Oleg B. Tarasov
NCSL / MSU

Development of the LISE++ code to simulate rare isotopes production

Fall Meeting of the APS Division of Nuclear Physics

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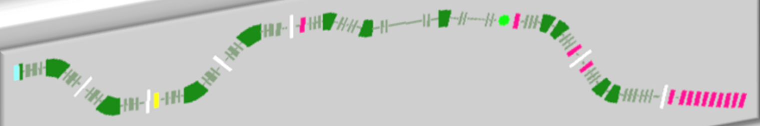
October 2021



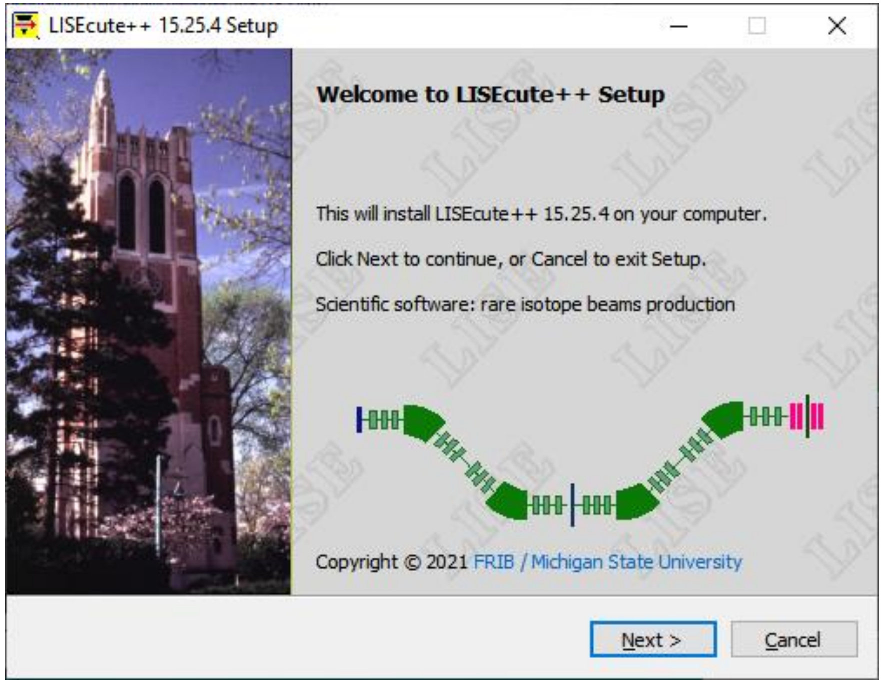
LISE++

LISE++

NSCL

1. Rare Isotope Beam Production with Fragment Separators
2. LISE package transportation
3. New features
4. New code implementation
5. Reaction mechanism models development updates
6. The LISE++ transportation team

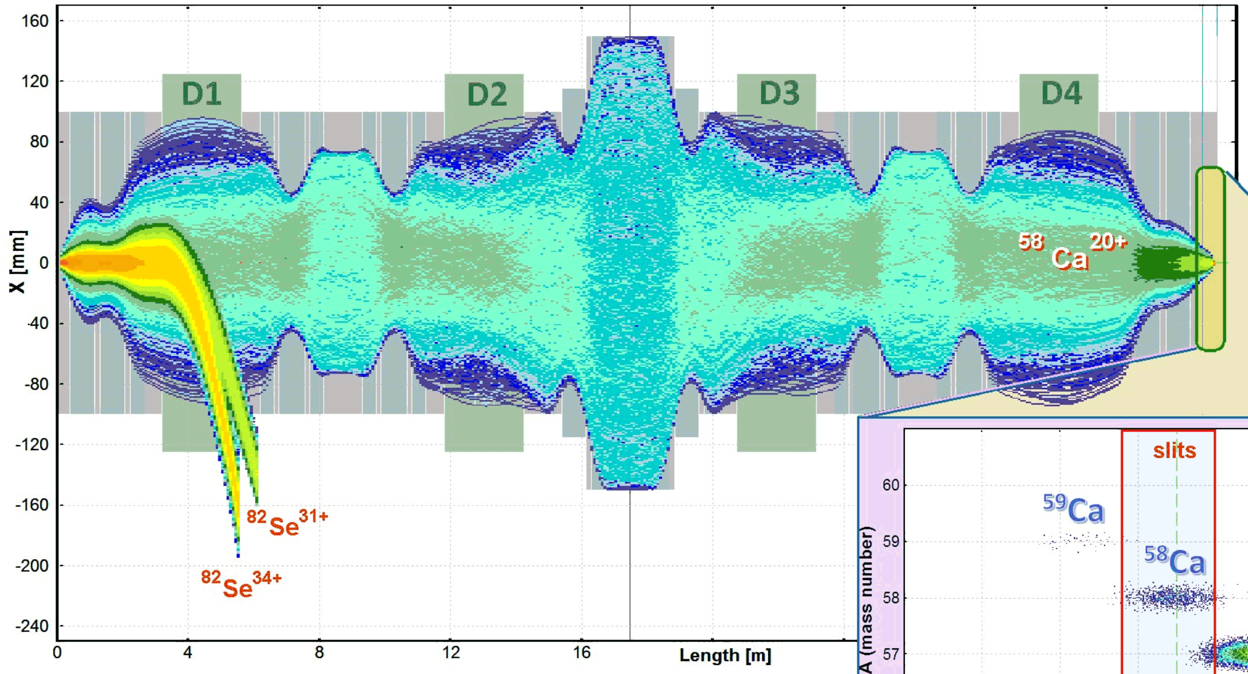
- The program LISE^{++} is designed to predict the intensity and purity of rare isotope beams (RIB) produced by In-flight separators
- The program is constantly expanding and evolving from the feedback of its users around the world
- Many “satellite” tools have been incorporated into the LISE^{++} framework
- It can be freely downloaded from the following internet addresses: http://lise.nscl.msu.edu



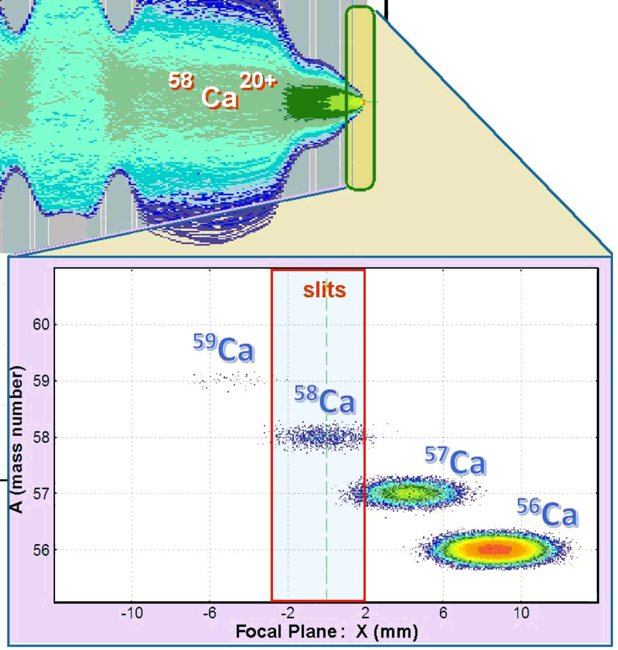
Main LISE++ Functions

- predict the fragment separator settings necessary to obtain a specific RIB
- predict the intensity and purity of the chosen RIB
- simulate identification plots for on-line comparison
- provide a highly user-friendly graphical environment

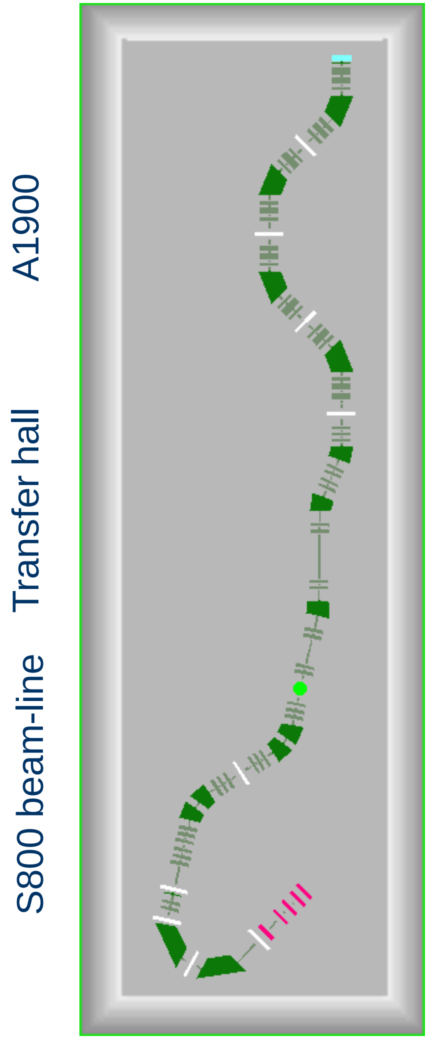
- allow construction of configurations for different fragment separators



X-envelope
$^{82}Se \rightarrow {}^{58}Ca$ @ A1900



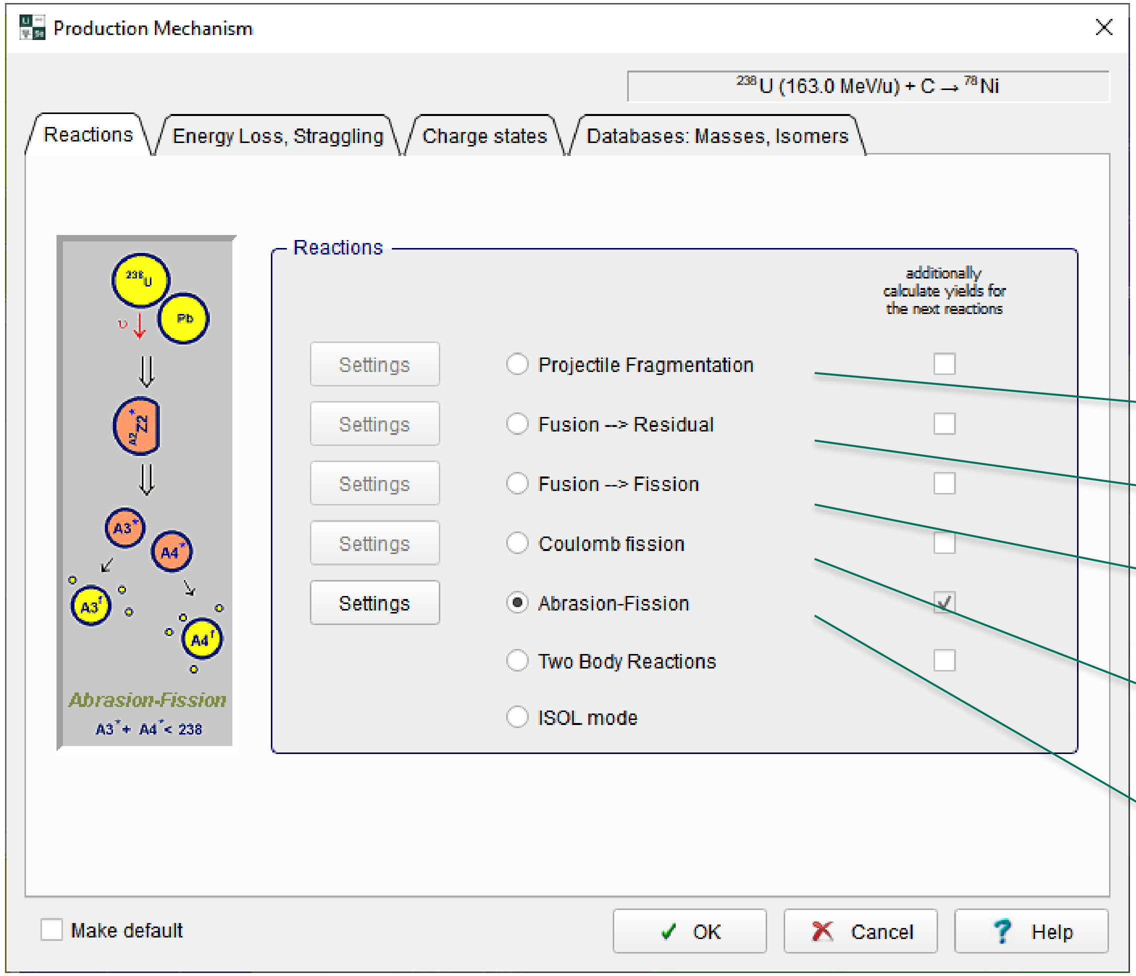
“wedge” selection



S800

Reaction Mechanisms

- Not only using classical reaction mechanism models, but actively developing fast and accurate in-house models of rare isotope production
- Includes secondary reactions in target
- Includes fragment production in materials (wedges, detectors)

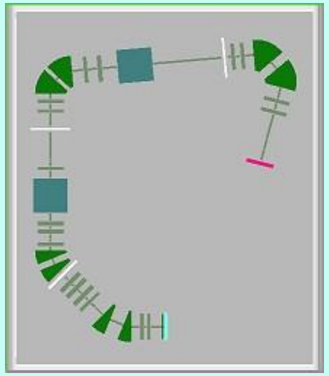


O.B.Tarasov	Analysis of momentum distributions of projectile fragmentation products	NPA 734 (2004) 536-540
O.B.Tarasov, D.Bazin	Development of the program LISE: application to fusion–evaporation	NIM B204 (2003) 174-178
O.B.Tarasov, A.C.C.Villari	Fusion–fission is a new reaction mechanism to produce exotic radioactive beams	NIM B 266 (2008) 4670-4673
O.B.Tarasov	LISE++ development: application to low-energy fission of projectiles at realtivistic energies	ENAM2004: EPJ A25 (2005) 751
O.B.Tarasov	LISE++ development: Abrasion-Fission	Preprint NSCL MSU, MSUCL-1300, 09.2005

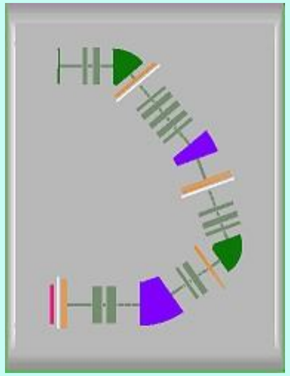
Application : Energy region and Facilities

The LISE^{++} code may be applied at low, medium, and high-energy facilities (fragment- and recoil-separators with electrostatic and/or magnetic selections)

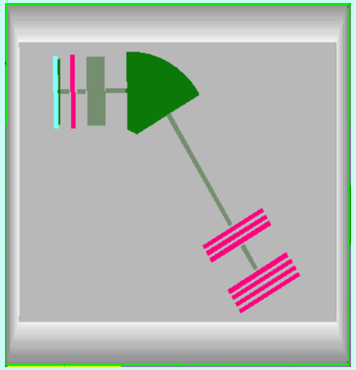
The LISE^{++} package includes configuration files for most of the existing fragment and recoil separators



