Borland C++ 5.02 IDE (integrating development environment), which is not compatible with the next Borland (Builder, Embarcadero C++) generations
- The LISE<sup>++</sup> software suite was ported to Qtframework in order to
  - Aid in sustainability of the code
  - Support modern compilers and computing methods:
    - ✓ 64-bit operation
    - Cross-platform compatibility (Windows, Mac, and Linux versions)
    - ✓ The ability to take advantage of computational progress (for example parallel computing methods)
    - Integration with control systems





LISE<sup>++</sup>, created using the Qt framework, is named LISE<sub>cute</sub> to indicate a new generation different from the previous Borland-based versions.



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### New Feature: 3-D Monte Carlo Transmission Plots







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#### **3-D Monte Carlo Envelope Plots**









#### ETACHA4 porting and development: evolution plots and corrections







## **GEMINI++** : **GUI** application





The Gemini++ code was implemented to the LISE++ package after porting to a GUI application using the Qt graphics framework.

The code was updated to use the AME2016 database and to plot calculation results with the LISE<sup>++</sup> code.

#### http://lise.nscl.msu.edu/gemini.html



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e About				
Execute	😅 Open	Save Save	<del> </del> About	
Compound Nucleus De	cay Fusion reaction			
Projectile           A=         16           Z =         8	N = 8 16 O	Target           A=         12           Z=         6	N = 6	$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$
N	NE (MeV) = -4.737	ME	(MeV) = 0	ME (MeV) = -21.4928
Beam Energy Lab Energy (MeV) 160	$\begin{tabular}{c c c c c } \hline Calculation & & \\ Q_{CN} = & 16.7558 \\ E_{CM} = & 68.5714 \\ E_{x} = & 85.3272 \end{tabular}$	Spin O Input max Max spin f	spin 23	Local settings Diffuseness of fusion spin distribution (ħ) 2 Number of fusion events 500
Masses Traditional Gemini AME2016 database	Evaporation m 0 = widths ( 1 = Hauser- 2 = Switche of the rai	ode & KE) calculated from Feshach formalism s bewteen options 0 io of rotational to th	m Weisskopf, S & L fro (H.F.) 9 and 1 depending ermal energy	m H.F. IMF emission — w use in calculations enhanced IMF emission

#### **Cross Sections (GEMINI)** EVAPORATION - Compound nucleus 172 Yb; Mode 2 Excitation energy 143.0 MeV; Max.compound nucleus spin 40.0 hbar



Ġ Gemini					
💾 Save 📑 Print					
Gen	nir	ni			
Statistical D	)ec	ay (	Cod	е	
Starting C	ond	itior	IS		
	z	Ν	Α	^EI	
Projectile	8	8	16	<sup>16</sup> O	
Target	6	6	12	<sup>12</sup> C	
Compound nucleus	14	14	28	<sup>28</sup> Si	
Bombarding energy (MeV)				160.00	
Center of Mass energy (MeV)				68.571	
Compound nucleus Excitatio	n en	ergy (	(MeV)	85.33	
Q-value of reaction (MeV)				16.756	
Compound nucleus recoil en	nergy	(MeV	9	91.429	
Compound nucleus recoil ve	locity	/ (cm/	(ns)	2.512e+00	
Compound nucleus recoil (β,	)			8.373e-02	
Beam velocity (cm/ns)				4.396e+00	
Beam velocity (β)				1.465e-01	

diffuseness	2.00	ħ
Fusion cross section	655.27	mb
Bass L	21.02	ħ
LO	20.85	ħ
Bass cross section	675.84	mb
Excitation energy	85.33	MeV
Critical spin	21.0	ħ

Fusion Product Summary

Result	Number
Intermediate Mass Fragments	268
Symmetric Fission	0
Residual Nuclei	232
TOTAL	500

		Yields	of Resid	ual Nuclei	
z	Name	Events	Percent	x-section (mb)	err(mb)
12	24Mg	11	4.7%	31.07	9.368
12	23Mg	28	12.1%	79.08	14.95
12	22Mg	44	19.0%	124.3	18.74
	Z 12 12 12	<ul> <li>Z Name</li> <li>12 24Mg</li> <li>12 23Mg</li> <li>12 22Mg</li> </ul>	Z         Name         Events           12         24Mg         11           12         23Mg         28           12         22Mg         44	Z         Name         Feederation           12         24Mg         11         4.7%           12         24Mg         26         12.1%           12         24Mg         24Mg         10.0%	Yields of Result         Nuclei           Z         Man         Evens         Parcen         x-socion(m)           12         24Mg         11         47%         31.07           12         24Mg         21         21.1%         79.08           12         24Mg         14.0         19.0%         124.3



