

Large Scale Computing for Beam Dynamics Simulations and Target Modeling*

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1 Introduction

Computer simulations have become very important in Nuclear Physics and start to emerge as a third research branch between Theoretical and Experimental Physics. They are especially important to study and precise the experimental conditions prior to planning for experimental measurements or building an experimental device such as detectors and accelerators. With the rapidly advancing Computer Technology, very fast and large-scale machines are now available reducing the computing time from months to days and days to hours. This paper discusses how this powerful tool could be used for simulations of great importance for the RIA project to help decide on the most performant and cost-effective design, first for the driver linac and second for targets to be used for the production of rare isotopes.

In the next section, a brief description of the beam dynamics calculation to be used for the simulation of different design options for the RIA Driver Linac is given. The scale of these simulations and the need for multi-process computing are discussed. First results using the Jazz cluster [1], recently inaugurated at Argonne's Laboratory Computing Resource Center (LCRC-ANL), are also presented. In section 3, a general description of the simulation used to optimize the geometry and arrangement of material inside ISOL targets, for better efficiency and minimal losses of short-lived isotopes, is given. The need for multi-process environment is discussed and ideas to reduce the memory load and computing time are proposed. National and International interest in these simulations through collaborative work is also discussed. Finally, a summary of the current situation of these large-scale calculations and future plans are presented in the last section of the paper.

2 Beam Dynamics Simulations

A dedicated beam dynamics code "Track" [2,3] is used for these simulations. The calculation is based on tracking ions from an ion source through the different elements of the accelerator system: accelerating cavities, quadrupoles, solenoids, bending magnets, strippers, etc. The transport of an ion through an electromagnetic element is performed by solving the corresponding equation of motion using a 4th order Runge-Kutta integration. The simulation of ions energy and angular straggling at the strippers is based on calculations using the code SRIM [4] with 5% fluctuation in the stripper thickness. For the simulation of the RIA Driver Linac, uranium is used as the reference beam due to

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its smaller charge-to-mass ratio. For uranium and most heavy ions, multiple charge states are accelerated simultaneously starting from the ion source. This results in a gain factor of about 20 in the output beam intensity for the same intensity at the ion source. In addition, accelerating multiple charge states simultaneously reduces the losses and consequently the shielding requirements at the strippers.

The purpose of these simulations is to study the performances and limitations of different accelerator design options in order to decide on the most performant and cost-effective design for the RIA Driver Linac. Multiple simulations of the same design using different values for errors such as the misalignment of accelerator elements and the fluctuations in the amplitudes and phases of the electromagnetic fields are necessary to study the sensitivity of the beam quality to these errors. The most tolerant design is the least sensitive to the same sets of errors.

Tracking individual ions through an entire accelerator is time consuming. The computing time increases linearly with the number of ions to track. Using the code "Track", tracking 1000 ions needs about 9 minutes on a 2.4 GHz PC. The typical number of ions to track for a given design and a given set of errors is 10 million, especially to study beam tail and halo. This corresponds to 1500 hours (63 days) on the same PC. Considering the number of errors sets to use for each design (up to 300) and that a new simulation is needed for every variation in the accelerator design, a very fast multi-process machine is absolutely needed. For these reasons, the code "Track" was parallelized using the Message Passing Interface MPI [5] and run successfully on the new Jazz cluster at the Laboratory Computing Resource Center of Argonne National Laboratory [1]. Jazz is a new teraflop machine (10^{12} floating point operations per second) with 350- 2.4 GHz processors. Half of the processors have 2 GB live memory or RAM and the other half have 1 GB RAM.

A first simulation was performed for the first design of the RIA driver based on the triple-spoke resonators [6] for the high-energy section of the linac. 100 different error sets were used. 10^5 ions were tracked for each error set corresponding to a total of 10 million ions. The calculation took about 15 hours on 100 processors. This is to be compared with 63 days on a single processor. The errors included in this simulation are the transverse (x, y) displacements of elements ends (± 0.3 mm for cavities, solenoids and quadrupoles), the quadrupole rotation about the beam axis (± 9 mrad) and the fluctuations in the RF fields phases (± 0.5 degrees) and levels (± 0.5 %). To compensate for displacements of the accelerator elements a beam steering and correction procedure is needed. The correction procedure in the version of "Track" used here is simply recentring the beam transverse position and angle after every other cryostat. A more realistic beam steering procedure [7] will be included in a future version of "Track".