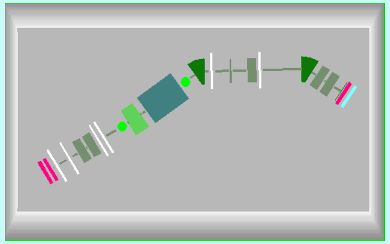
SECAR, *MSU*



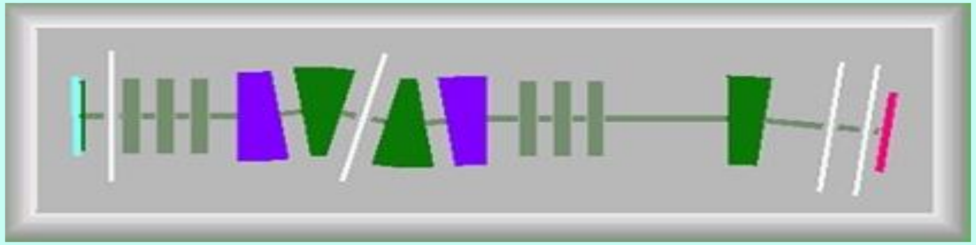
DRAGON, *Canada*



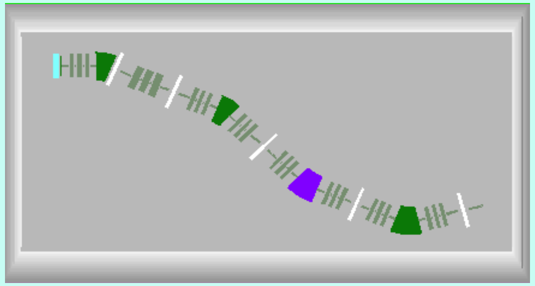
PRISMA, *Italy*



MARS, *TAMU, USA*

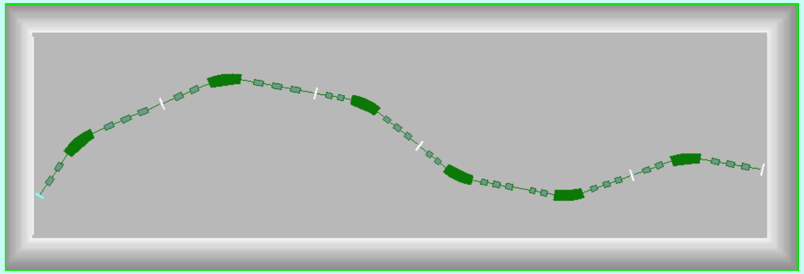


SHELS, *Russia*



S^3, *France*

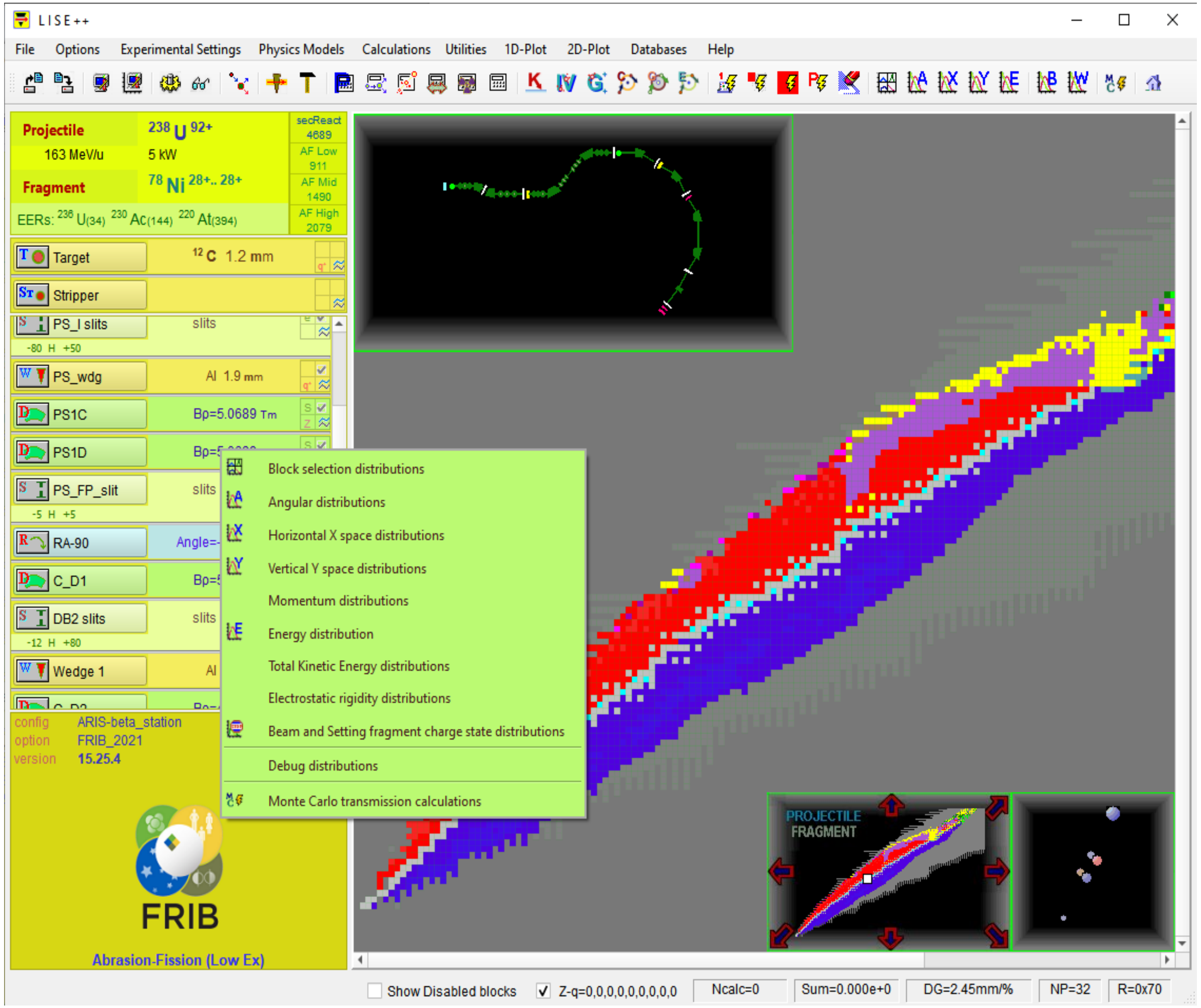
BigRIPS+ZeroDegree, *Japan*



SuperFRS_HEB, *Germany*

LISE^{++} transportation → LISE$^{++}_{cute}$

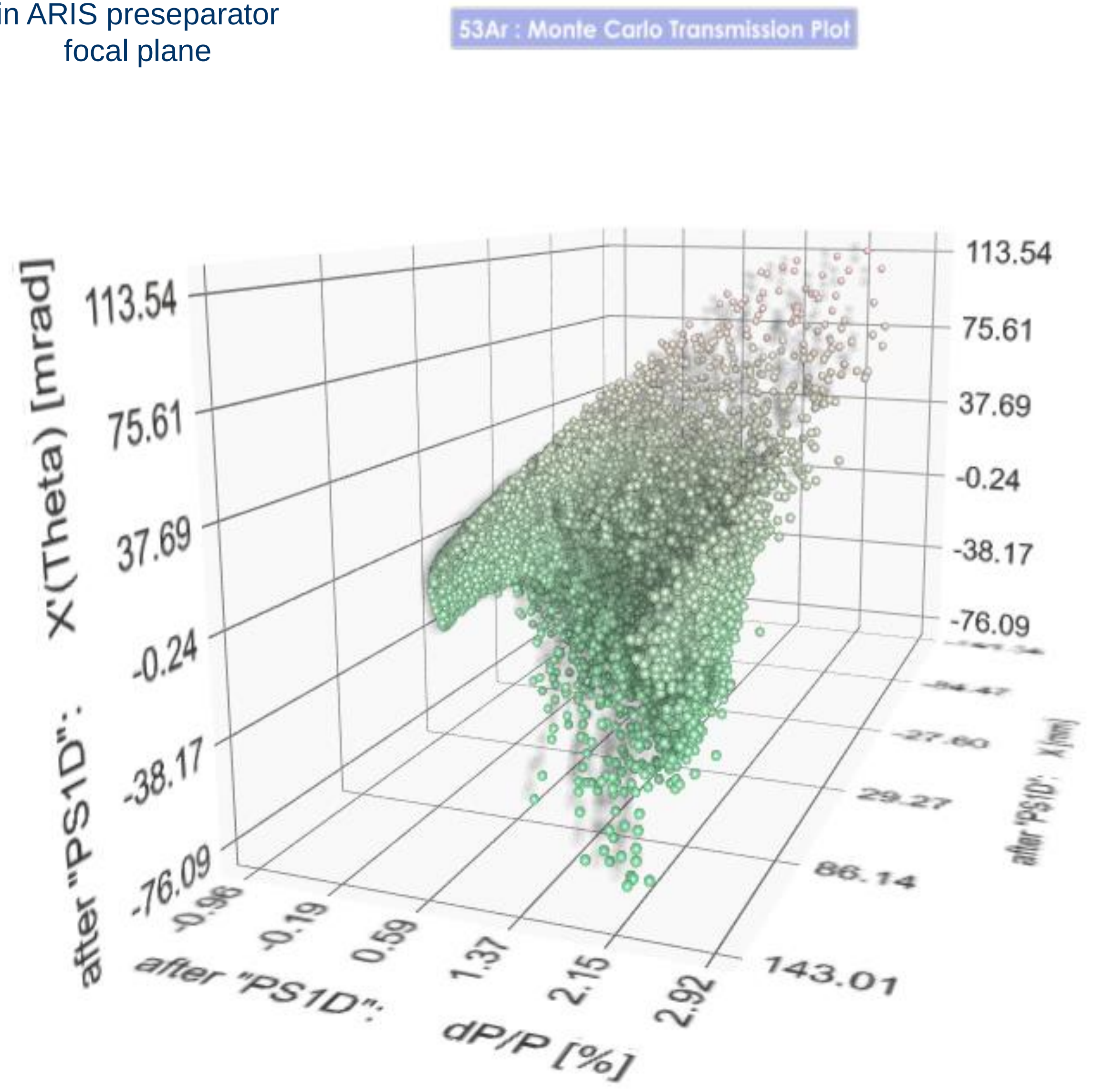
- The LISE^{++} code (v.6-13) was developing at Borland C++ 5.02 IDE (integrating development environment), which is not compatible with the next Borland (Builder, Embarcadero C++) generations
- The LISE^{++} software suite was recently ported to Qt-framework in order to
  - Aid in sustainability of 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^{++} version 15, created using the Qt framework, is named **LISE$_{cute}$** to indicate a new generation different from the previous Borland-based versions.*

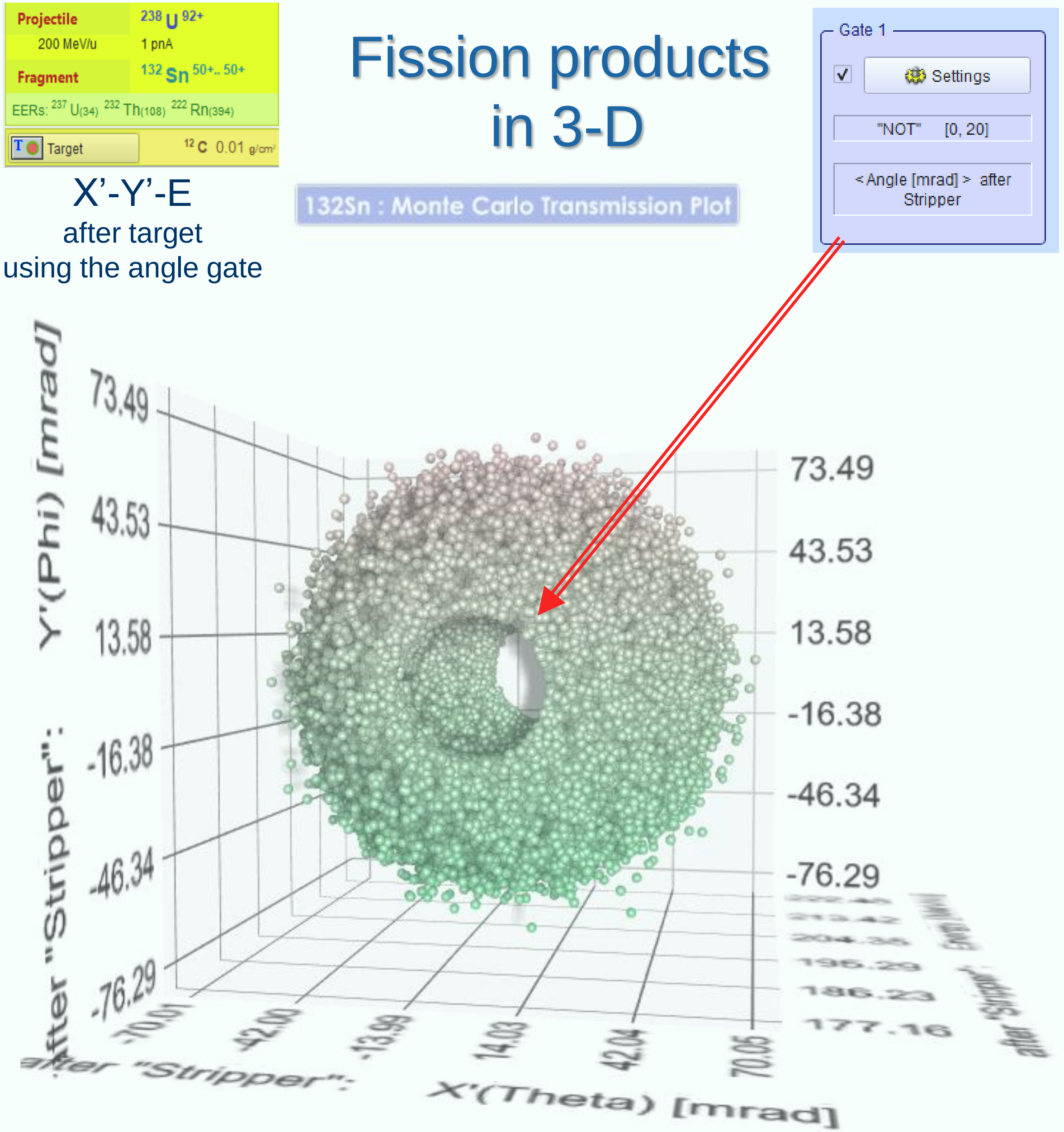
New Feature: 3-D Monte Carlo Transmission Plots