#### ATIMA 1.4 implementation in LISE $_{cute}^{++}$



#### **Implementation of ATIMA1.4 (catima1.5)**

Complete agreement with site results were obtained

ATIMA 1.4 is set as default Energy loss model in version 15

Production Mechanism
4e Ca (140.0 MeV/u) + Be -> 42 S     Reactions      Energy Loss, Straggling      Charge states      Databases: Masses, Isomers
Prefragment and Evaporation options
Energy Loss — Energy Loss model 4 - ATIMA 1.4 H.Weick, improved mean charge formula for HI •
Energy straggling Energy Straggling model 1 - ATIMA 1.2 (LS-theory)
Shape     Calculation method     O Gaussian     Calculation method     o integration
Moyal approximation of the Landau distribution     interpolation from table
Angular Straggling Angular Straggling method 1 - Moliere et al. (ATIMA 1.2)
Coefficients for GM.'s energy straggling calculations         Slope       0.217         (default 0.217)       Free member         1.12       (default 1.12)
Make default V OK X Cancel ? Help



#### Acknowledgements to Drs. H.Weick and A.Prochazka

ATIMA website: http://web-docs.gsi.de/~weick/atima/



### LISE\*\* development chart





**Fig.** A schematic diagram of the LISE<sup>++</sup> development plans. *M.P. Kuchera et al.*/*Nuclear Instruments and Methods in Physics Research B* 376 (2016) 168–170



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# Enhancing LISE++

# **Through Student Research Contributions**



### **Research group**

#### LISE<sup>++</sup> Assistance Team

#### https://lise.frib.msu.edu/porting/assistance\_team.html

Research - Sherrill - Group	
Name	Title
Sherrill, Bradley (M)	University Distinguished Professor
Tarasov, Oleg (M)	Senior Research Physicist
Ray, Arjun	Student Research Assistant I
Kaloyanov, Daniel	Student Research Assistant II
Matthews, Holly	Graduate Assistant
Watters, Shane	Graduate Assistant
Richardson, Isaiah	Graduate Assistant
Tarasova, Sasha	Student Research Assistant II

6 from 8-person list @ this workshop with 4 talks and 4 posters





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### The LISE<sup>++</sup> Assistance Team : Daniel

#### Daniel Kaloyanov (joined in 2023)



- $\cdot \ \tt{LISE}^{++}$  package maintenance in github
- $\cdot \ \tt{LISE}^{++} \, \rm{color} \ \rm{palette} \ \rm{update}$
- $\cdot~\texttt{LISE}^{++}$  Isomer database update
- $\cdot\,$  Migration of the  $\tt LISE^{++}$  databases from DBF to SQLite
- $\cdot$  LISE<sup>++</sup> for Excel:
  - Using DLLs created with Qt in MS Excel 64, Creation of libraries in the  $\tt LISE^{++}$  package
- $\cdot \ \tt{LISE^{++}}$  site statistics analysis
- $\cdot\,$  SpecTk: Improvement and maintenance

#### see Daniel's poster for LISE for Excel and SpecTk,

see LISE website statistics at the end of this presentation

#### https://lise.frib.msu.edu/16/16\_Databases.pdf

#### $\textbf{DBF} \rightarrow \textbf{SQLite}$

#### Cu → Te MICHIGAN STATE UNIVERSITY

#### Problem

Li 🎂 🐺 Se

- in the old system we stored data in dbf-format what are essentially text files (Excel: only read).
- While this works there are many issues with this primarily Scalability, Security, and Usability.

#### Solutions

- Using a library like libxl to read from an excel file
- The better choice: using SQL to read from a database file
- We Initially chose to use Access .accdb files as our databases, but ran into some issues and decided to switch.
- We then began to use SQLite because it was light weight, high performance, and had cross platform support.
- SQLIte files are also significantly smaller than Access files.

#### **Post-Implementation**

- There is now more versatility thanks to SQL queries
- Each query takes significantly less time to search for data than the old dbf code
- GEMINI++ reads in the data about 5x faster than before
- PACE4 reads data in about 2x quicker
- LISE<sup>++</sup> : the start is faster, the performance is slightly better
- Overall, there were slight performance improvements, but the databases in LISE and other codes overall is now more future proof, safe, and easier to work with

#### Hope, that Daniel joins our graduation program



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#### The LISE<sup>++</sup> Assistance Team : Sasha

Alexandra Tarasova (joined in 2023)

- $\cdot\,$  Package benchmarks & optimization (profiler, memory check)
- $\cdot\,$  Adaptation of the  $\tt LISE^{++}$  "new version" utility to SSL connection
- $\cdot\,$  FRIB logo application using Qt Design studio
- Creation of a LISE<sup>++</sup> video tutorial,
   "How to Make Rare Isotope Beams at Home", to be used on YouTube
- $\cdot \ {\rm Sound} \ {\rm support} \ {\rm for} \ {\tt LISE}^{++} \ {\rm code}$
- $\cdot\,$  Porting the  $\tt LISE^{++}$  package to Android Operating System
- · Development of the ARIS Beam dump utility [3D-graphics]