Figure 1.a shows projections of the coordinates of the 10 million ions in the six dimension (6D) phase space at the accelerator exit. It is important to note that there were no beam losses and that the limits in the phase space are well within the acceptance of the accelerator. Figure 1.b shows the evolution of beam envelopes in the transverse directions (x, y) and phase. The figures are superpositions of the curves obtained for different error sets. We clearly notice the beam size jumps in the post-stripper magnetic transport system

(MTS) as it is expected for a multiple charge state beam. Only few particles are lost along the MTS at the location of designated collimators. Figure 1.c shows the beam emittance growth, both transverse and longitudinal, with distance. A significant increase is seen at the strippers but still well within the acceptable limits.

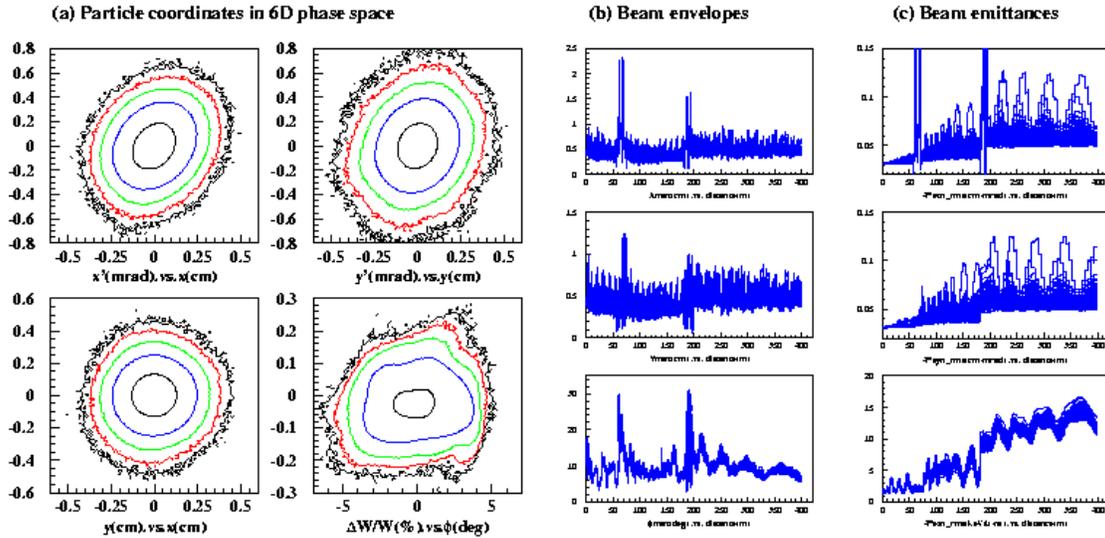


Figure 1. (a) Coordinates of the simulated 10 million ions in the 6D phase space. (b) Beam envelopes in x , y and phase as function of distance. (c) Beam emittance growth with distance.

3 ISOL Targets Modeling

A Monte-Carlo approach has recently been developed [8] for the simulation of ISOL Targets. It is based on tracking the nuclei produced by the beam inside the target until they are released from the ion source. The processes involved are the diffusion, which is the transport of particles through material and the effusion the transport through vacuum. The detailed geometry and tracking are implemented using the Geant-4 Library [9]. The effusion process has been added to Geant-4 to consider the sticking time and the cosine law governing particle's emission from the surface to the target volume. The diffusion process is treated analytically using the appropriate diffusion equation [10].

The purpose of these simulations is to optimize the target geometry and the arrangement of material inside the target for better efficiency and minimal losses of short-lived isotopes by radioactive decay. This could be achieved by simulating different target design options and different possible forms of target material: thin foils, fibers or grains. The optimal design corresponds to minimum delay time from production to release.