X-X'-dP/P
in ARIS preseparator
focal plane

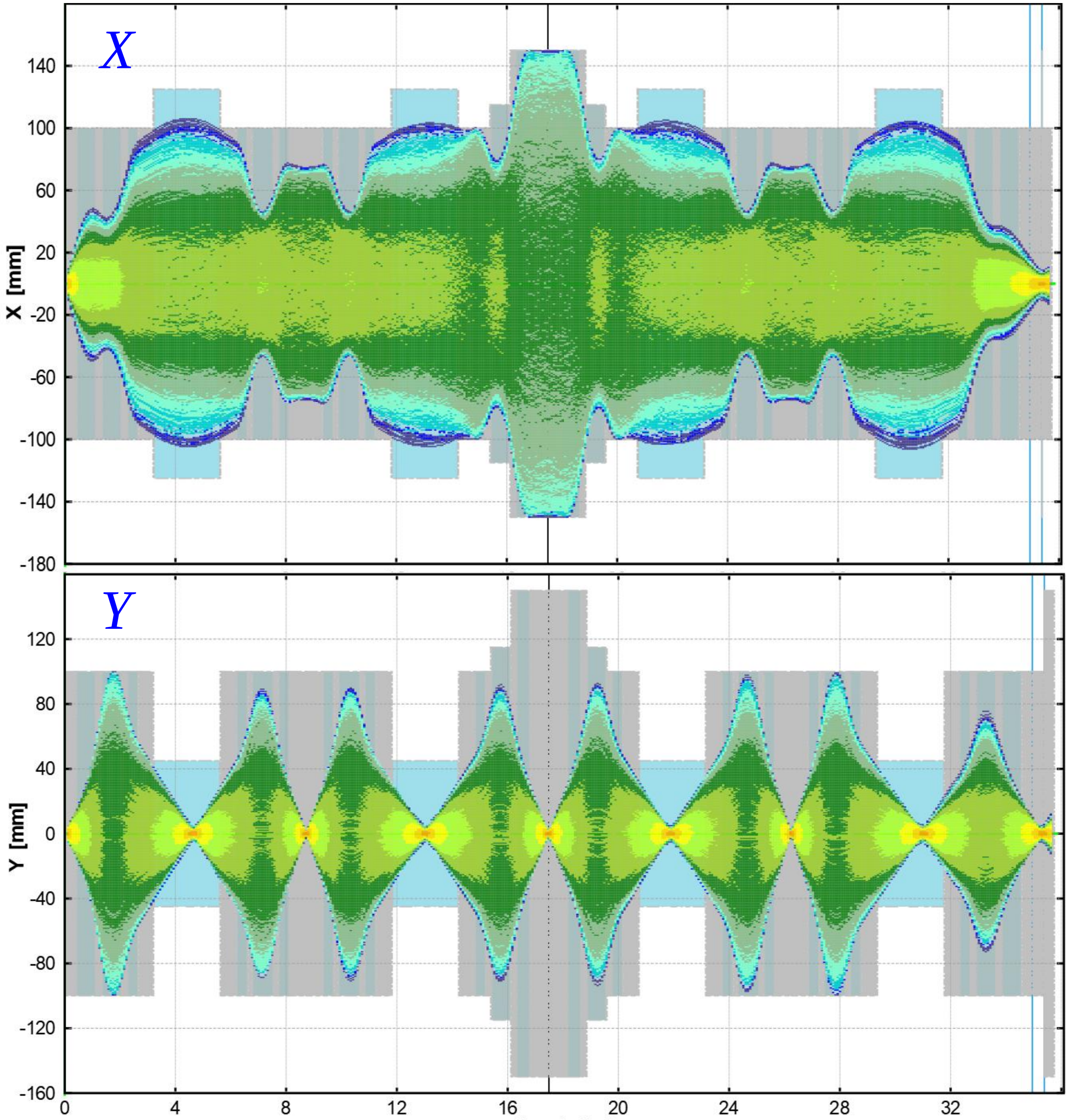


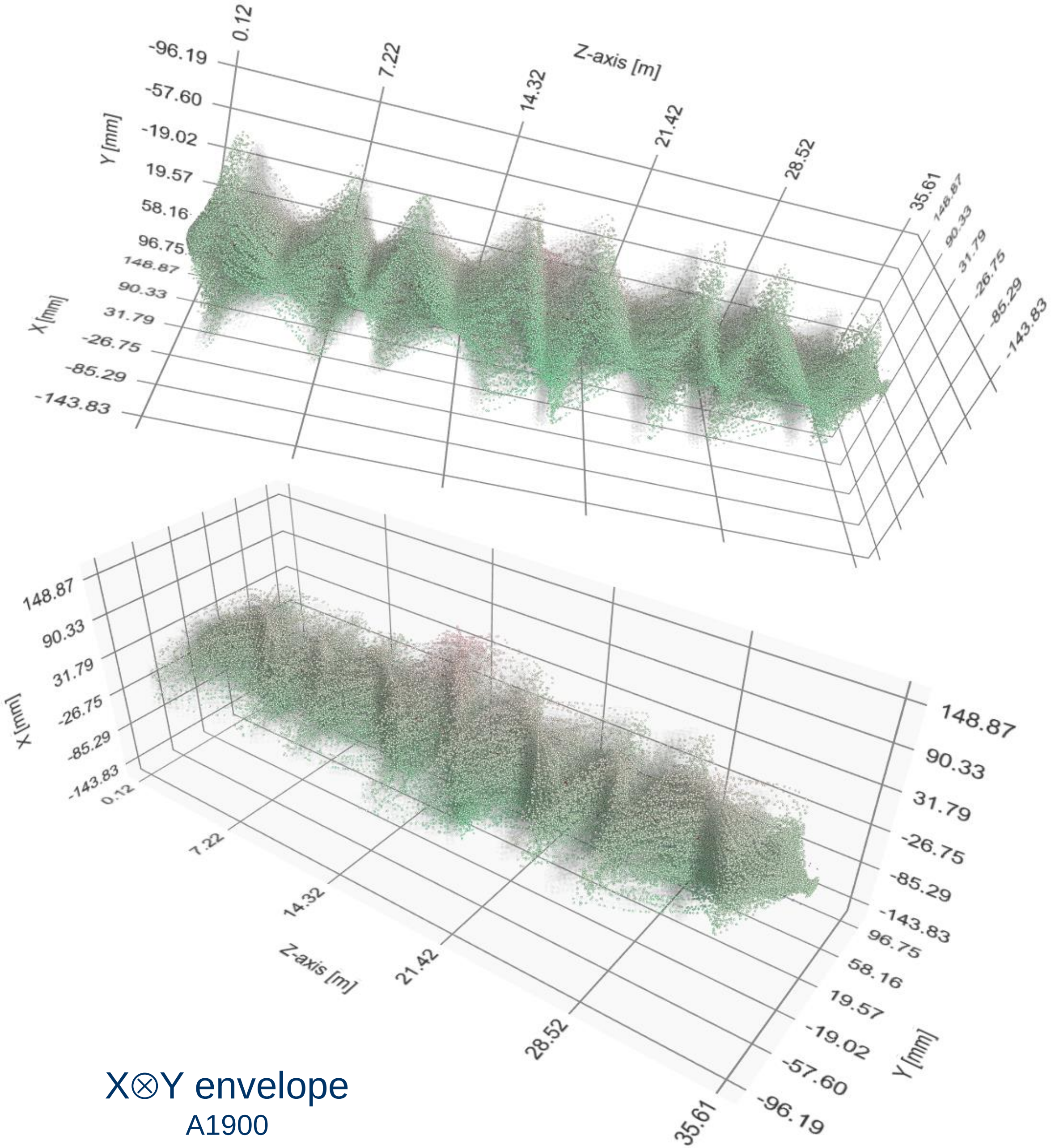
X'-Y'-E
after target
using the angle gate

Fission products
in 3-D



3-D Monte Carlo Envelope Plots





X⊗Y envelope
A1900

LISE^{++} development chart

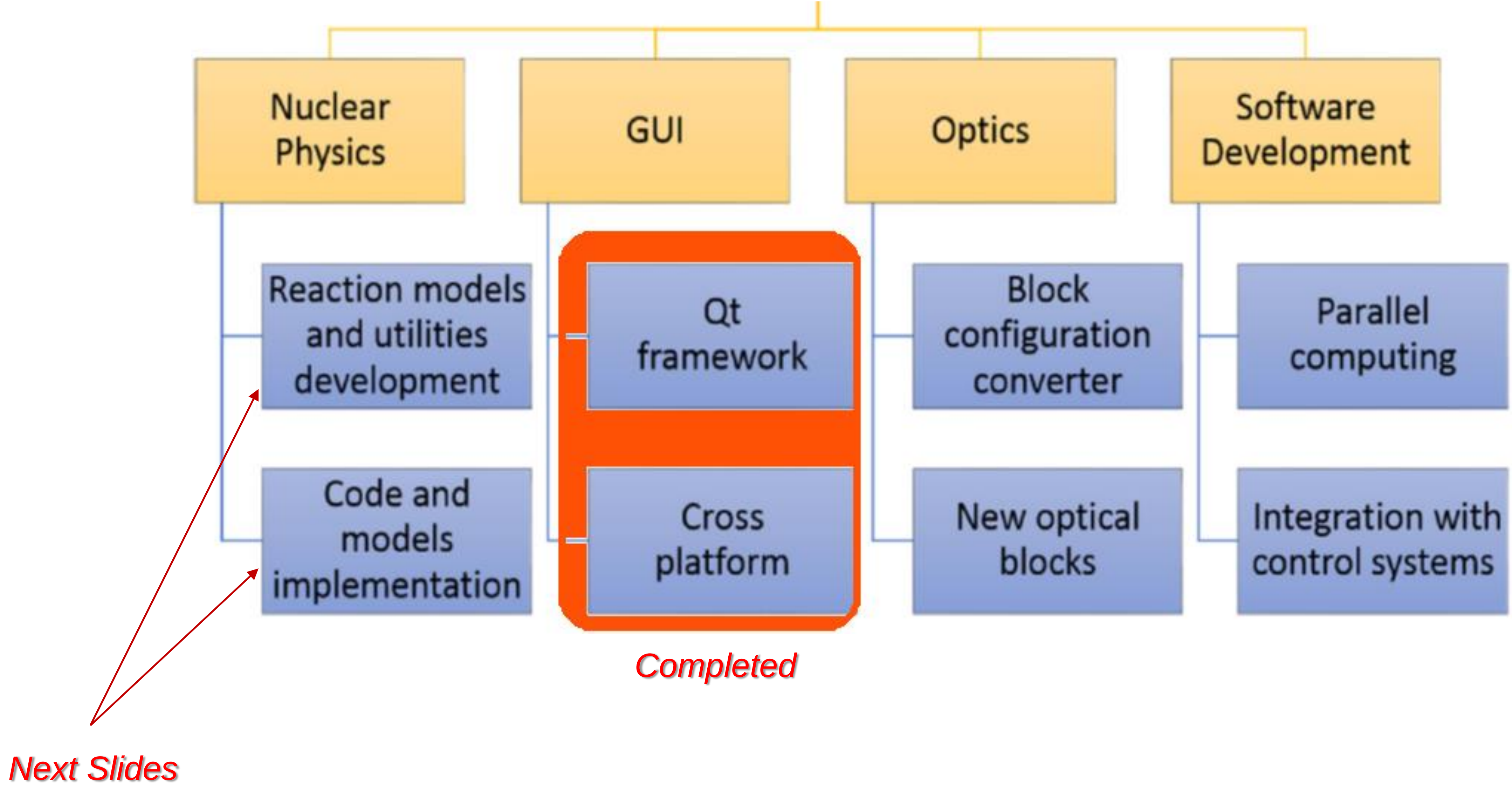
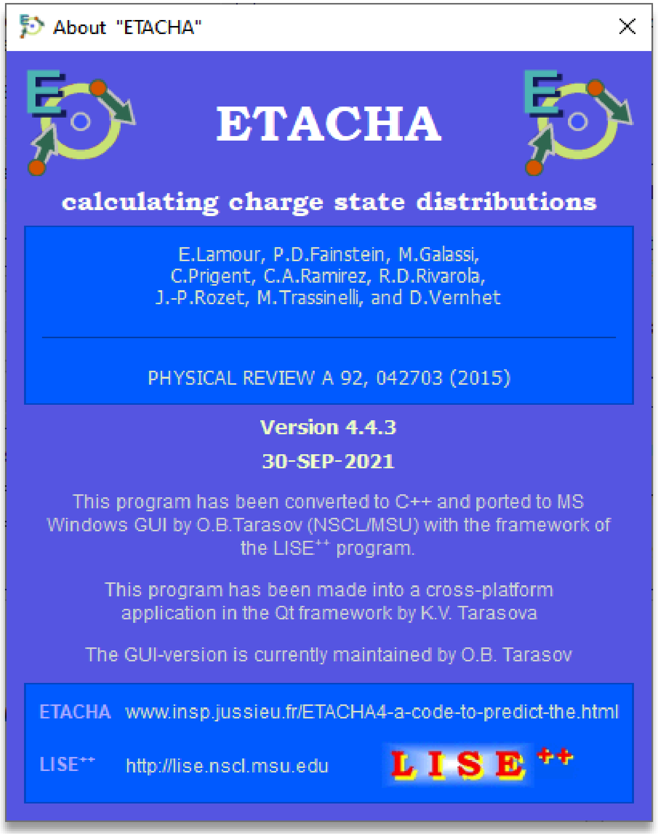
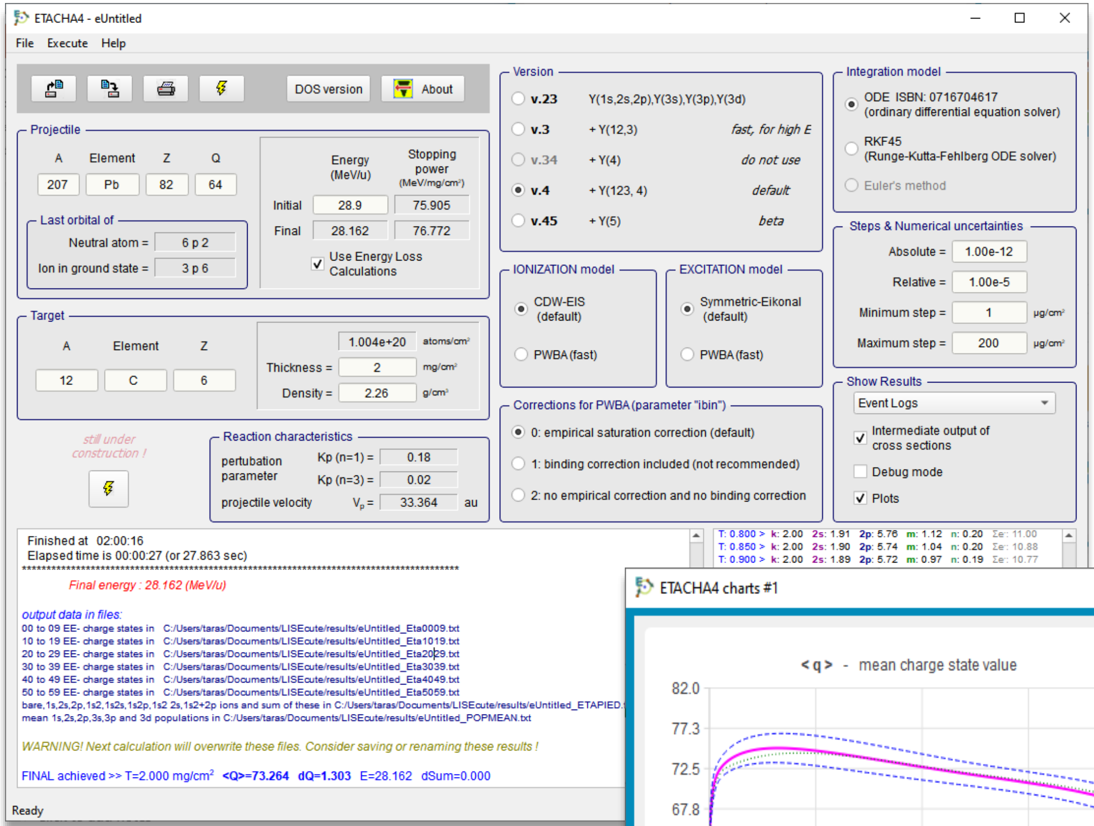


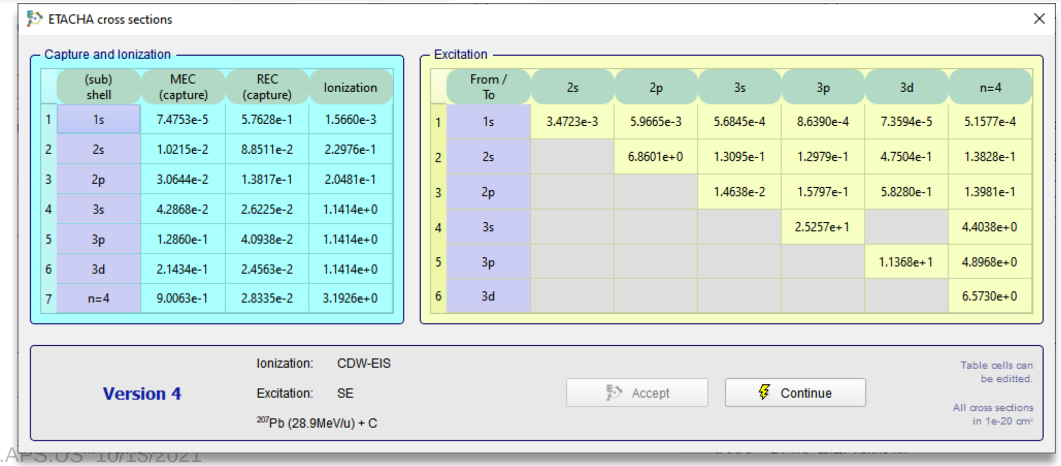
Fig. A schematic diagram of the LISE^{++} development plans.