#### 3D ARIS BeamDump











### Sasha's project : LISE<sup>++</sup> performance optimization

Profiler (links)	Latest Release	os	Languages	Integration	Setup	Overhead	Tools	Licensing	Support			Inte	er2 <mark>Old</mark> and	New
Intel VTune	Intel 2023	Windows Mac OS Linux	C/C++ Python Java .NET	Standalone Visual Studio	Easy	Low	Performance CPU/GPU MemoryEvent-based sampling Call graph analysis Threading analysis	Free	Documentation Community Forum		17 18 19 19 19 10 10 10 10 10 10 10 10 10 10	ion2::inter2(double x, int method, bool FlagLog, boo method<2) //check stupid warning in stacks window lue = inter2_New (x, method, FlagLog, OnlyPositive);	Class::Method C distribution2:inter2	Call Count         Call Cou         Function         Children         Children %         Total         Total %           327,340         1.38%         1.946.06         0.77%         \$5,252.99         37.78%         \$7,199.05         38.56%
MS Visual Studio	Microsoft 2023	Windows	C/C++ Python Java .NET	Visual Studio	Easy	Low	Performance CPU/GPU Memory Concurrency Visualizer Threading analysis	Free	Documentation Community Forum		20         27         300         40         1.0         2	<pre>p = interuid (x, mende, Figues, univestive;) heckylaueid) [] (gi=0 &amp; (checkvalue=-0) heckylaueid) &amp; grabs (checkvalue=-p)/n bs(checkvalue) &amp; &amp; grabs(checkvalue-p)/n bs(checkvalue) &amp; &amp; grabs(checkvalue-p)/n bs(chec</pre>	Class::Method distribution2:inter2	Call Count         Function         Function         Children         Children %         Total         Total %           327.371         1.79%         1,700.86         0.88%         23.945.29         12.44%         25,646.15         13.33%
Very Sleepy	Richard Mitton 2021	Windows	C/C++	Standalone	Easy	Low	CPU Call graph analysis	Free	Documentation		36         3         0.00         else p = C           37         38         //         //           39         30         327,340         180.92         return p;	v 16.16.11	Eurctions called by function: distribution2:: Class::Method C	inter2
Relyze	Relyze 2022	Windows	C/C++ Delphi	Standalone Visual Studio	Easy	Moderate	Memory Resource allocation Extensive graphs/ representations	Free	Documentation		42 //return Check 43 }; 44 }; 16 // 17 double distribu	Value; www.www.www.www.www.www.www.www.www.ww	distribution2::inter2_Old distribution2::inter2_New	327,340 1.38% 13,883.89 5.51% 34,107.87 13,53% 47,991.77 19,04% 327,340 1.38% 11,277.79 4.47% 35,983.43 14,27% 47,261.22 18,75% inter2
	SmartBear	Windows	C/C++ Java	Standalone Visual Studio			Performance CPU/GPU		Documentation		18         327,371         25,666.156,74           19         327,371         182.95         if (methods4           20         327,371         24,387.48         double pN = 3           21         327,371         24,387.48         double pN = 3	<pre>   method&lt;2) method=2; inter2_New (x, method, FlagLog, OnlyPositive); coston +16-16-16</pre>	Class::Method C distribution2::inter2_New	Call Count         Call Count         Function         Function         Children         Children         Total         Total         Total %           327.371         1.79%         14,984.74         7.79%         8,960.55         4.66%         23,945.29         12,44%
AQTime Pro	Software 2023		Delphi	RAD Studio	Moderate						time ela	apsed (sec)		<b></b>
Deleaker	Softanics 2023	Windows	C#/C++ .NET Delphi	Standalone Visual Studio RAD Studio QT Creator	Easy		version	con	npiler	release date	124Xe,	198Pt,	Average factor	Int         Call Cou         Function         Function         Children         Children         Total         Total %           3820         1.20%         1.821.21         0.72%         111,559.25         44.25%         113,380.46         44.97%           3644         0.02%         205.93         0.08%         13,390.26         5.31%         13,596.19         5.39%
Performance Validator	Software Verify 2023	Windows	C/C++ .NET Delphi	Standalone	Easy						charge states	charge states		t         Call Cou         Function         Function         Children         Children         Total         Total %           20         1.56%         2.461.68         1.28%         26,137.36         13.58%         28,599.04         14.86%           46         0.03%         281.71         0.15%         4.309.83         2.24%         4.591.54         2.39%
							13.4	Borla	and(32)	5/5/2020	206	685	12.40	Children 🖡 Total 🖡
Profi	ler C	om	pari	son	Cha		16.3.1	Mi	nGW	4/6/2022	99	290	5.60	An example of identifying bottlenecks and performing
							16.14.20	Mi	nGW	4/26/2023	50	187	3.20	subsequent optimization
							16.16.14	Mi	nGW	7/25/2023	48	167	2.96	
							16.16.34	Mi	nGW	8/12/2023	35	90	1.86	
							16.17.2	Mi	nGW	8/18/2023	28	87	1.63	
							16.17.2	М	ISVC	8/18/2023	17	54	1.00	



