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

Contents lists available at ScienceDirect

Nuclear Inst. and Methods in Physics Research, B

journal homepage: www.elsevier.com/locate/nimb

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

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ARTICLE INFO

Keywords:
$\mathtt{LISE}^{++}$
Fragment-separator
Simulation
Rare isotope production

ABSTRACT

The $\mathtt{LISE}^{++}$ software for fragment separator simulations has undergone a major update. The package, widely used at rare isotope beam facilities, can be used to predict intensities and purities of rare isotope beams and for planning and running of experiments using in-flight separators. It is especially useful for radioactive beam production as its results can be quickly compared to on-line data. The $\mathtt{LISE}^{++}$ package has been ported to the Qt-framework in order to support modern compilers and computing methods. The benefits include 64-bit operation and $\mathtt{LISE}^{++}$ availability on three different platforms: Windows, MacOS and Linux. In addition, the porting provides the ability to take advantage of future computational improvements. The updated package is named $\mathtt{LISE}^{++}_{cute}$ to indicate a major step forward from the previous Borland-based versions. In addition to porting to the new platform, new main features and modifications have been added, mostly devoted to improving models and implementing other codes involved in rare isotope production at FRIB. A summary of modifications completed to improve the functionality of the code are discussed in this work, as well as future plans.

1. The code performance and sustainability

$\mathtt{LISE}^{++}$ is the standard software used at in-flight separator facilities for predicting beam intensity and purity [1,2]. The code simulates nuclear physics experiments where fragments are produced then selected with a spectrometer. According to our plans for performance and model improvements in the $\mathtt{LISE}^{++}$ software [3], the $\mathtt{LISE}^{++}$ software package is being transported to a modern graphics framework with new compilers to aid in the performance and sustainability of the code. The benefits include 64-bit operation, and make $\mathtt{LISE}^{++}$ available on three different platforms: Windows, macOS and Linux. In addition, the porting gives us the ability to take advantage of future computational improvements. The $\mathtt{LISE}^{++}_{cute}$ package remains essentially identical for all platforms, keeping all previous versions functionality with implementation of new features and utilities.

2. New features

In addition to porting to the new platform, new features and modifications have been added. Most features are devoted to improving models and implementing other codes involved in rare isotope production at corresponding facilities across the world. Creation of in-house reaction models and implementation of powerful modern algorithms in the code remain important priorities for $\mathtt{LISE}^{++}$ development. Detailed information about all the new features can be found on the $\mathtt{LISE}^{++}$ website [1]. In this paper, we highlight the main updates.

2.1. Codes

Three auxiliary programs are now available in $\mathtt{LISE}^{++}_{cute}$.

- The GEMINI++ statistical decay code [4] was transferred into an interactive Graphical User Interface (GUI) program and incorporated into the $\mathtt{LISE}^{++}$ package. This also allows for the plotting of results directly within $\mathtt{LISE}^{++}$.
- ETACHA4 [5,6] has been converted into C++ and $\mathtt{LISE}^{++}$ users are able to interact with this new version via a GUI. Within this new ETACHA4-GUI, users are now able to plot calculated charge state evolution distributions (see Fig. 1).
- Lastly, the new version 1.4 of the energy loss code ATIMA [7] is now available in $\mathtt{LISE}^{++}$.

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https://doi.org/10.1016/j.nimb.2023.04.039
Received 17 February 2023; Received in revised form 23 April 2023; Accepted 23 April 2023