M.P. Kuchera et al. / Nuclear Instruments and Methods in Physics Research B 376 (2016) 168–170

ETACHA4 porting and development: evolution plots and corrections

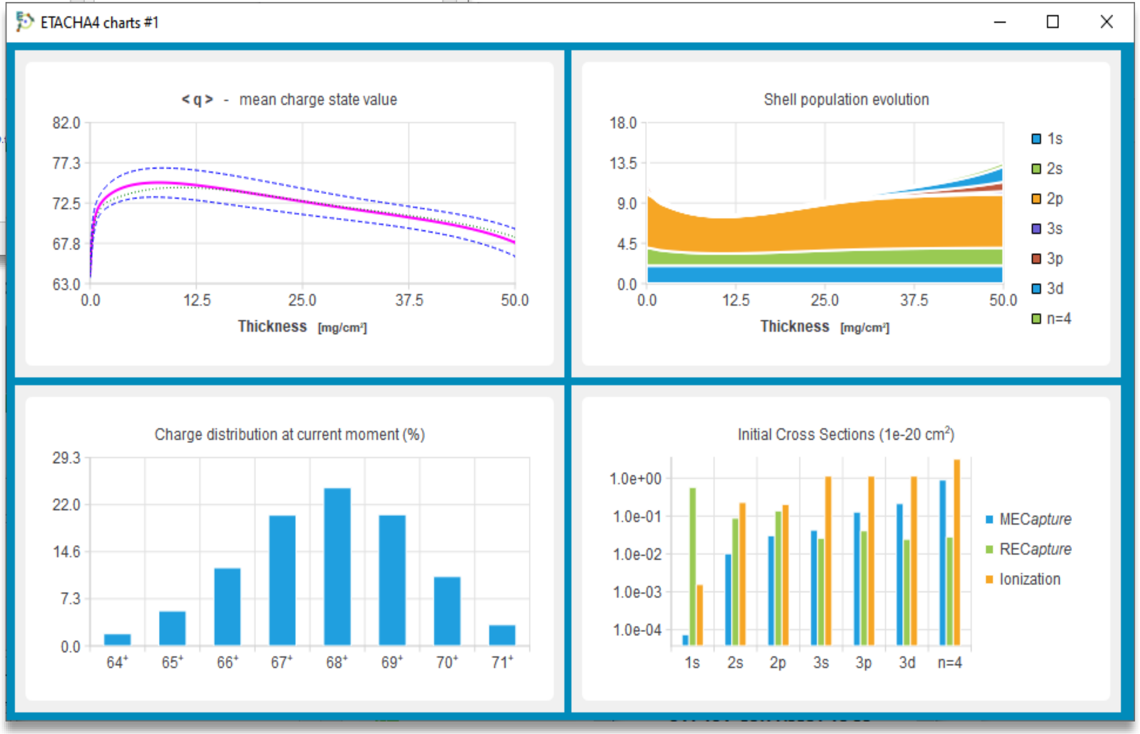






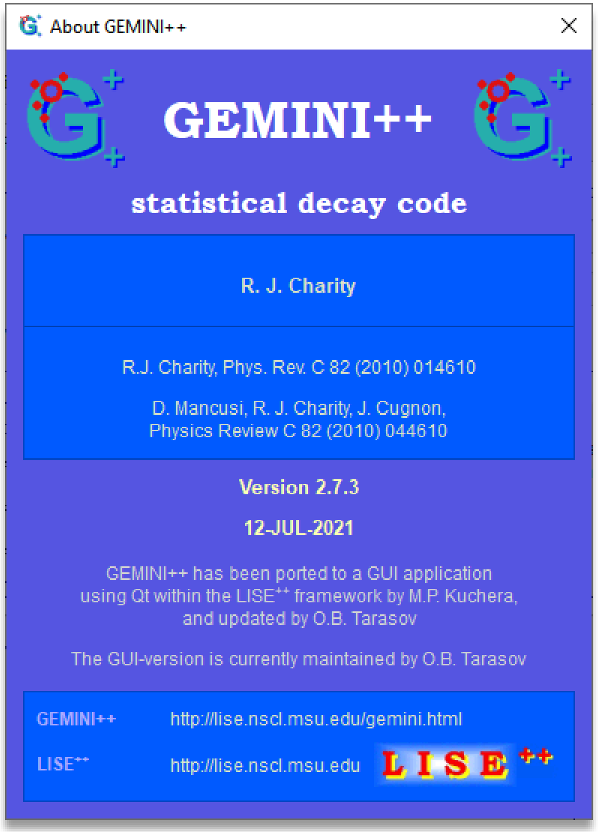
	(sub) shell	MEC (capture)	REC (capture)	Ionization
1	1s	7.4753e-5	5.7628e-1	1.5660e-3
2	2s	1.0215e-2	8.8511e-2	2.2976e-1
3	2p	3.0644e-2	1.3817e-1	2.0481e-1
4	3s	4.2868e-2	2.6225e-2	1.1414e+0
5	3p	1.2860e-1	4.0938e-2	1.1414e+0
6	3d	2.1434e-1	2.4563e-2	1.1414e+0
7	n=4	9.0063e-1	2.8335e-2	3.1926e+0

	From / To	2s	2p	3s	3p	3d	n=4
1	1s	3.4723e-3	5.9665e-3	5.6845e-4	8.6390e-4	7.3594e-5	5.1577e-4
2	2s		6.8601e+0	1.3095e-1	1.2979e-1	4.7504e-1	1.3828e-1
3	2p			1.4638e-2	1.5797e-1	5.8280e-1	1.3981e-1
4	3s				2.5257e+1		4.4038e+0
5	3p					1.1368e+1	4.8968e+0
6	3d						6.5730e+0



We are very grateful to Dr. Toshiyuki Sumikama (RIKEN) for the fast and quality analysis of bug locations during the porting process

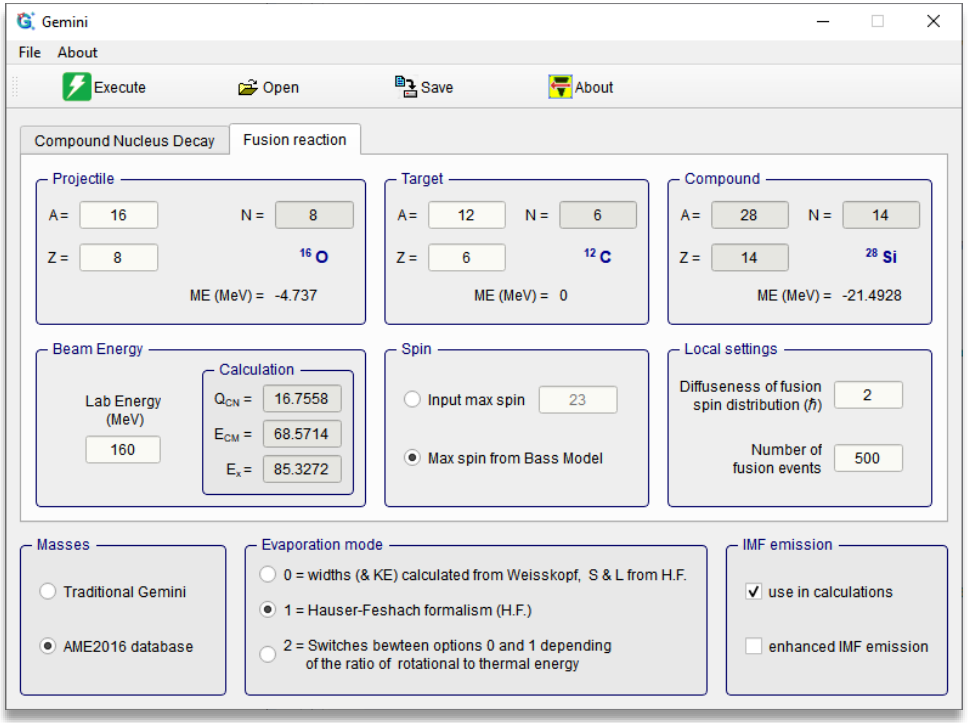
GEMINI++ : GUI application

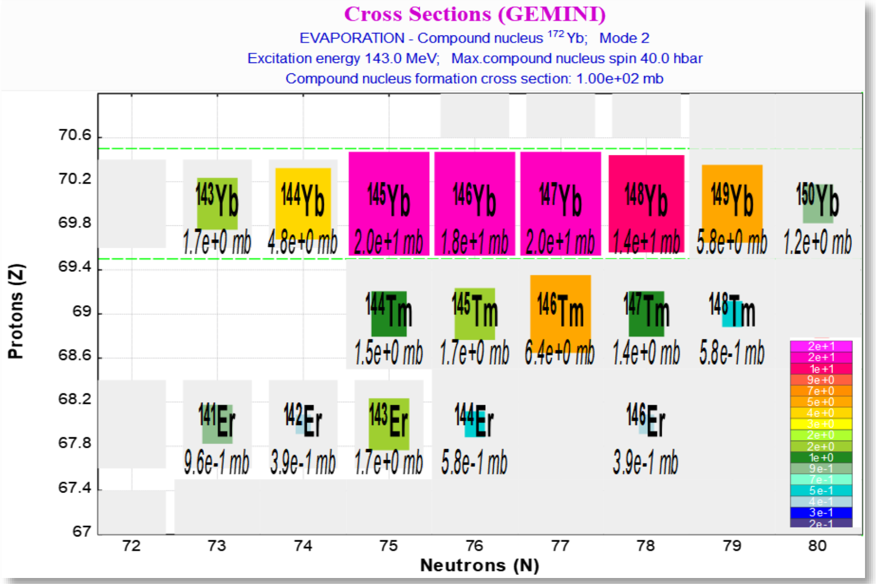


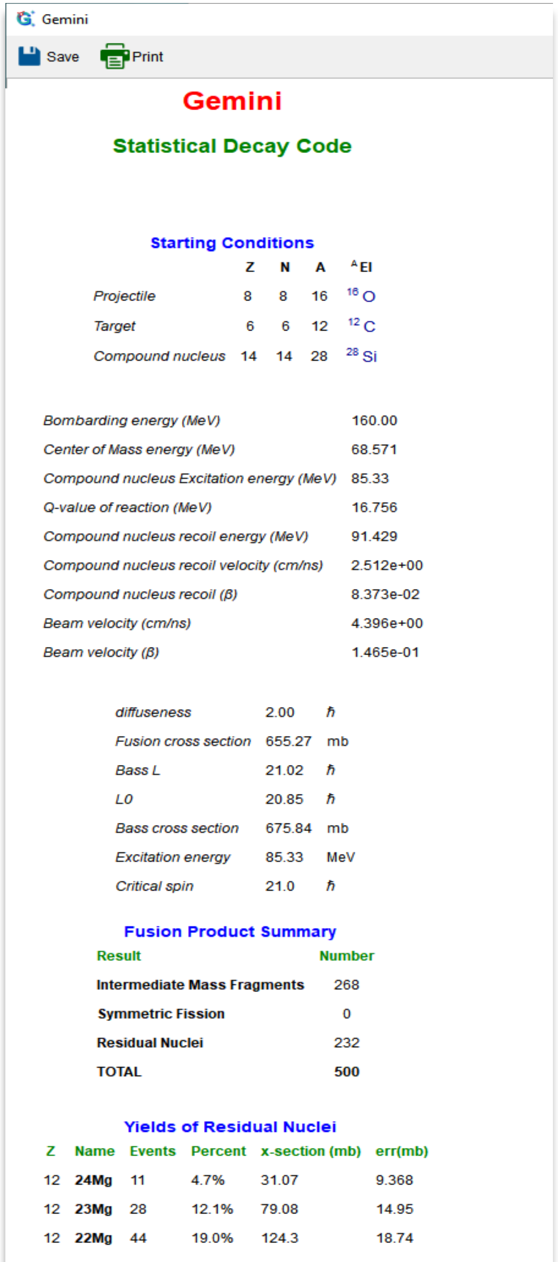
The Gemini++ code was implemented to the LISE++ package after porting to a GUI application using the Qt graphics framework.