### **Applying Graduate Research in the LISE development**



#### Excitation energy distribution study with BeAGLE Analysis of events generated by BeAGLE for <sup>238</sup>U, <sup>208</sup>Pb, <sup>136</sup>Xe, <sup>124</sup>Xe, <sup>90</sup>Zr, <sup>64</sup>Ni, <sup>58</sup>Ni projectiles Isaiah Shane to deduce an excitation energy model to be used in LISE\*\* Watters Richardson Z/N - data A=231, Z=87 43 22.86 24.42 21.83 23.17 23.86 23.58 23.58 23.86 23.97 24.23 23.37 22.80 -LogNormal fit 92 21 23 22 60 22 90 21 62 22 45 22 21 21 53 21 47 21 35 20 95 20 59 19 97 19 14 17 63 15 33 8 33 4 -EEE distribution fit ILISE 'D' 91 20.53 21.90 21.96 21.22 21.58 21.48 21.04 20.99 20.65 20.52 19.97 19.56 18.96 18.25 17.18 15.87 13.44 19.55 19.56 21.95 21.02 20.67 20.84 20.71 20.33 20.12 20.00 19.65 19.39 18.75 20.48 20.52 20.62 20.37 20.12 19.86 19.76 19.55 19.17 18.96 18.57 18.10 17.52 16.95 16.07 15.77 17. 87 20 22 20 02 19 81 20 03 19 82 19 48 19 16 19 02 18 80 18 29 18 09 17 52 17 01 16 44 16 20 17 3 configurations for 20 11 19 67 19 54 19 89 19 59 19 25 19 17 18 97 18 46 18 53 18 20 12 89 17 48 17 19 Excitation energy [MeV 84 20.23 19.95 19.58 19.2 0.39 19.41 19.37 19.72 19.34 19.45 19.16 16.89 16.51 16.44 16.11 17.97 17.43 17.35 17.23 18.01 18.73 17.86 19.03 18.70 19.83 19.17 19.45 19.43 19.25 18.81 18.58 18.70 18.16 17.99 17.96 17.64 17.26 16.73 the 2<sup>nd</sup> order 18.06 18.66 18.93 20.06 19.76 19.93 19.22 19.41 18.89 18.89 18.41 18.27 18.06 17.27 18.16 17.18 16.18 18.89 Our first outlines from BeAGLE results 81 20.04 17 35 18 66 19 11 18 68 19 11 19 26 19 55 18 31 18 67 18 31 17 38 16 77 15 31 16 56 17 7 No events in 0-20 MeV range (dA=7) 17.33 18.63 18.11 18.53 17.78 18.68 19.34 17.99 18.36 17.83 18.36 17.16 18.17 16.82 · LogNormal distribution, not Gaussian 17.78 17.29 17.88 17.78 18.68 19.56 18.02 17.99 15.99 17.50

17.41

20.02 17.84 18.69 17.92

#### **Optics calculations for PID reconstruction**

- Trajectory reconstruction required for PID analysis
- · Fast updates of optics settings to analysis
- Creation of reliable transport calculations of
- It can be used to study **ARIS** optics



minimization results (Dipoles: COSY maps, Quads; effective lengths from calibration)



see Shane's poster

New Shane's project: **Reverse trajectory reconstruction** with fragment-separators

# FRIB

N/Z dependence of modes (statistics)

see Isaiah's poster

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# **Trajectory reconstruction**



#### Using trajectory reconstruction to benchmark

- The reverse ray-tracing technique provides valuable benchmarks of the analysis providing the beam-optics constraints of fragments passing through a spectrometer.
- Reverse rays should be inside of beam optics element, that can be seen from reverse envelopes in dispersive and nondispersive planes plotted

https://lise.nscl.msu.edu/9\_10/ReverseConfiguration.pdf

- Blue and grey shadow areas demonstrate aperture sizes of multpipole and drift elements correspondingly.
- These envelopes demonstrates how well rays fit in apertures of two quadrupole located after a target





### **Reconstruction of fission fragment trajectory at S800**

- LISE<sup>++</sup> now supports reverse mode, allowing experimental data to be input for simulation, with reaction product properties extrapolated **back to the target**
- Data extracted from a ROOT tree (or SpecTcl) are converted to text and processed in LISE<sup>++</sup>, using 5<sup>th</sup>-order COSY maps for ion-optical transformations.



• This reverse ray-tracing technique provides valuable benchmarks for beam optics as fragments traverse the **fragment separator** 



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# Reaction mechanism:

# **Abrasion-Fission**



### LISE<sup>++</sup> 3 Excitation-Energy Regions (3EER) model





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#### **Disadvantages of LISE++ AF 3EER model : high Z settings**



https://lise.nscl.msu.edu/10\_1/10\_1\_127\_highZ\_AF.pdf

Limitations of the 3EER model due to averaging on more probable fragments

- Use manual cross sections as BigRIPS CS table
- New model development to use pre-calculated tables (in process, see IFN analyzer slides)



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## Initial Fissioning Nuclei (IFN) Analyzer

Abrasion-fission

A3\*+ A4\*< 238



- The utility, Initial Fissioning Nuclei (IFN) Analyzer, calculates the contribution from all possible parent Fissioning nuclei to the final fission fragment, which allows to calculate
  - fission fragment production cross section as contribution of all Fissioning parents,
  - more probable parent Fissioning nuclei,
  - fragment velocity in CMS (provide kinematics),
  - excitation energy of the initial fission fragment,
  - number of nucleons released to reach the final fission fragment.
- Still under development:
  - Overprediction reported by BigRIPS requires the Global revision of the de-excitation process (mathematics & physics, constructed in 2003)
  - creation of pre-calculated tables to use in production rate calculations (CS value and velocity<sub>CMS</sub> array)