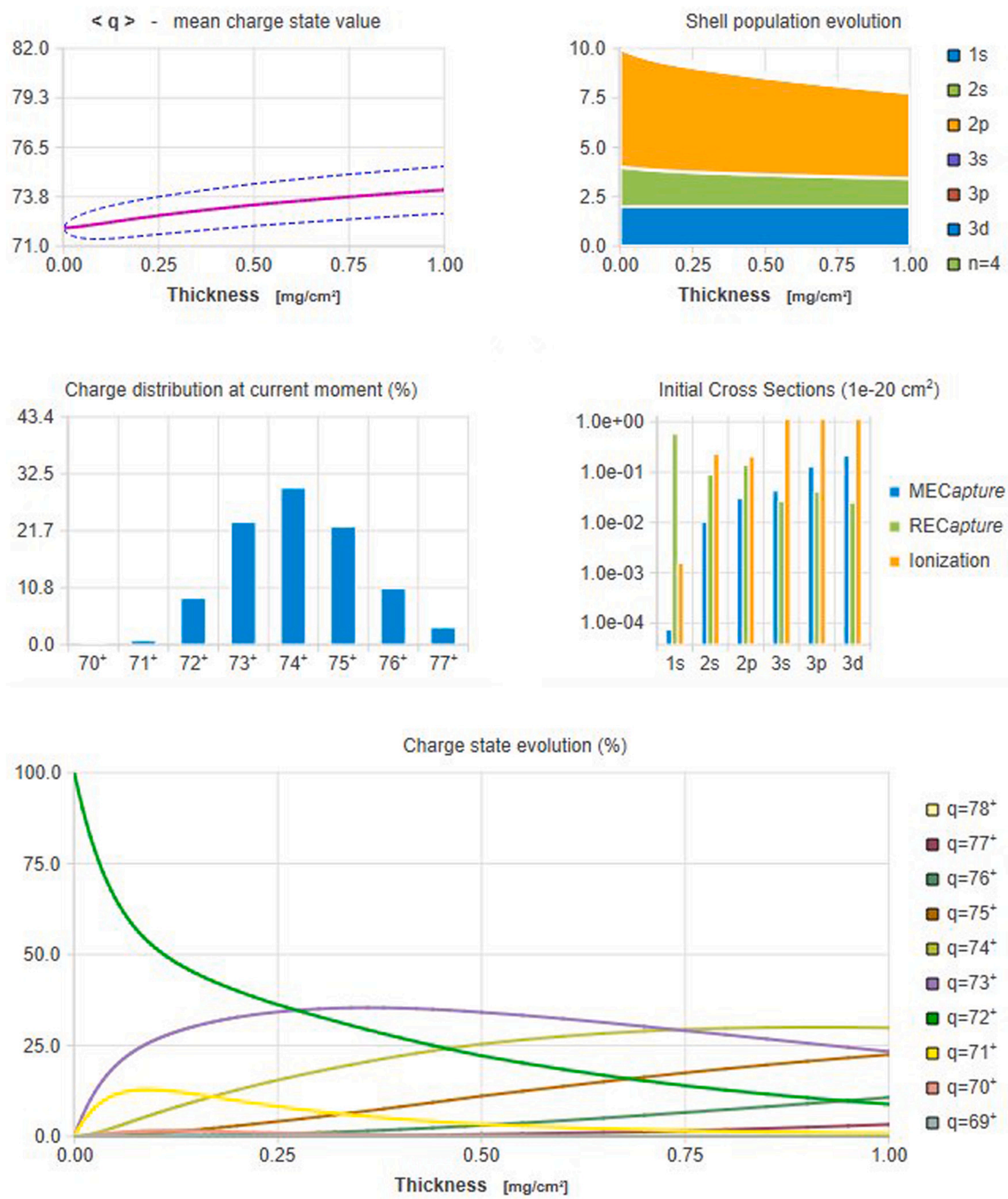

Fig. 1. Charge state evolution distributions calculated by the ETACHA-GUI code for $^{207}Pb^{72+}$ at 28.9 MeV/u passing a carbon foil of 1 mg/cm^2.

2.2. Utilities

LISE^{++} provides a collection of tools, or utilities, to assist with calculations. Here, we summarize updates to existing utilities and new utilities that are available in the newest version of LISE^{++}.

- The minimization procedure of the LISE^{++} Abrasion–Ablation model [8] was modified to adjust its parameters based on experimental projectile-fragmentation cross-sections. For example, using the updated utility together with the HFB22 mass table, the cross sections for more neutron-deficient germanium and selenium isotopes were predicted in the recent work [9].
- The *Two Fission Fragments* utility calculates the probability of simultaneous detection of fission fragments after passing through the spectrometers. The utility can be run in the batch mode.
- A new utility, *power deposition and rate analysis in blocks*, calculates the power deposited per block for both primary and secondary beams.
- A new utility, *Beam energy scanning*, determines the optimal beam energy for the selected separator settings.
- A new utility, the *Initial Fissile Nuclei (IFN) Analyzer*, calculates more probable fissile nuclei for the final fission fragments. To overcome the "averaging" effect intrinsic to the LISE^{++} three excitation energy regions (3EER) model [10,11], the IFN analyzer