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

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



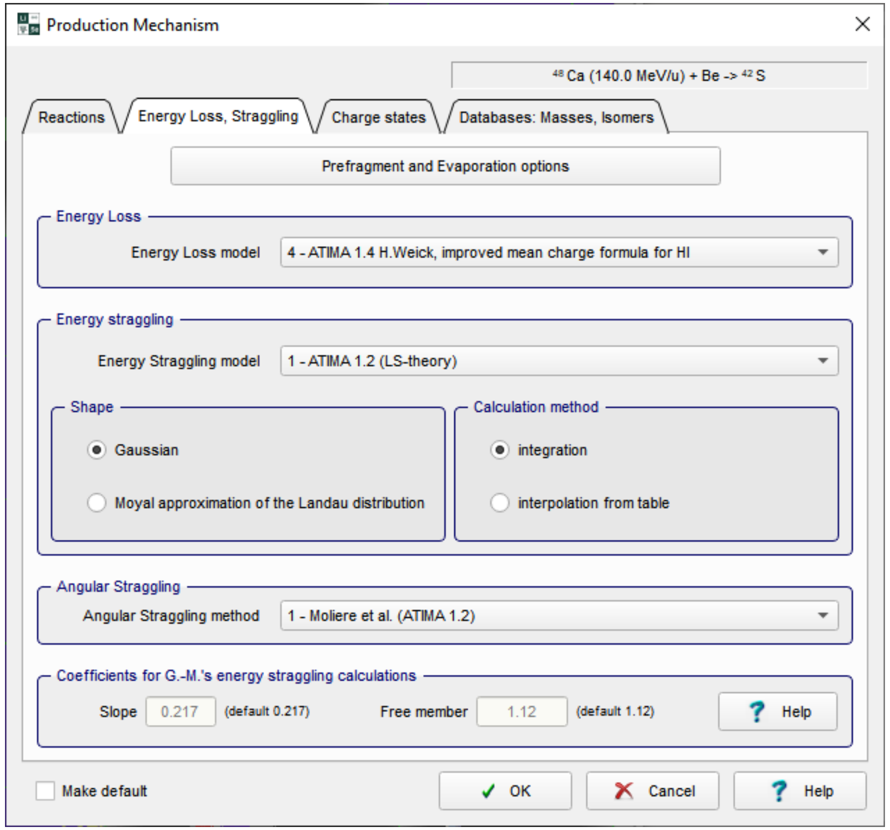


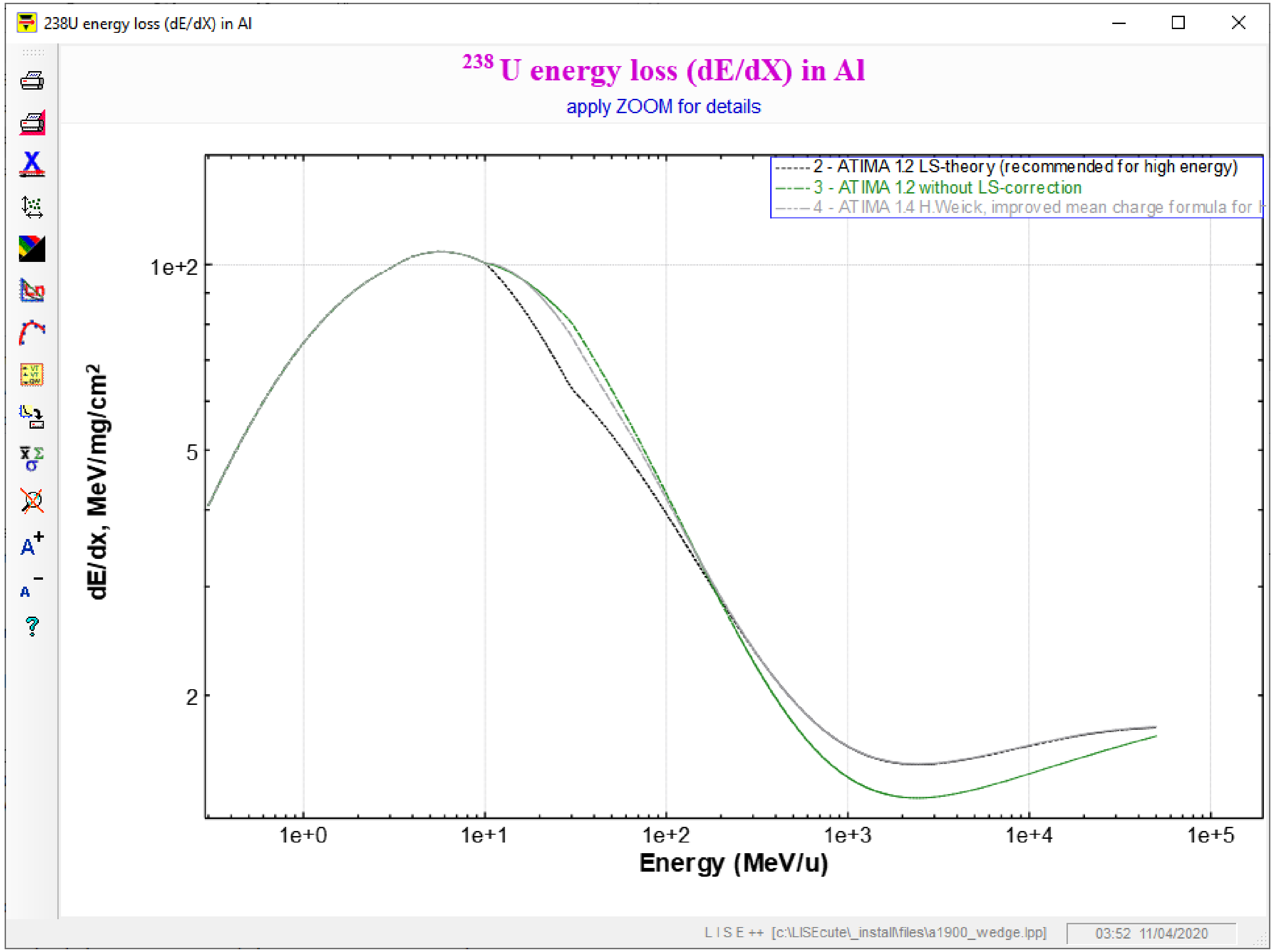


Implementation of ATIMA1.4 (catima1.5)

Complete agreement with ATIMA14 site results were obtained

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





Acknowledgements to Drs. H.Weick and A.Prochazka

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

Initial Fissile Nuclei (IFN) Analyzer

- The standard LISE 3EER (excitation energy region) model uses only 3 fissile nuclei to calculate fission fragment cross sections. Fast, but there is a large discrepancy for exotic nuclei production, as it is aimed at obtaining the main fission yield.

- The new utility, Initial Fissile Nuclei (IFN) Analyzer, calculates the contribution from all possible parent fissile nuclei to the final fission fragment, which allows to calculate
  - fission fragment production cross section,
  - more likely fissile nucleus,
  - fragment velocity in CMS,
  - excitation energy of the initial fission fragment,
  - number of nucleons released to reach the final fission fragment.

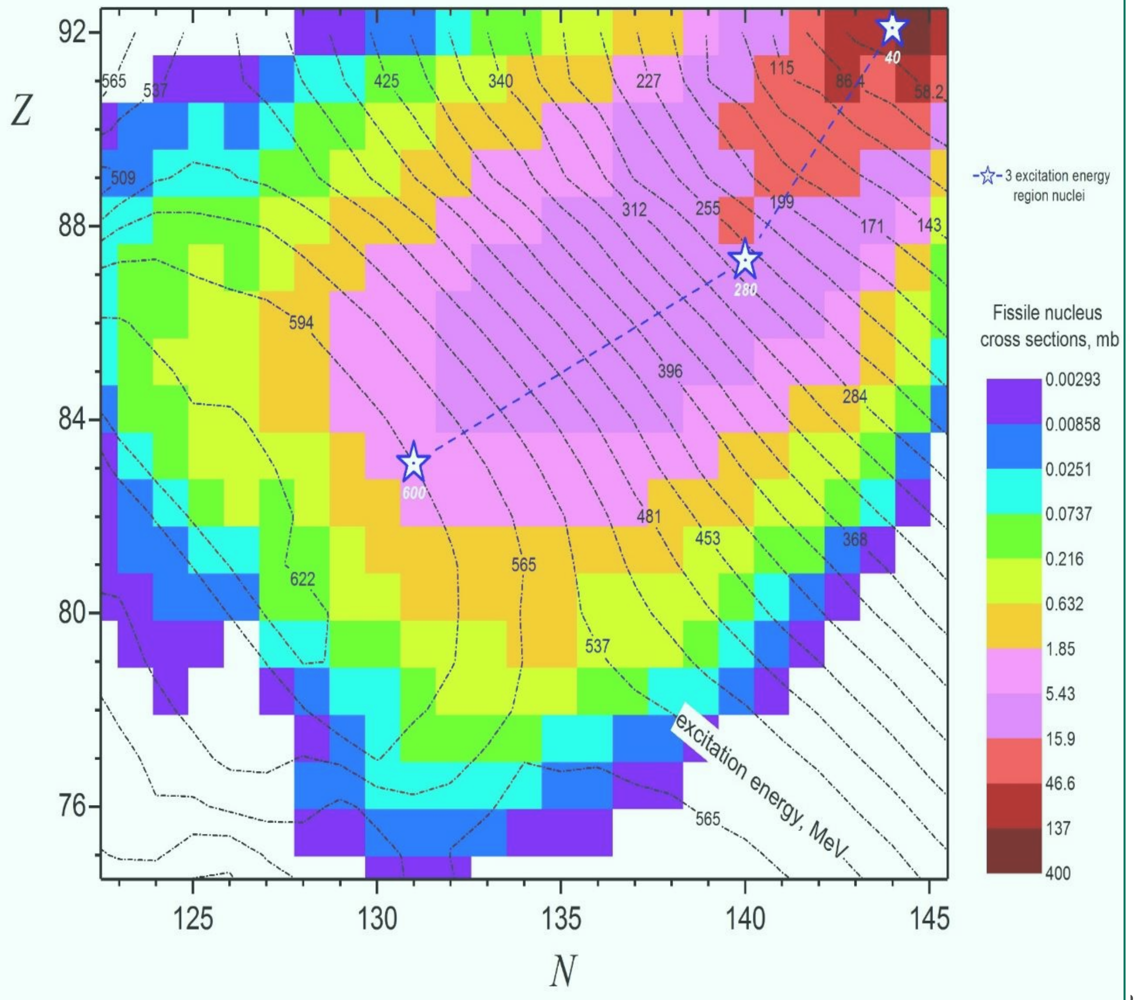
- Knowledge of the parent fissile nuclei helps to choose a reaction to maximize production of the isotope of interest, transmission factor

http://lise.nscl.msu.edu/10_1/11_0_28_IFN_search.pdf

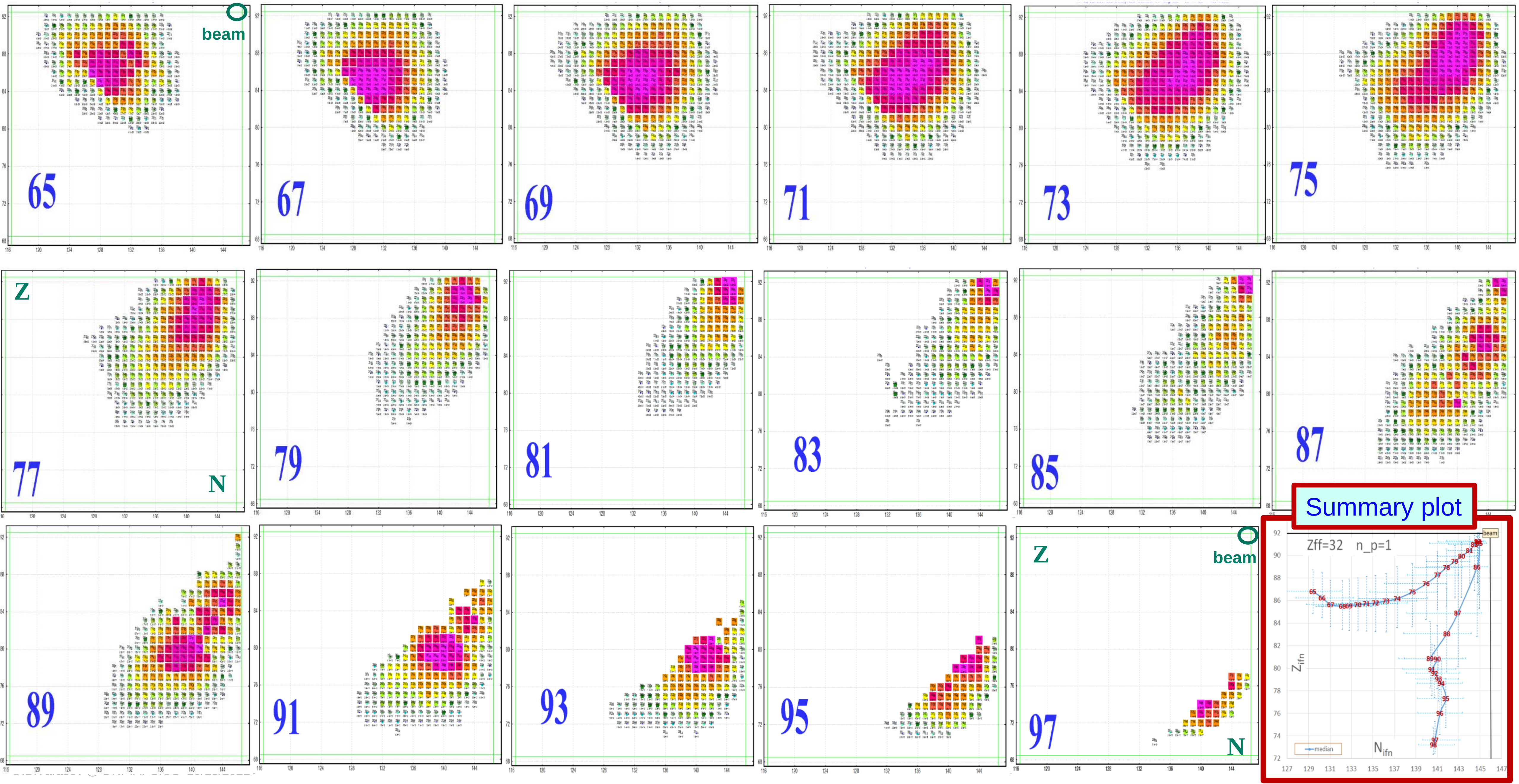
Abrasion-Fission 3EER model

- Fast Analytical model
- Averaging → substitution of more than 1000 fissile nuclei by **3** nucleus