	http://lise.nscl	l.msu.edu/10_1/11_0_28_IFN_search.pdf
Abrasion-Fiss	ion Initial fission nuclei	×
	<sup>238</sup> U (79.6 MeV/u) + C	Settings - I (Select region) coef for $Z_b = 0.75$ 0.1 < coef ≤ 1; recommendation: 0.75 Z_stop = 69
Choose	e Final fission fragment 87Kr	coef for N <sub>b</sub> = $0.8$ 0.1 < coef ≤ 1; recommendation: 0.80 N_stop = 117
	Calculate - I : Fission channels after Abrasion* + CF	✓ Include Coulomb fission channel determine low Z (element number) where Abrasion-Ablation stops. Z <sub>stop</sub> = coef ⋅ Z <sub>beam</sub>
Calcul: <i>G</i> ALL I & II	Calculate - II :	Settings - II Cross-section minimum threshold to use a nucleus in calculations (mb) 1.0e-08
	Fission of nuclei gated on Final Fragment **	Number of excitation energy points         Statistical values to show in the result frames           distribution to use in calculations         Mean value and Standard Deviations           1         Deviations
	* - takes ~ a minute; ** ~ 10 minutes - a hour	1. Unity mean value <2>     1. Unity mean value <2>     1. Unity mean value <2>     1. Unity mean value and its variances     1. Unity mean value and its variances
	Evaporation settings	Detailed ouput ✔ 23892_01206_08736_p3m_v4 Browse Show
	Prefragment excit.energy	General log file 🗸 IFN_v4 📑 Browse 🚥 Show
Batch file m	ode	Results - I (Fissile channels after abrasion) Total fission cross section in the region (mb) 1.67e+03
	no file or bad file	Number of fissile nuclei is the region (1) 1130 Key Fission Channels cross sections
	V Run the batch life: Takes time	Number of fissile nuclei used 690 690
Make defaul	Results - IIa: Initial Fissile Nuclei	Results - IIb: Final Fission Fragment
I OK	Gated on the Final Fission Fragment	Final fragment 7.68e+00 mb mdn (-vrns; +vrns), where cross section 7.68e+00 mb "mdn": median; "vrnc":variance
	2D: Fissile Nuclei CS	Initial fiss.fragment excitation energy 47.5 (-21.7; +59.2) MeV 1D: Excitation Energy
X Cancel	E*, MeV 109.1 (-56.3; +146.1)	Velocity in CMS 1.407 (-0.101; +0.043) cm/ns 🗽 1D: Velocity in CMS
? Help	N 142.74 (-3.10; +1.42)	Number of nucleons emitted to reach FFF 5.47 (-2.05; +2.86) 📐 dA, dN, dZ









## IFN-analysis for final Ge-isotopes (Z=32) : summary plot







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### **Reaching limit with one-step fission reactions**





LISE<sup>++</sup> 3EER model: Fissioning channel map after abrasion

Time to think about the multi-step reactions?



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# Reaction mechanism:

# **Abrasion-Ablation**





#### **Abrasion-Ablation model**





- AA is the most advanced method, modeling final fragment production in two steps.
- Its applicability is limited by the extensive input requirements and insufficient data on prefragment excitation functions.
- The excitation function is critical for setting energetics in the ablation step.
- Abrasion-Ablation calculations are highly sensitive to mass model input. Considered as mass model benchmarking.





#### Obtaining excitation energies from experimental cross-sections with mass model variation



O. B. T. et al., PHYSICAL REVIEW C 87, 054612 (2013)

<sup>82</sup>Se + Be E\* = 15

 $E^* = 15 \text{ MeV/dA}$ 

A.Kubiela et al., PHYSICAL REVIEW C 104, 064610 (2021)

<sup>78</sup>Kr + Be

E\* = 13.3 MeV/dA





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#### LISE\*\* Abrasion-Ablation minimization utility



The new minimization utility allows to deduce Abrasion-Ablation model parameters from comparison of AA-calculation results with experimental cross-sections with selection one from 28 mass models distributed with the LISE<sup>++</sup> suite. The utility is based on the levmar package using the Levenberg-Marquardt nonlinear least square algorithm.

User Cross-Section analysis using the Abrasion	-Ablation model : MINIMIZATION ==> (	uss_Z30_hfb22.mfit	– 🗆 X
Excitation energy model #3 (gaussian parameter E* : quadratic polynomial <e*> - excitation energy per abraded nuc 0 1 0 + 13.722 * d abb</e*>	rization) sigma(E*) : quadr Excitation energy 2 5 + (-0.0775) * d abr <sup>2</sup> 3 3 3 3 3 4 3 3 3 3 4 3 3 3 3 3 3 3 3	Common parameters AA X-section dR correction - polynomial Maplitude factor 2 + 0.5161 1/2 * d abr	al
Use in Fitting process Use Bounds constraints Lower bound 0 10 Upper bound 15 30	V     V       -2     0       2     10	V     V       V     V       V     V       0.5     -2       1.5     6       1	V         V         V           .0.5         0.5         10         5
Calculate down to Z = 22	Fitting         N iterations =         10         Image: Show condition         Restore previous values	Operations This utility can be used if — Make items 1-3 1. "Projectile Fragmentation" reaction mode is selected 2. Abrasion-Ablation is the selected CS method 3. "File" cross section option is set to "on" 4. There are more than 2 user CS in memory	- Cascade Info & Dialog operations Press "Escape" to interrupt the analysis. "d_abr" is the number of abraded nucleons mass model User's ME file [hfb22] + LDM#3
Weights Analysis X <sup>2</sup> LoD Value 0.5 1	Plot Product values from the chi Target value = 8.11e	able     Image: Load Settings       1     Image: Evaporation Settings	decay channels Np=128; Modes=1011 1000 010; Q
Global 1 2	Number of user CSs = 9(10	Prefragment excitation energy	E* model 3 - Parametrized Gaussian distribution
✓ Use experimental CS errors in analysis ✓ Use Reduced chi-square (divide by "n-p") if exp.error is absent, then error=coef*CS where coef is	Show intermediate results	Analysis Log-file Browse Gauss_Z30_hfb22	Clear AA Make default