Target simulations could be also very time consuming. Considering for example the case of the RIST target [11] which is an 18 cm long- 2 cm diameter tantalum tube filled with 3600- 25 μ m thick discs. The target is connected to a 3.5 cm long- 3 mm diameter

tungsten ionizer tube. The simulation of 1000 events using this geometry [8] needs about 15 hours on a 2.4 GHz PC. The limiting factors are the numbers of discs or foils and the aperture of the ionizer tube, making the simulation of a reasonable number of events (typically a million) almost impossible on a single PC. In addition to the long computing time, the memory needed to run the calculation becomes a limitation when the number of foils, fibers or grains goes above certain limits, typically 100,000 to millions. For these reasons we are planning to use the Jazz cluster for future target simulations. Meanwhile we are proposing ideas to reduce the memory load and the computing time. The basic idea is that instead of defining the whole target filled with millions of grains for example, see figure 2.a, we only define the grains of a small cell moving inside the target, see figure 2.b. This will first reduce the memory needed for the calculation to run and second reduce the computing time because the tracking will be done inside the small cell instead of the whole target. There is also the possibility to replace the tracking procedure by an analytical model for effusion within the cells. Implementations and tests of these ideas are in progress.

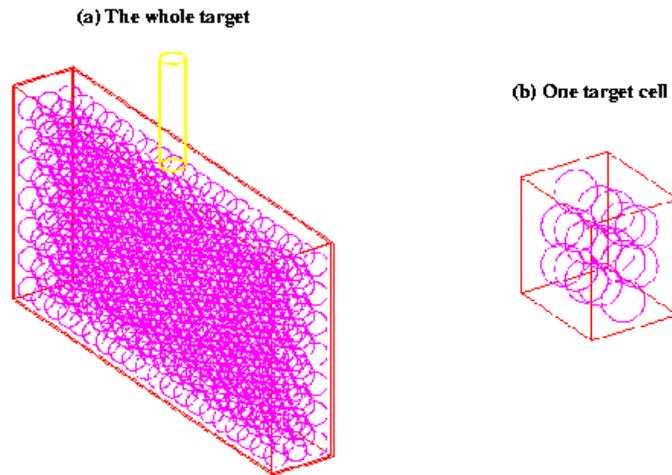


Figure 3. (a) Sample of a target filled with grains. (b) One target cell.

Groups from US and International Laboratories with existing ISOL facilities are more and more interested in these target simulations. Simulations of effusion from different Target/Ion Source systems tested at Oak Ridge National Laboratory [12,13] were performed recently and presented at the last INTDS conference [14]. A reasonable agreement with the data was obtained as a benchmark of the approach. Diffusion measurements are planned in collaboration at the UNISOR facility, ORNL. At GANIL, France, the target group of the SPIRAL facility is now using the effusion simulation package developed at Argonne to simulate their targets. Future experimental tests are planned in collaboration.

4 Summary and Perspectives

Considering the large scale of the beam dynamics simulations for the RIA driver linac, the beam dynamics code "Track" developed at Argonne is now parallelized and run successfully on the new multi-process Jazz cluster at Argonne's Laboratory Computing

Resource Center. Results from simulations of the first design of the RIA driver, based on the triple-spoke resonators in the high-energy section of the linac [6], are encouraging and promising. Future end-to-end simulations of different design options with multiple sets of errors are needed to decide on the most performant and cost-effective design. These simulations are planned after updating the code "Track" with more realistic beam halo formation at the strippers and a real beam steering and correction algorithm [7]. Eventual contamination of the beam by nuclear reactions products in the strippers as well as ways of cleaning the beam will be investigated.

ISOL targets simulations necessary to optimize the target geometry and the arrangement of material inside the target for better efficiency and minimal losses of short-lived isotopes are also very time consuming. Modeling targets made of thousands of very thin foils or millions of fibers or grains is memory consuming also. Tracking the produced nuclei inside a small cell moving inside the target or developing analytical models for effusion within cells has the potential of reducing both the memory load and the computing time. The implementations and tests of these ideas are in progress. The Jazz cluster will also be used for future ISOL targets simulations.

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