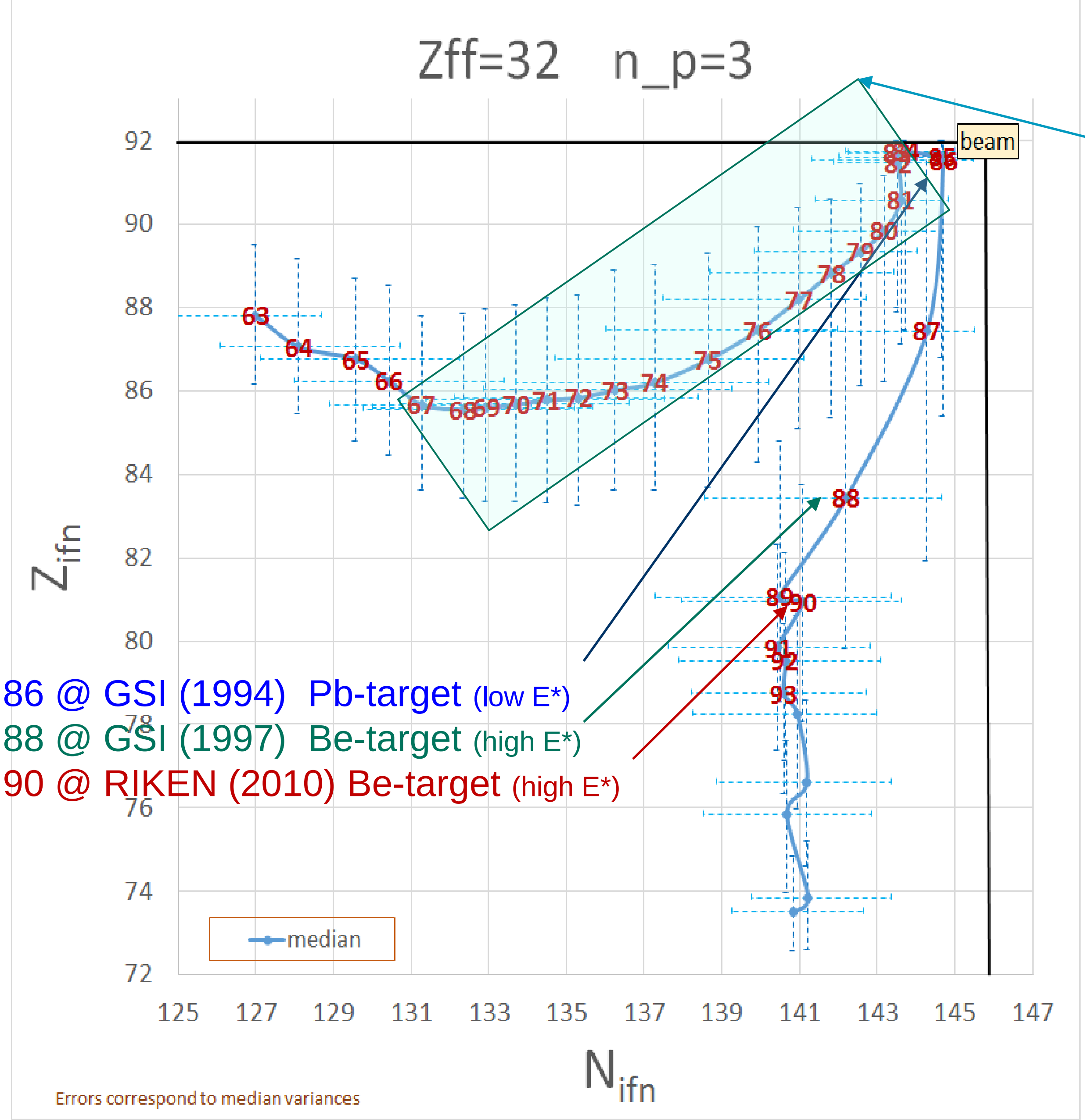
Fissile nuclei map after abrasion of ^{238}U

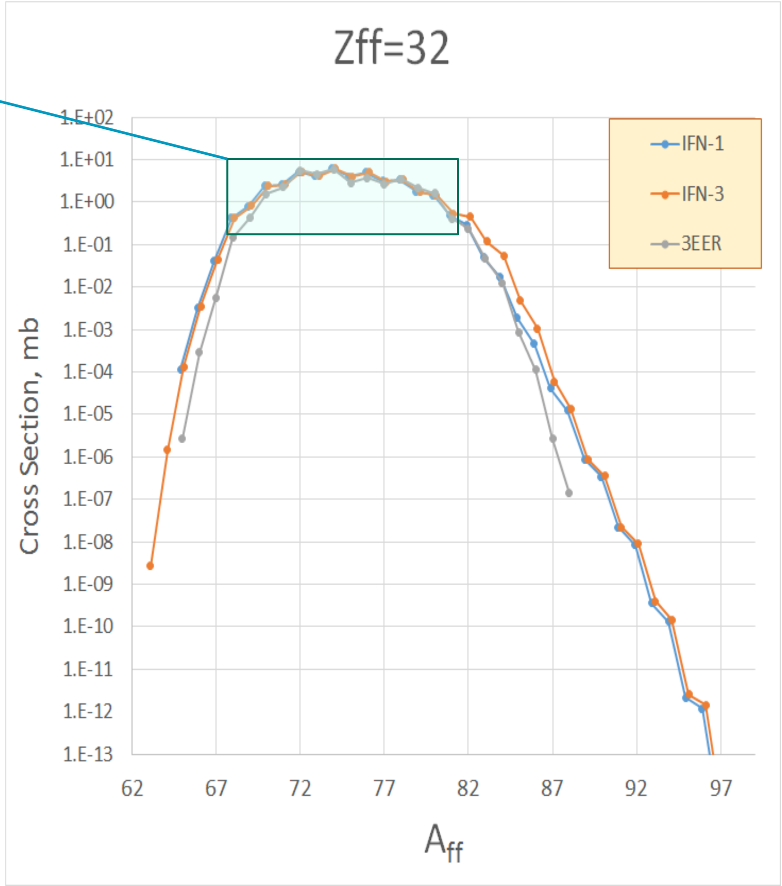


Initial Fissile Nuclei (IFN) for final Ge-isotopes (Z=32)



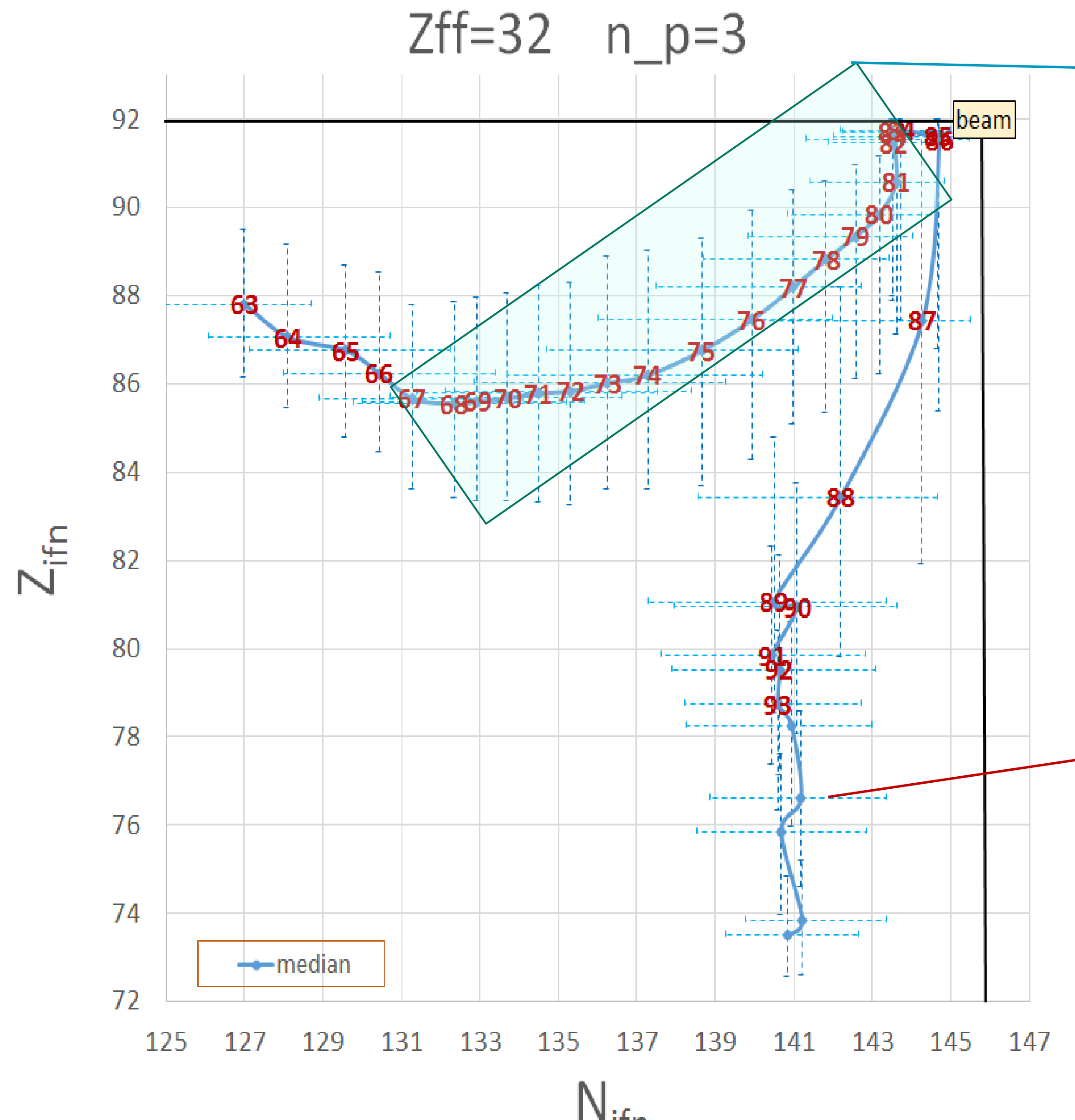
IFN-analysis for final Ge-isotopes (Z=32)





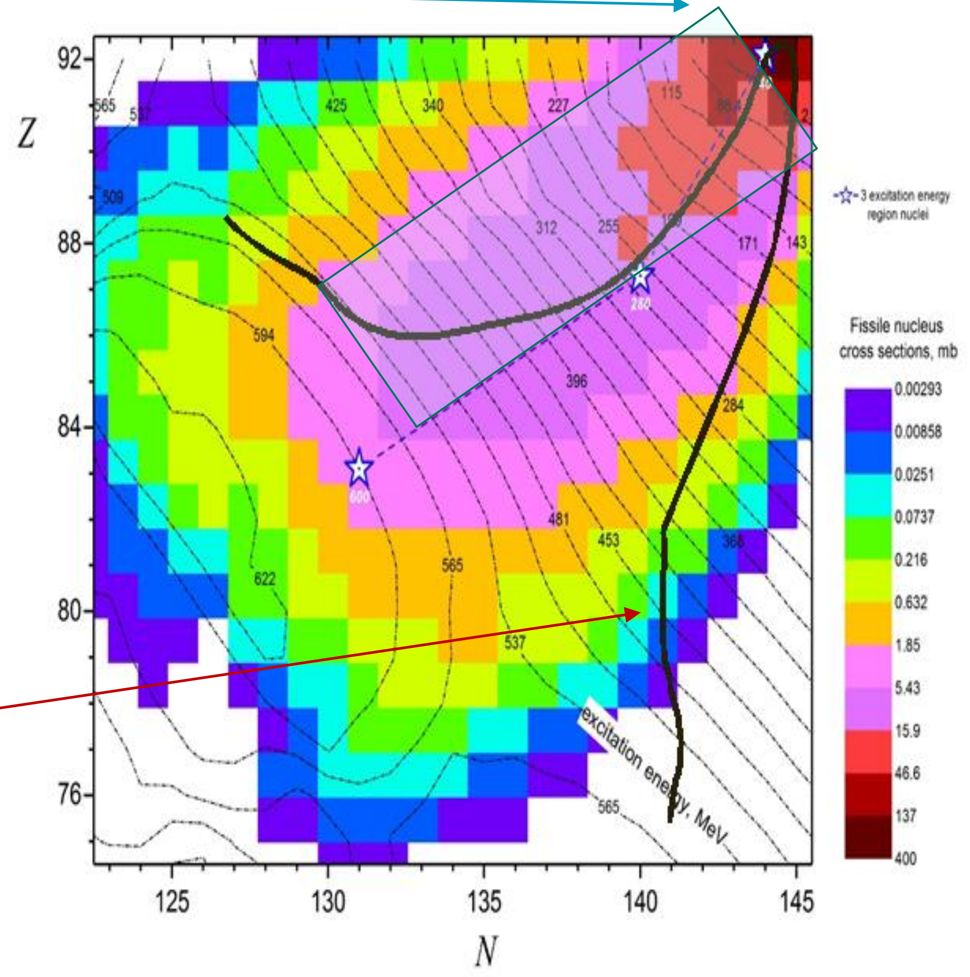
Very neutron-rich isotopes produced in high excitation fission of nuclei with Z<82. Light Z-target should be used.

IFN-analysis for final Ge-isotopes (Z=32)



Errors correspond to median variances

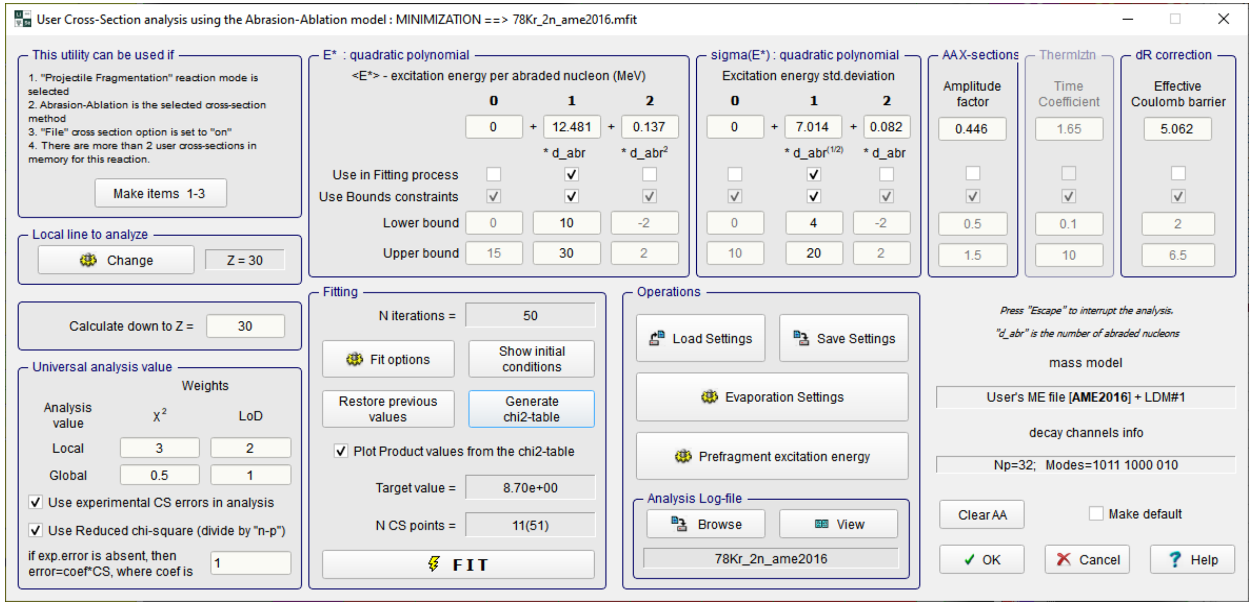
Fissile nuclei map after abrasion of ^{238}U

