LISE++ Software Updates and Future Plans

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Abstract. This paper describes capabilities and future upgrade plans for the isotope production and simulation software that is used at many in-flight fragmentation facilities, namely LISE++. We highlight the process and methods of updating the software while retaining the computational integrity of the code. The calculations of beam transport and isotope production are becoming more computationally intense with the new large scale facilities. Computational improvements as well as the process of updating this large code is discussed.

1. Introduction

Production of new isotopes is one of the opportunities at the intensity frontier of nuclear physics. The associated science ranges from tests of the Standard Model to exploration of the origin and evolution of the chemical elements in the universe. Leading facilities in this effort are RIBF at RIKEN, TRIUMF in Canada, and ISOLDE at CERN. New large scale facilities under development at the nuclear intensity frontier include FAIR in Europe, FRIB in the United States, and others in countries including China, France, Korea, and Italy. Simulation of isotope production at these facilities is crucial for experiments in this field.

LISE++ is software used to predict beam intensity and purity of rare isotope beams produced in-flight by magnetic and electric separators. The primary use of LISE++ at most facilities is to predict and identify the composition of Radioactive Nuclear Beams [1]. Intensity and purity of a desired beam can be predicted, along with the separator magnet settings. Included in the LISE++ package are models of isotope production mechanisms, ion optical transport through magnetic and electric systems, and ion interactions in matter. The suite contains a set of tools to assist in the simulation of many components of projectile fragmentation experiments. Users include designers of spectrographs and fragment separators, experimentalists at existing facilities, and beam physicists involved in tuning beams through such systems.

2. The LISE++ Software Suite

LISE++ provides models for reaction mechanisms for isotope production: projectile fragmentation, fusion-residual, fusion-fission, coulomb fission, and abrasion-fission. For spectrometer design, construction of a spectrometer is implemented through the use of material and optical blocks. These blocks can consist of detector and target materials, dipole magnets, and other materials commonly used in these experiments. The software suite has a Graphical User Interface (GUI) from which the user sets up and completes all calculations. The main GUI screen with a particle identification plot is shown in Fig. 1. Another widely used component of LISE++ is the Physical Calculator, shown in Fig. 2. This is used to calculate energy loss through
Figure 1. The LISE++ main GUI with a $\Delta E$ vs Total Kinetic Energy particle identification simulation plot overlaid.

Figure 2. The physical calculator is a widely used utility in the LISE++ framework. It calculates the energy loss through an unlimited number of material blocks.

Figure 3. Horizontal space envelope of the A1900 fragment separator at NSCL calculated with LISE++. This represents the beam ray paths through the spectrometer.

material and optical blocks. The LISE++ suite provides a complete analysis framework for isotope production. It allows for the input of ion-optical maps from other codes, such as COSY Infinity for higher order calculations [2]. Also included in the suite are stand-alone utilities for other calculations useful in these experiments such as charge state calculations, fusion-evaporation calculations, and a spectrometric calculator. These utilities implement popular independent codes within the LISE++ framework.
3. Software Update

3.1. Motivation
LISE++ is currently distributed as a Windows executable with support for 32-bit compilation. The program was developed within the Borland C++ framework. Since its inception in 1998, the code has grown immensely. It started on MS-DOS with 14 C++ files and less than 10,000 lines of code and grew to 606 files on MS Windows today. The calculations of beam transport and isotope production are becoming more computationally intense with the new large scale facilities. For example, the 90 m long FRIB separator will have around fifty magnetic elements and ten points of beam interactions with matter. In order to perform the calculations in acceptable time, updates to the current software are desired. In order to meet computational demands of new large scale facilities, the software is being converted to a new development environment. A new compiler is necessary to implement parallel computing, which is not available in the current framework. In addition, a native Linux version is desired for integration with control systems at labs such as GSI and NSCL. With over 350 thousand lines of code, this is a significant undertaking and the verification and validation of the conversion is a very important process.

3.2. Updates and Future Plans
To ensure longevity of the LISE++ program for future operating systems, the LISE++ program will be transported to a modern graphics framework with cross-platform support that allows the use of various compilers. Additional benefits include providing a 64-bit application, cross-platform compatibility, and the ability to take advantage of computational advances. To achieve the speedup desired by new large-scale facilities, numerical optimization and parallel methods will be applied. Fig. 4 outlines the areas of the LISE++ software where updates are planned.

![Figure 4](image_url)

**Figure 4.** Development scheme for the LISE++ update. The plan is to first do a graphics framework transportation, verify the new code, then implement improvements.

Qt was chosen as the graphics framework for its feature set and widespread use in cross-platform C++ applications. Future plans include improved numerical optimization methods in areas such as ion optics and reaction models. To start, optimization of quadrupole fields using the Levenberg-Marquardt algorithm has been implemented and will be released with the next version of LISE++ [3]. OpenMP is planned for parallelization of Monte-Carlo calculations to exploit multi-core personal computers. Afterwards, an extension for use on supercomputers is planned for large-scale computations using MPI. Lastly, integration with control systems is planned.

4. Current Progress
The first release of the new LISE++ software suite was the LISE++ Utilities Package, released March 4, 2015. It is available from the LISE++ website [5]. This is a cross platform transportation of the satellite utilities in LISE framework to Qt. The package consists of five stand-alone programs useful for experiment design: PACE4, Charge, Global, Spectrometric Calculator, and a units convertor. Fig. 5 shows the package along with the program PACE4 with results.
PACE$4$ is a Monte-Carlo code for coupling angular momentum for use in fusion-evaporation reactions. **Charge** calculates atomic charge-changing cross sections, charge-state evolutions, and equilibrium-charge-state distributions for bare, H-, and He-like relativistic heavy ions penetrating through matter. **Global** is for calculation of charge state distributions. The **Spectrometric Calculator** contains many calculations expressed in Kantele's Handbook of nuclear spectrometry [4]. Work is now underway to convert the entire LISE$^{++}$ program to Qt with ISO C++. 

5. Summary

Work is underway to revamp the LISE$^{++}$ software suite. New code capabilities such as parallel computing, cross-platform functionality, and integration with control systems are planned and work is in progress. In order to implement these changes, the code is being transferred to a new graphics framework, Qt, and work is being done to ensure compliance with ISO C++ for use with modern compilers. The first release within the new framework is the LISE$^{++}$ Utilities Package, which was first released on March 4, 2015 [5]. The package contains five satellite utilities that are distributed in the LISE$^{++}$ software suite. Computational speedup has become highly requested from users at many facilities, and computation time becomes even more crucial with the new large-scale nuclear physics facilities in production now, such as FRIB. Facilities such as NSCL and GSI have keen interest in integrating the LISE$^{++}$ software with their control systems. With the completion of this work, we aim to address many requests of the LISE$^{++}$ user base.
References
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