#### <sup>78</sup>Kr + Be H.Suzuki et al., submitted to PTEP

mass table	chi2
ws4_rbf	1.60
hfb22	1.91
ktuy	1.91
frdm12	2.02
ws4	2.49
tuyy	2.85
ame2016	2.95
ame2020	3.22
hfb27	3.87
unedf1	4.81
unedf0	13.88



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#### Excitation Energy (theory) : "Exotic nuclei" collaboration BNL-FRIB







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## **Excitation Energy (theory) : INCL Liege**



PHYSICAL REVIEW C 96, 054602 (2017)



This schematic depicts the Liège event process. The interacting particles are composed of spherical nucleons which interacts via a peripheral collision and cascades through the nucleus resulting in an excited prefragment.



Mo/dA

dΖ

0

1 2

3

5

6

10

11

dN

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15.0415.8115.5915.9216.0616.2916.3416.2516.7816.0416.4216.8618.02

7 14.77 15.5014.96 15.03 15.72 15.67 15.63 16.28 15.87 16.07 15.93 16.82 16.03 17.17 13.21 15.4614.54 15.22 15.09 15.45 15.79 16.16 15.34 15.67 15.41 16.45 18.84

9 14.80 14.16 14.27 15.00 14.67 14.50 15.14 14.86 14.30 15.57 15.07 15.01

14.03 12.77 10.31 15.45

13.3914.5314.5114.2215.3814.5615.7414.2612.51



## **Excitation Energy: Theory vs. Experiment**





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## <sup>78</sup>Kr + Be : Momentum distributions



## Velocity distribution modes (peak location) of Prefragment\* & Final Fragment are the same. (\* before de-excitation)

 Probably for systematics: ∆A should be equal to A<sub>beam</sub> - A<sub>prefragment</sub>

#### <sup>63</sup>Se is most probable initial prefragment for <sup>54</sup>Zn







### <sup>78</sup>Kr + Be : Momentum distributions vs. *E*\*



## Prefragment velocity @ corresponding E\* should be considered $v(A_{PF}) = f(E^*)$ (Convolution model mechanism)



If  $E^* / dA = const$ , dv / dA = constbut according to INC results  $E^* / dA = const$ 