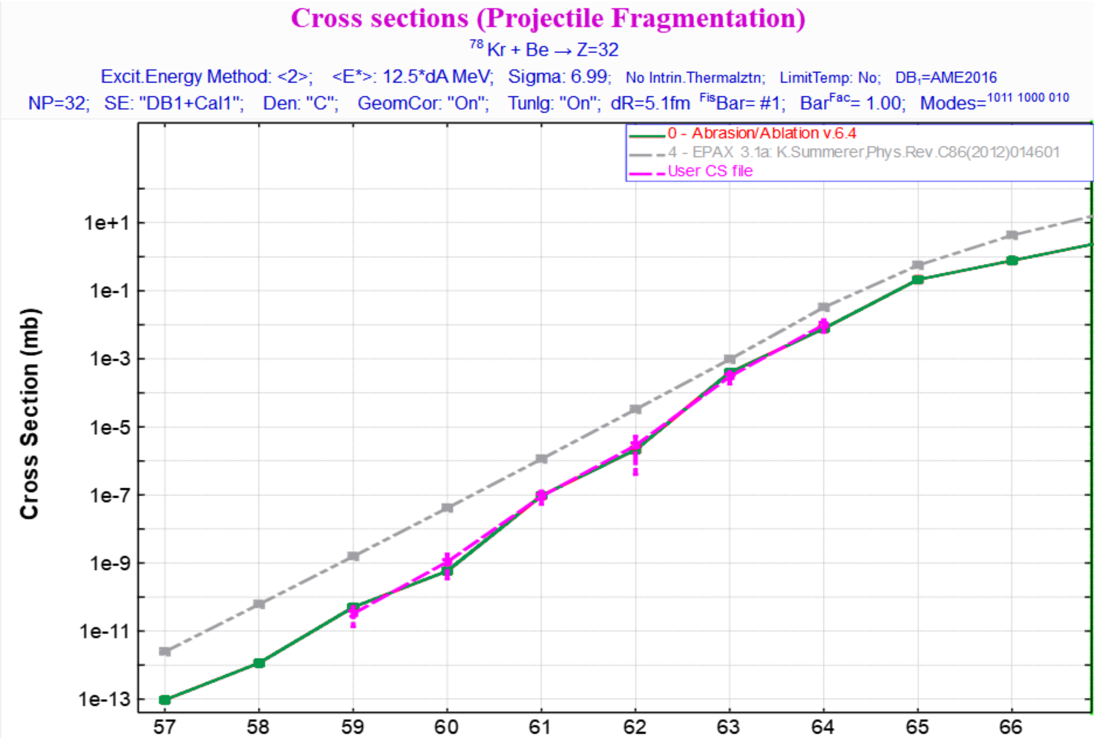


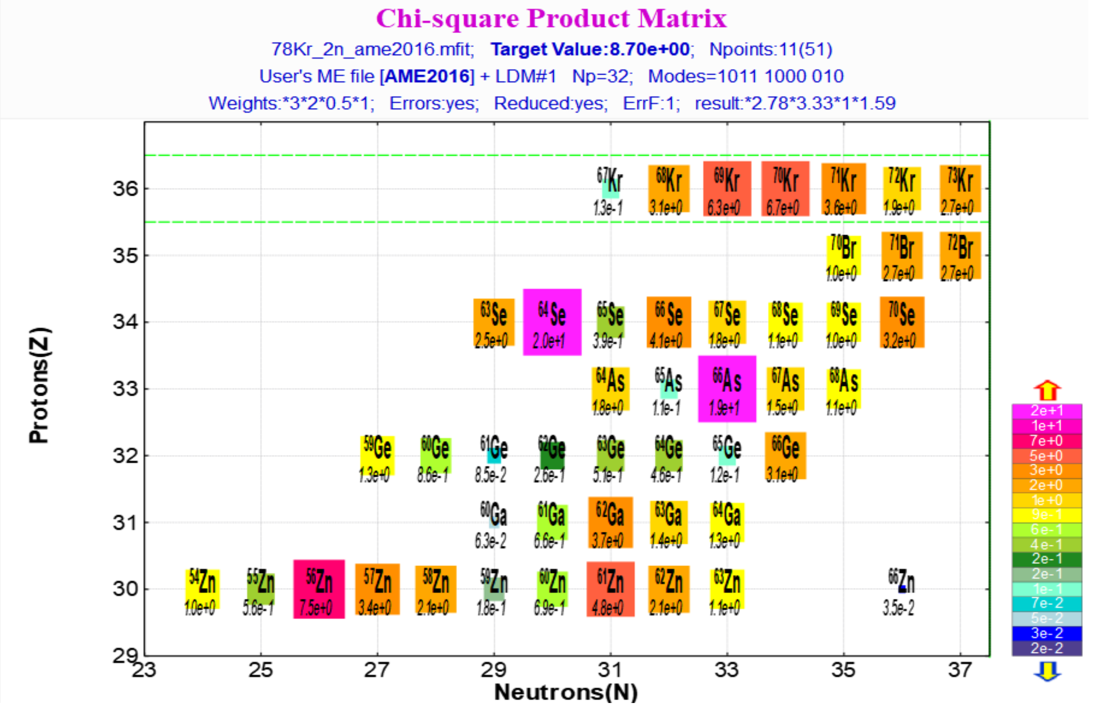
LISE^{++} Abrasion-Ablation : minimization to describe experimental cross sections

The new minimization utility recently developed in the LISE code 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^{++} suite. The utility is based on the levmar package using the Levenberg-Marquardt nonlinear least square algorithm.

Abrasion-Ablation: http://lise.nscl.msu.edu/AA.html
AA minimizer: http://lise.nscl.msu.edu/10_1/11_0_45_AA_min.pdf







Reaction Models Development Plans

- Improvement of the fast model for multi-step reactions
- Creation of fast and accurate Abrasion-Fission model based on the Initial Fissile Nuclei Analyzer tables
- Intermediate Dissipation step in the Abrasion-Ablation model
- Implementation in LISE^{++} 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
- Theoretical study of prefragment excitation energy
- Systematization of experimental production cross-sections
- Creation of Monte Carlo de-excitation cascade utility to benchmark the analytical LISE^{++} cascade subroutine and to create condition (gating) options
- Investigate charge-exchange and pick-up reactions in RIB production

Summary

- The program LISE^{++} is designed to predict the intensity and purity of rare isotope beams (RIB) is widely used at heavy ion collision facilities
- The program is constantly expanding and evolving from the feedback of its users around the world
- Fast and accurate models of rare isotope production mechanism are being developed in the LISE^{++} framework
- The LISE^{++} software suite has been transferred to a new graphics framework, Qt, to use with modern compilers, that provides cross-platform functionality, 64-bit operations
- New code capabilities such as parallel computing, and integration with control systems are planned, so the next step to be undertaken will be the creation of a LISE$_{core}$ library. This library will allow the integration of LISE^{++} with control systems for direct assistance in the tuning of fragment separators. These developments are planned to be tested at FRIB in the near feature
- Computational speedup is requested from users at many facilities, and becomes more crucial with the new large-scale nuclear physics facilities under construction, such as FRIB and FAIR, that have keen interest in integrating the LISE^{++} software with their control systems
- The release of official version 16 is expected in late autumn (currently v.15 is beta-version)

The LISE^{++} Transportation Team

Members working on the transportation of the LISE^{++} Software Suite to Qt.

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
P. Ostroumov	supervision, funding acquisition
M. Portillo	physics & ion optics consulting, benchmarks
B. Sherrill	supervision, funding acquisition
O.B. Tarasov	leading porting process worker
K.V. Tarasova	source porting, benchmarks
T. Zhang	process administration, IT consulting, adaptation to Linux

This work was supported by the U.S. National Science Foundation under Grants No. PHY-1565546, PHY-2012040

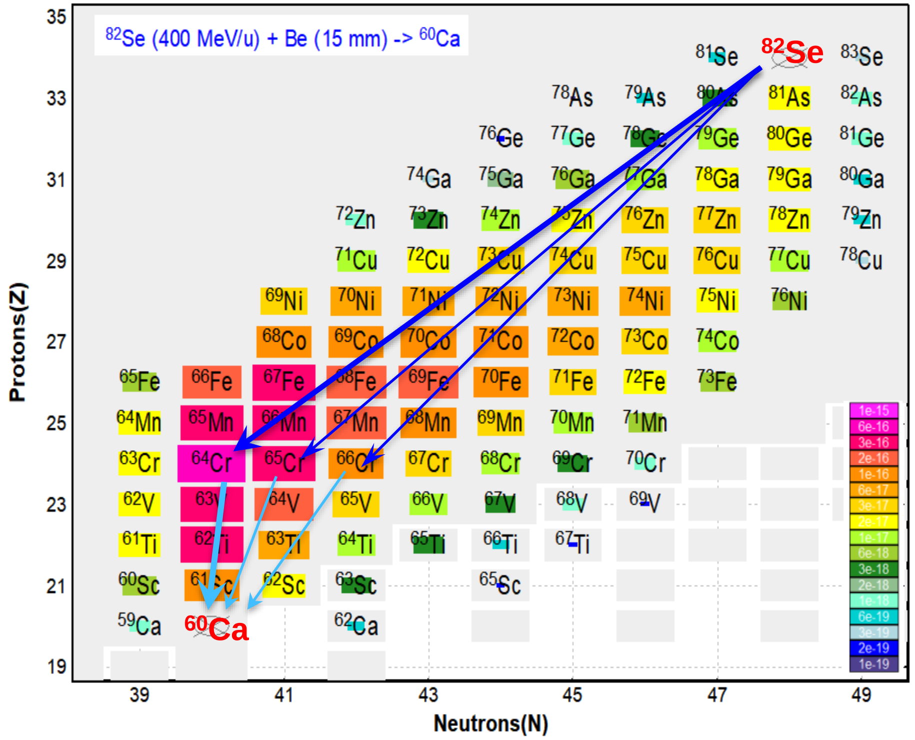
BACKUP

Multi-Step Reactions

- Multi-step reactions in thick targets is process then the projectile undergoes a series of successive reactions until the fragment of interest is produced

- For the second and next reactions we assume always a projectile fragmentation mechanism and uses the EPAX parameterization to speed up calculations

Parent nuclei: multistep production probability

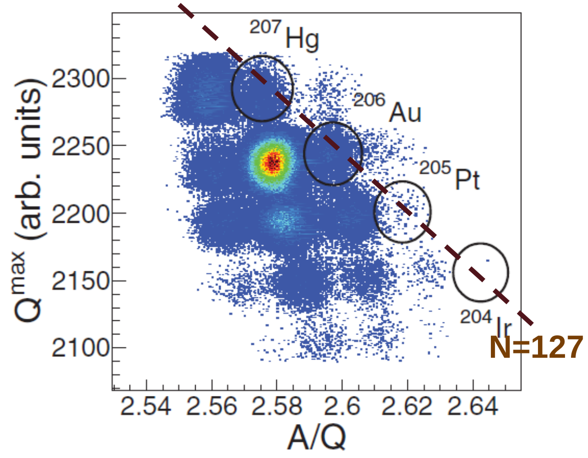


LISE^{++} → ^{64}Cr is more probable second-step projectile to produce ^{60}Ca with a ^{82}Se beam (400 MeV/u) on Be (15 mm).
Total Multi-step reaction factor is equal to 10.1

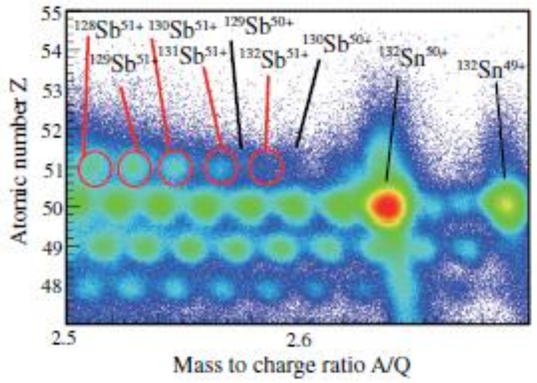
Charge-Exchange Reactions (1)

- The study (experimental and theoretical) of the charge-exchange mechanism as a **step for rare isotope production**

- (p,n)
  - A. I. Morales, J. Benlliure et al., PRC84, 011601(R) (2011)
    $^{208}Pb_{126}$ (1 AGeV) + Be



- (n,p)
  - J. Yasuda, M. Sasano, et al., PRL 121, 132501 (2018)
    ^{132}Sn (200 MeV/u) + H → **Sb
  - D.Kostyleva, I.Mukha et al., PRL 123, 092502 (2019)
    ^{31}Ar (620 MeV/u) + Be → ^{31}K



Multi-Step Reactions Study

- The study (experimental and theoretical) of the multi-step reactions:
  - the development of a fast model for multistep reactions
  - the measurement of experimental secondary cross sections
- Important to approach the nucleon drip-lines
  - So, more probable path for ^{70}Ca production at FRIB is a three-step process:

    1. Abrasion of ^{238}U to low-excited ^{237}U (E*~32 MeV) with sequential fission to ^{81}Ga (2e-2 mb)
    2. First projectile fragmentation step : ^{81}Ga $\rightarrow$ ^{76}Fe (-5p, ~1e-5 mb)
    3. Second projectile fragmentation step : ^{76}Fe $\rightarrow$ ^{70}Ca (-6p, ~1e-6 mb)

- MSU-RIKEN collaboration recent experiments with multi-step reactions analysis in process:
  - Production of neutron-rich isotopes around ^{60}Ca by projectile fragmentation of a beam of ^{70}Zn at 345 MeV/u *(O.Tarasov et al., PRL 121 (2018) 022501)*
  - Production of very neutron-rich Pd isotopes around *N* = 82 by projectile fragmentation of a RI beam of ^{132}Sn at 280 MeV/u *(H.Suzuki et al.)*

Charge-Exchange Reactions (2)

- Recent “^{60}Ca” experiment at RIKEN

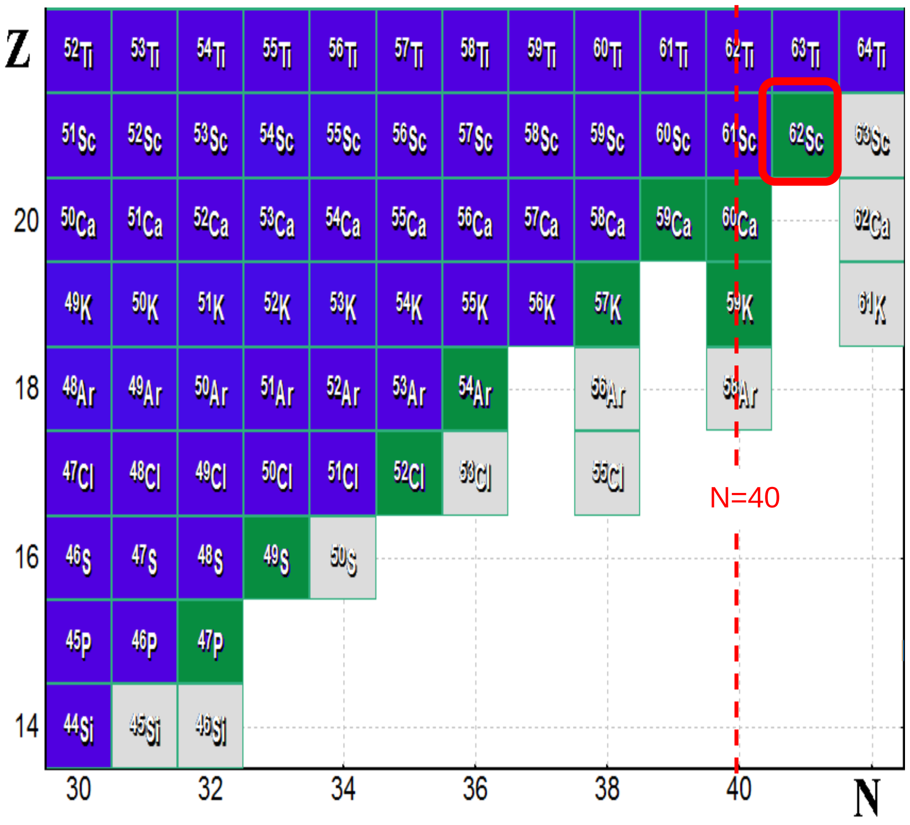
O.Tarasov et al., PRL 121 (2018) 022501

- Production of ^{62}Sc is -9p,+1n
- Pickup is suppressed at these energies
- Two-step reactions through a charge-exchange channel?