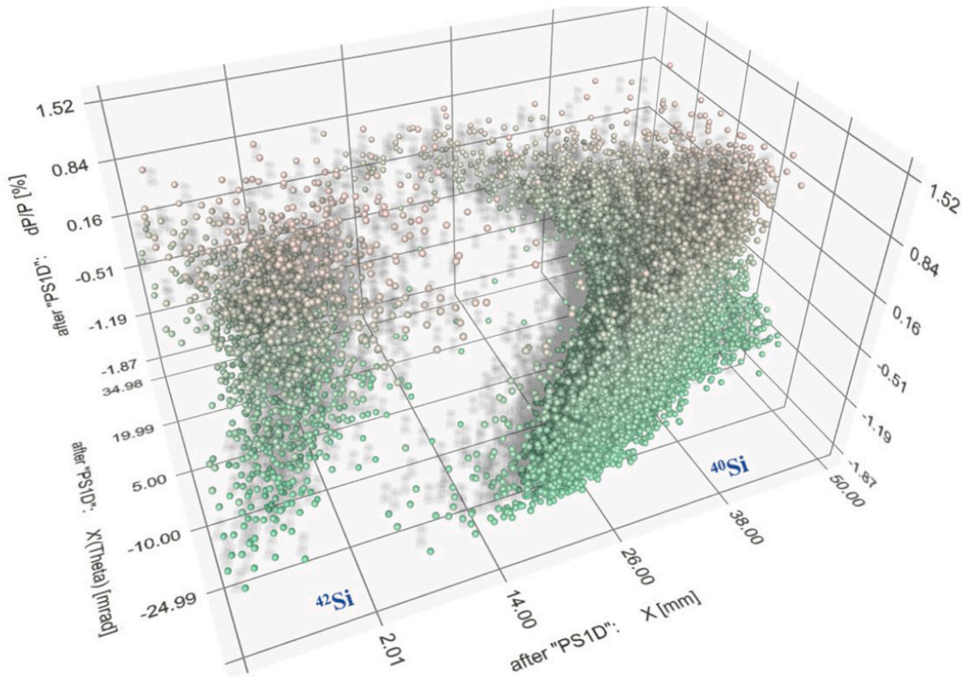

Fig. 2. 3-D plots of the X, X', dP/P distributions of ^{40}Si and ^{42}Si fragments in front of the ARIS preseparator final focal plane slits calculated by Monte Carlo method with 5th order maps use in the reaction ^{48}Ca(251 MeV/u) + ^{12}C(10 mm). The separator set to produce ^{42}Si uses a 6-mm special shape aluminum degrader located in the dispersive focal preseparator plane, which compress fragment momentum distributions by a factor 3. Calculated transmission through the next slits ($\pm$8 mm) are 0.03% and 87.2% for ^{40}Si and ^{42}Si, respectively.

takes into account contributions for all possible fissile nuclei, follows an abrasion-fission production model in LISE^{++}. This choice was made after benchmarking and performance optimization.

2.3. New features

Additional improvements were made in the central LISE^{++} program.

- Monte Carlo transmission outputs may now be rendered as a three-dimensional point-cloud distribution (see Fig. 2). This feature includes the plotting of 3-D envelopes.
- Angular straggling contributions are now included in ion optics calculations.
- Material length is now taken into account in optics calculations.
- Shape calculation of two angle wedges is implemented to pass neighboring isotopes besides a setting fragment in the case of thick momentum compression degrader.
- The source code was ported to C++17 and the code now utilizes safe pointers. This improves the safety and future compatibility of the code base.
- The LISE package installer on Windows is now signed with a digital certificate.

3. Development plans

In the near future, the creation of a LISE$^{++}_{core}$ library and code parallelization will be undertaken. This library will allow for the integration of LISE^{++} calculations in control systems, which is an essential feature to assist the tuning of fragment separators. This functionality will be tested at FRIB. For example, the direct integration of LISE^{++} software with the ARIS controls at FRIB will enable operators to update inputs to calculations based on experimental measurements.

To take advantage of modern computing architecture, parallel computing methods are essential in achieving faster computation. This work aims to address the increased computational demands associated with more complicated devices at new large scale facilities. In order to perform the necessary calculations in an acceptable time, code optimization and parallel methods will be applied. As a first step, the LISE^{++} code parallelization process will be implemented on the Monte Carlo and *Distribution* analytical methods for fragment transmission calculation.

Additionally, three tools are planned for development:

- *Beam optics tuner:* Inspired by the program TUNER [12], this new utility will calculate second order optics of beam line configurations dynamically with the ability to plot envelopes of setting fragment kinematic distribution widths and optical matrix elements.
- *Block configuration converter:* A new tool will be built around a new type of block, labeled "G"(Group), which allows the grouping (and ungrouping) of "E"(Element) blocks (see for details the work [2]).
- *Beam dump utility:* This Monte Carlo-based tool will calculate the primary beam charge state locations in a beam dump plane using fifth order optics of beam line configurations, with a 3D option for plotting rays and locations.

4. Summary

The LISE^{++} software suite has been transferred to Qt, a modern graphics framework, to aid in the performance and sustainability of the code. The benefits include 64-bit operation, and ability to deploy LISE^{++} on three different platforms: Windows, MacOS and Linux. In addition, the porting gives us the ability to take advantage of future computational improvements as integration with control systems and code parallelization.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Acknowledgments

This work was supported by the U.S. Department of Energy, Office of Science, Office of Nuclear Physics and used resources of the Facility for Rare Isotope Beams (FRIB), which is a DOE Office of Science User Facility, operated by Michigan State University, United States, under Award Number DE-SC0000661, and by the US National Science Foundation under Grant Nos. PHY-20-12040 and PHY-2012865.

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