										-	
				E	Se/	٩Ċ	SLE	Ξ: '	<sup>′8</sup> k	(r+	-e
	Mo/dA	dN									
	dZ	9	8	7	6	5	4	3	2	1	0
	0		20.25	20.84	21.54	20.09	19.64	18.14	17.23		
	1		20 34	20.00	20.61	19 51	19.63	18 54	18.09	16 34	
	2	10.96	20.34	20.00	20.01	20.00	20.50	10.04	10.05	12.00	17 /6
	2	19.00	21.45	20.03	20.12	20.00	20.50	19.09	19.00	10.09	17.40
	5	20.09	20.69	21.92	20.95	20.71	20.53	19.83	19.68	18.21	17.67
	4	19.32	22.26	21.74	21.59	21.12	21.45	20.03	19.97	18.66	19.24
	5		20.24	20.66	21.36	21.30	20.03	19.66	19.63	18.81	18.52
	6			20.29	21.08	21.36	20.93	20.63	20.06	19.08	18.07
	7			21.42	19.95	20.14	19.33	20.17	20.24	17.31	19.87
	8				22.10	20.13	19.82	19.21	18.01		
dZ 28 27	26 25 24	23 2	2 21	20 19	18 17	16 15	14 13	12 11 10	9	8 7	6 5
1							18	.22 17.77 17.6	16.82 19.7	117.2616.3	37 14.87 13.4
2						1	5.37 11.61 <mark>21</mark>	.12 17.75 20.29	18.89 18.5	017.2316.4	9 15.24 14.8
3					17	20.371	9.48 20.31 20 0.75 20 37 19	.91 19.67 19.54 56 19.67 19.7	18.3318.3	317.2116. 517.6417.2	9 16 24 15 9
5				19	.51 21.17 17	.50 19.91 2	0.43 20.31 19	.51 19.86 19.03	3 18.50 18.2	3 17.42 17.2	7 16.78 16.4
6			20	21.39 18	1.66 21.35 21	.10 20.81 2	0.42 19.09 19	.56 19.11 19.20	18.47 18.6	017.8417.8	117.2317.5
8			20.22.20.	84 19.90 20	.17 19.93 20	.00 20.14 2	0.27 19.49 19	.52 19.41 19.3	3 19.17 18.6	0 18.40 18.0	5 17.84 17.9
9		18.7	7 18.82 19.	95 19.70 20	.39 20.13 20	.45 19.88 1	9.50 19.66 19	.64 19.20 19.0	5 19.01 19.2	2 18.87 18.7	6 18.65 19.3
10	10.77	19.72 20.0	120.9419.	87 20.31 20	.72 20.41 19	.87 20.03 2	0.13 19.49 19	.67 19.16 19.3	5 19.46 19.5	719.3619.6	7 19.67 18.7
12	19.77	20.06 20.0	6 19.35 20.	24 20.22 19	.10 20.21 19	.18 19.792	0.13 19.80 19	.86 19.96 19.8	5 19.51 19.1 5 19.61 19.6	8 20.29 19.7	1 20.23 20.2
13	19.32 19.91	20.02 19.9	3 20.13 19.	70 19.79 20	0.02 19.82 19	.81 19.80 1	9.80 19.71 19	.77 19.95 19.5	3 19.73 19.9	4 20.01 20.5	0 19.83 19.9
14 1	18.56 19.20 19.67	20.00 19.7	5 19.75 19.	54 19.64 19	.97 19.71 19	.89 19.83 1	9.82 19.71 19	.84 19.68 19.8	7 19.47 19.9	8 20.59 19.2	6 20.86 18.5
15 18 79 1	18.5519.1219.63	19.36 19.8	1 19.46 19.	68 19.49 19 47 19 48 19	48 19 51 19	90 19.68 1	9.64 19.53 20 9.82 20 01 19	60 19 73 20 24	20.2520.5	3 20.26 21.1 0 20 36 19 2	3 19.64
17 18.241	18.69 19.20 18.67	18.77 19.0	7 19.04 19.	17 19.29 19	.29 19.41 19	.69 19.76 1	9.85 20.03 19	.76 20.42 19.6	520.14 22.0	8 20.38	.5 10.05
18 <mark>19.41</mark> 17.82 1	19.63 18.69 18.72	18.63 19.0	8 18.94 19.	46 19.06 19	.46 19.47 19	.75 19.36 1	9.95 19.52 20	.46 20.65 20.1	7 20.29 9.1	0	
19 16.95 17.75 1	19.03 18.47 18.57	19.06 18.9	2 18.79 18.	76 19.17 19	11 19.35 19	59 19.81 1	9.51 19.76 20	.00 18.90 18.9	1 18.56		
21 17.53 18.17 1	18.13 18.65 18.29	18.99 18.5	518.7018.	77 19.08 18	.80 18.77 20	15 19.431	8.41 19.01 20	.52	•		
22 16.02 17.77 1	18.3317.8218.54	18.65 18.4	6 18.51 18.	83 19.01 19	.16 19.16 19	.00 18.33 1	4.55 18.23 18	.59			
23 17.351	17.2317.4718.72	18.57 18.5	518.7818.	75 18.08 18	1.16 17.89 17	.07 17.97					
25	17.26	17.99 18.0	317.1318.	61	.54 10.50	(	Cour	tesv	of I.I	Rich	ards



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- This shift can be attributed to an intermediate step—Dissipation (Friction)—between the Abrasion and Ablation processes, which contributes to the appearance of the low-energy exponential tail.
- Discrepancy in results: Is the measurement reflecting the mean value or the mode (peak location)?
- Further investigation is needed on the neutron-rich side.



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# <u>Multistep reactions</u> (see NI presentation)



# LISE site statistics





#### 2024 LISE<sup>++</sup> site statistics



France

2%

, Slide 42

Germany

5%

2%

India.

6%

Japan

6%



Russia

4%



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## **2023: Downloading the LISE package: Countries**







 $\mathbf{r}$ 

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## By countries per year (1)







## By countries per year (2)





	difference	)	difference
country	<22,23>	-21 country	24-23
China	1296	USA	2631
other	1088	China	2141
USA	895	USA-MI	490
Russia	503	Other	408
Germany	493	Spain	211
India	421	Germany	170
France	296	Canada	105
S.Korea	152	Italy	78
Canada	124	Russia	75
USA-MI	118	UK	69
Romania	83	Belgium	50
UK	70	Brazil	39
Turkey	39	Japan	34
Vietnam	37	Thailand	11
Brazil	23	Iran	10
Thailand	16	Romania	5
Belgium	8	Saudi Arabia	-2
Saudi Arabia	8	Vietnam	-7
Italy	-16	India	-14
Iran	-21	Kazakhstan	-14
Kazakhstan	-50	Turkey	-78
Spain	-69	S.Korea	-168
Japan	-168	France	-293
bot	-21	bot	92
Total no bots	5547	Total no bots	5951
Total w ith botl	5525	Total with botl	5475



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## Laboratories (absolute values) : 2024







## **Private/Phys IPs by years**







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# LISE ++ Development Plans



### LISE\*\* development chart







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## LISE <sup>++</sup><sub>cute</sub> software development



#### In the near future:

- The creation of a LISE <sup>++</sup><sub>core</sub> library
  - This library will allow to integrate LISE<sup>++</sup> calculations within control systems, in order to directly assist the tuning of fragment separators.
  - LISE for Excel-64 (just completed)
- The code parallelization will be undertaken (project of A.Ray)
  - To take advantage of modern computing architecture, parallel computing methods are essential in achieving faster computation. As a first step, the LISE<sup>++</sup> code parallelization process will be implemented on the Monte Carlo and "Distribution" analytical methods for fragment transmission calculation.
- Block configuration converter

- This new tool will be built around a new type of block, labeled G (Group), which allows the grouping and ungrouping of E blocks. The tool can be applied to create sector configurations for fast analytical calculations.