^{70}Zn(p,n)^{70}Cu → ^{70}Cu(-8p)^{62}Sc
or
^{70}Zn(-8p)^{62}Ti → ^{62}Ti (p,n)^{62}Sc

- Cross sections are under analysis
- Charge-exchange reactions become an important mechanism for the Rare Isotopes production

$^{70}Zn_{40}$ (345 MeV/u) + Be → $^{62}Sc_{41}$



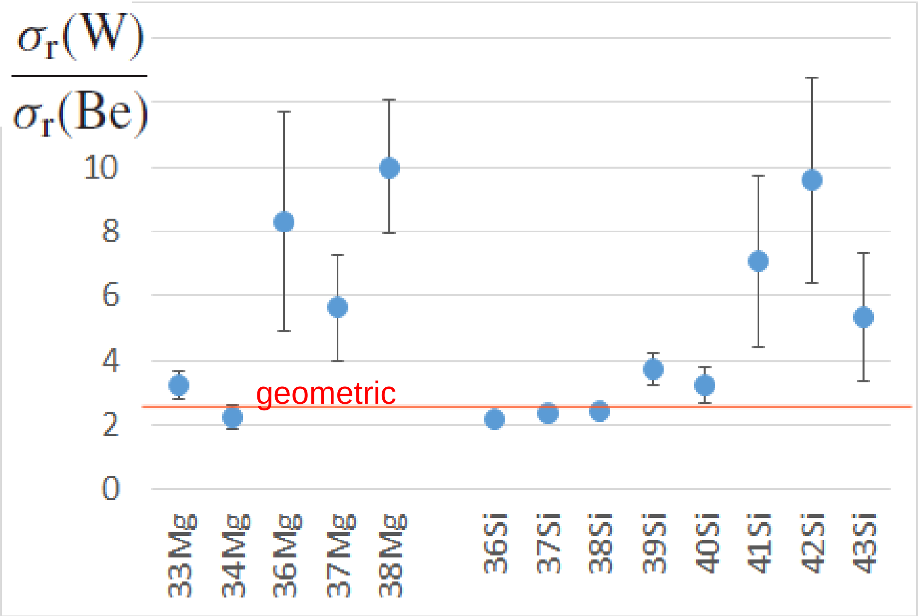
Target factor

- The study of the target factor in rare isotope yields for energies 50–150 MeV/u

- ^{48}Ca(140 MeV/u) + Be,W
  - ^{40}Mg, ^{42,43}Al:
    T. Baumann, et al.,
    Nature 449 (2007) 1022
  - ^{44}Si:
    O.B.Tarasov, et al.,
    PRC75 (2007) 064613

- ^{198}Pt (85 MeV/u) + Be, NI
  NCSL/MSU, 2019
  O.Tarasov et al, under analysis

^{48}Ca(140 MeV/u)+Be,W



The cross sections for reaction with the tungsten target are larger than those with beryllium by factors that range from approximately 2.5 at A = 36 (Z=14) to about 10 at A = 42, values that become significantly larger than the ratio of the geo-metric reaction cross sections equal to 2.66

LISE^{++} Powerful Tools

Besides analytical calculation of the transmission and yields of fragments

- Monte Carlo simulation of fragment transmission,
- Monte Carlo simulation of fission fragment kinematics,
- Ion Optics calculation and Optimization ,
- LISE for Excel (MS Windows, Mac OS - download)

LISE^{++} calculators:

- "Physical Calculator",
- "Relativistic Kinematics Calculator",
- "Evaporation Calculator",
- "Radiation Residue Calculator" *(new)*,
- "Ion Mass calculator" *(new)*,
- "Matrix calculator"
- "Initial Fissile Nuclei analyzer" *(new)*

Implemented codes:

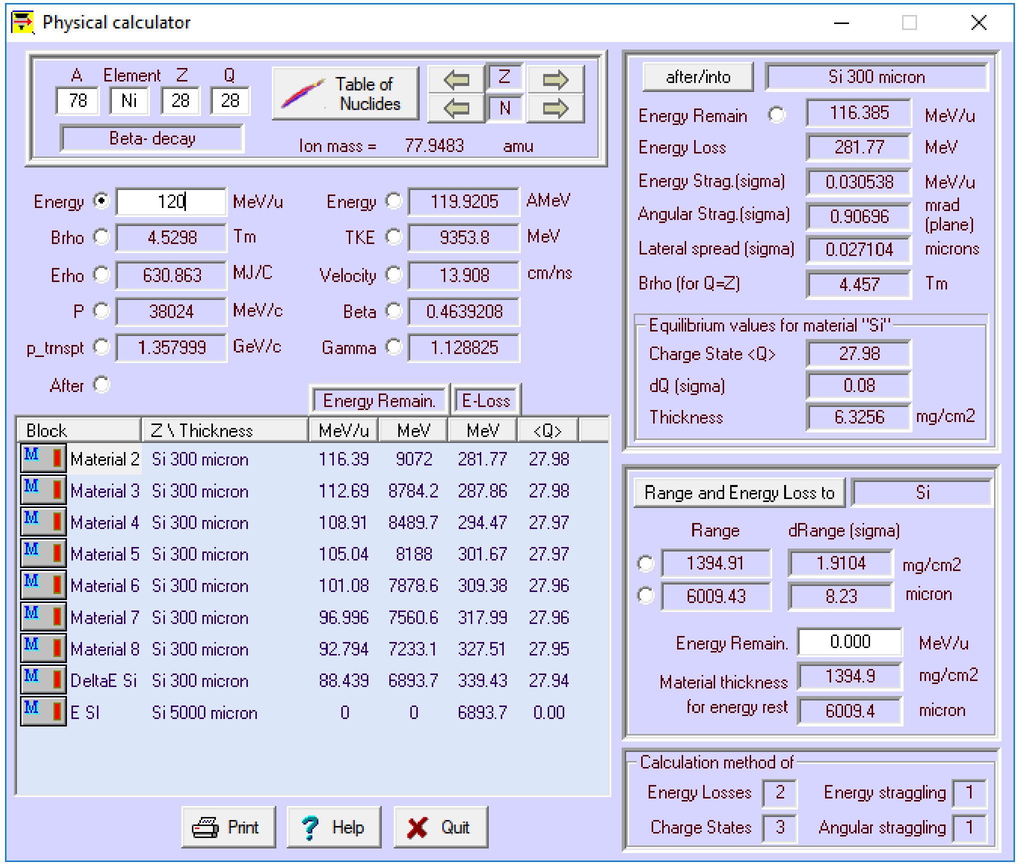
- «PACE4» (fusion-evaporation code),
- «MOTER» (raytracing-type program for magnetic optic system design)
- «ETACHA4» (charge-state distribution code) *(new)*,
- «Global» (charge-state distribution code),
- «Charge» (charge-state distribution code),
- «Spectroscopic Calculator" (of J.Kantele»)

LISE^{++} Utilities:

- Stripper Foil Lifetime Utility,
- Brho Analyzer,
- Twinsol (solenoid) utility,
- Units Converter,
- ISOL Catcher,
- Decay Analysis (includes Proton, Alpha, Cluster, Sp.Fission half-lives calculation),
- Reaction Utilities (Characteristics, Converters, Plots),
- «BI»- the automatized search of two-dimensional peaks in spectra

Databases:

- Nuclide and Isomeric State databases with utilities,
- Large Set of Calculated Mass Tables (includes FRIB mass tables),
- Ionization Energy database (used with the Ion Mass calculator),
- Decay Branching Ratio database (used with the Radiation Residue calculator)



Fragment Separator Construction

- with different sections called "blocks" (magnetic and electric multipoles, solenoid, velocity filter, RF deflector and buncher, material in beam, drift, rotation element, and others).

- a user-friendly interface that helps to seamlessly construct a fragment separator from the different blocks.

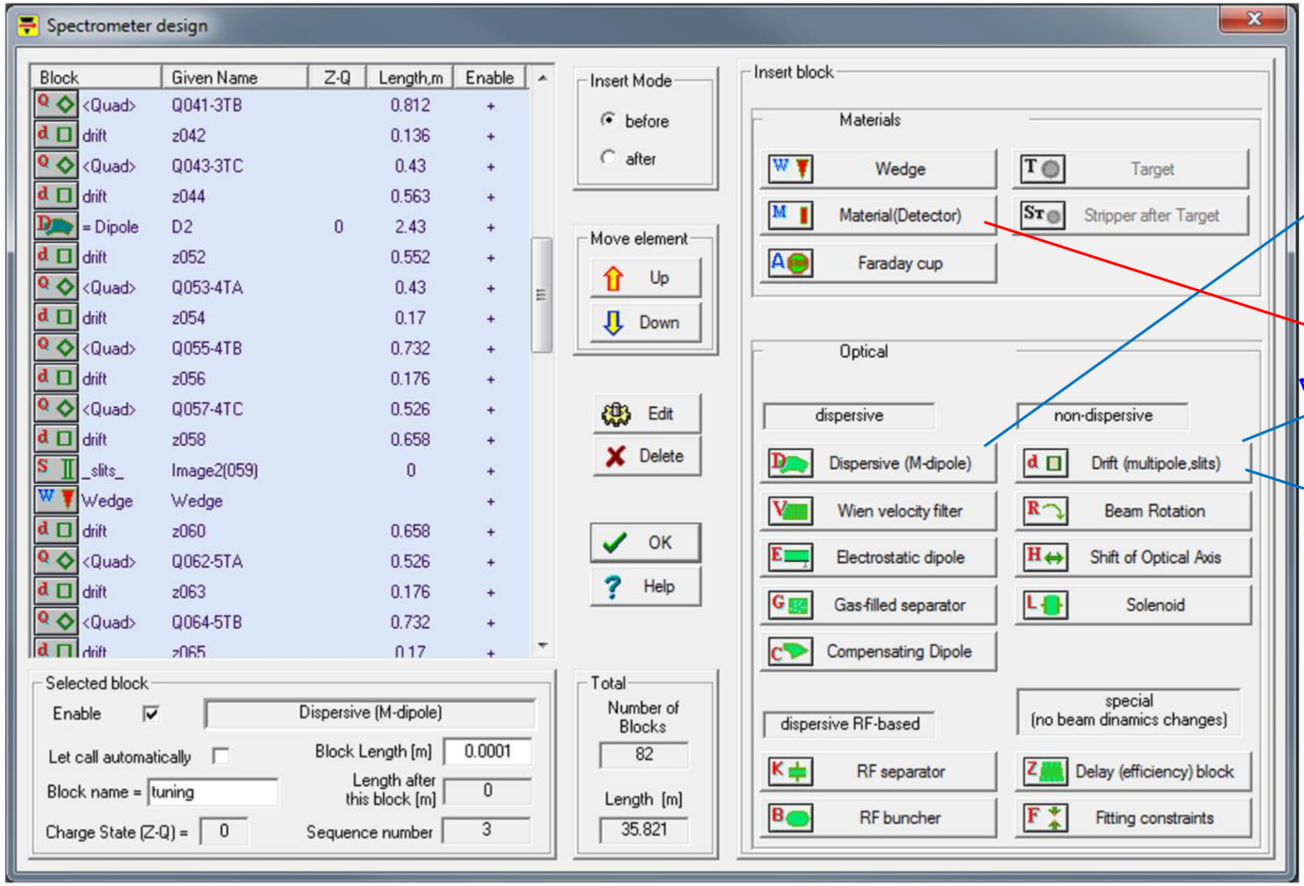
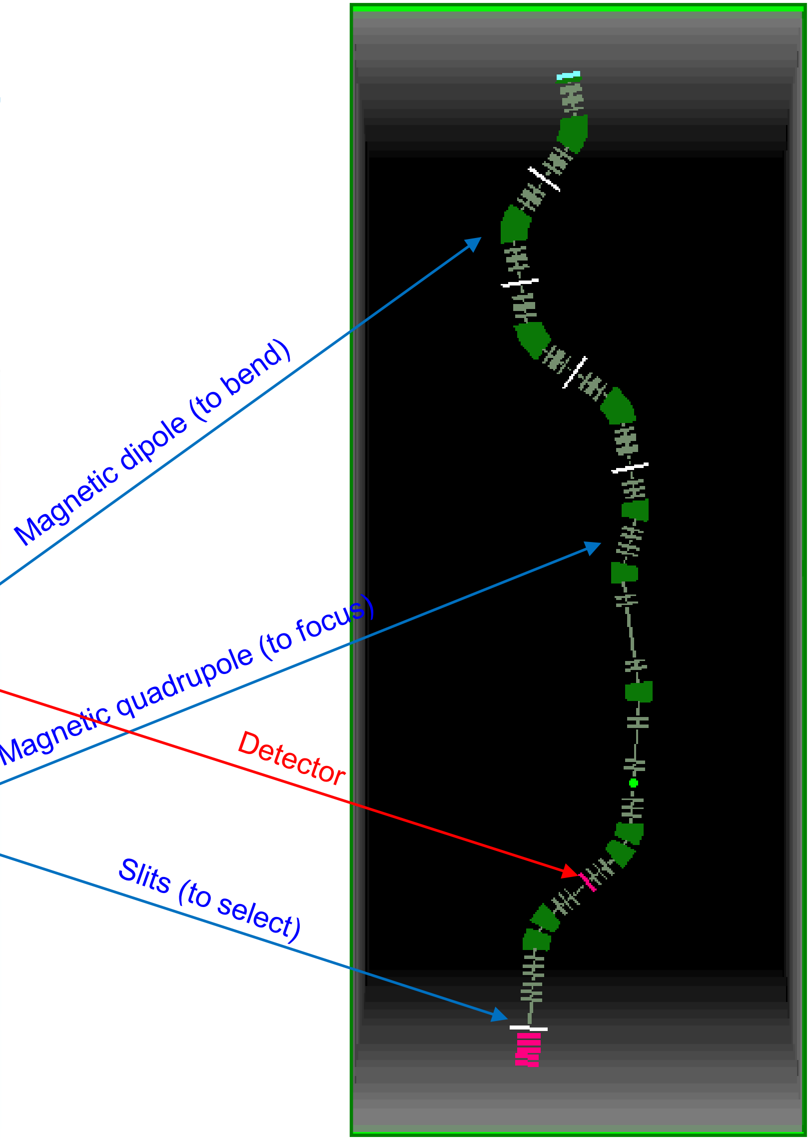


Fig. 1. Updated view of the "Spectrometer Design" dialog window.



Configuration: A1900_S800BL (2nd order) 164 blocks