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The new LISE<sup>++</sup> feature for converting a series of extended blocks to a single segmented block.





- Creation of fast and accurate Abrasion-Fission model based on the IFN Analyzer tables
- Abrasion-Ablation:
  - Global revision of the de-excitation process (mathematics & physics, constructed in 2003)
  - Improvement of the fast model for multi-step reactions (implementation of the AA for second step)
  - Intermediate Dissipation step in the Abrasion-Ablation model
  - Theoretical investigation of prefragment excitation energy with BeAGLE and INC-Liege models, incorporating in-house developments
- Direct model implementation in LISE<sup>++</sup> code for transmission and cross section calculations
  - ETACHA4: Low-energy non-equilibrium charge state evolution
  - PACE4: Projection Angular-momentum coupled evaporation
  - INC: intranuclear cascade model to use at higher energies with light targets
- Creation of Monte Carlo de-excitation cascade utility to benchmark the analytical LISE<sup>++</sup> cascade subroutine and to create condition (gating) options
- Systematization of experimental production cross-sections (  $\Delta BE$ , ..)
- Investigate charge-exchange and pick-up reactions in RIB production









### LISE <sup>++</sup><sub>cute</sub> : Powerful tool of the FRIB scientific program







The latest official version 17.11 has been released 01/06/2025

#### Nuclear Instruments and Methods in Physics Research B 541 (2023) 4-7

 $LISE_{cute}^{++}$ , the latest generation of the  $LISE^{++}$  package, to simulate rare isotope production with fragment-separators

O.B. Tarasov <sup>a,\*</sup>, D. Bazin <sup>a,b</sup>, M. Hausmann <sup>a</sup>, M.P. Kuchera <sup>c</sup>, P.N. Ostroumov <sup>a,b</sup>, M. Portillo <sup>a</sup>, B.M. Sherrill <sup>a,b</sup>, K.V. Tarasova <sup>a</sup>, T. Zhang <sup>a</sup>

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#### 03/17/23 openAI: Write an essay about LISE++ code

LISE++ is a computer code designed for the simulation of nuclear reactions and the calculation of ion beam transport.

Overall, the LISE++ code is a powerful tool for the simulation of nuclear reactions and ion beam transport. Its ability to accurately model these processes has made it an essential tool for researchers in a range of fields, from nuclear physics to medical imaging. As the field of nuclear science continues to evolve, it is likely that the LISE++ code will continue to play a critical role in advancing our understanding of the underlying physics.



### **Team & Acknowledgements**



The LISE <sup>++</sup> Transportation Team		The LISE <sup>++</sup> Assistance Team	
Members working on the transportation of the LISE <sup>++</sup> software suite to Qt		Members assisting on the LISE <sup>++</sup> code development	
D. Bazin	physics & ion optics consulting, benchmarks, adaptation to macOS		
M. Hausmann	physics & ion optics consulting, benchmarks		
M. Kuchera	source porting, development of porting process base	I. Richardson grad	
P. Ostroumov	supervision, funding acquisition	S. Watters grad	
M. Portillo	physics & ion optics consulting, benchmarks	D. Kaloyanov undergrad (senior)	
B. Sherrill	supervision, funding acquisition	A.O. Tarasova undergrad (senior)	
O.B. Tarasov	leading porting process worker	A. Ray undergrad (sophomore)	
K.V. Tarasova	source porting, benchmarks		
T. Zhang	process administration, IT consulting, adaptation to Linux		

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# Upgrading to 400 MeV/u







- Upgrading FRIB to 400 MeV/u will significantly increase the production probability of neutron-rich isotopes in multistep reactions by an order of magnitude
- **Target Production Research:** Utilizing a liquid lithium target can further enhance the multistep factor, improving isotope production efficiency

#### 1 week run

<sup>66</sup>Ca @ E200 ~ 1 event: C-target
<sup>68</sup>Ca @ E400 ~ 1 event: C-target
<sup>70</sup>Ca @ E400 ~ 1 event: Li-target



1 – FRIB 2024 (20 kW, 1 day, dP/P=4%, FOI as 50%) a 1/700 factor compared to E200





#### <sup>70</sup>Ca production in 3-steps reaction: ${}^{238}U \rightarrow {}^{237}U^* \rightarrow {}^{81}Ga \rightarrow {}^{76}Fe \rightarrow {}^{70}Ca$







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A lot of uncertainties, where main one is PF production cross sections in exotic regions

O.B.Tarasov@mnt.rkien.jp, 05 July 2024, Slide 58

<sup>70</sup>Ca

70

60

<sup>76</sup>Fe