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ELECTROMAGNETIC SIMULATIONS OF A NOVEL PROTON LINAC USING VSim ON HPC

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Abstract

We discuss electromagnetic simulations of accelerating structures in a high performance computing (HPC) system. Our overarching goal is to resolve the linac operation in a large ensemble of initial beam conditions. This requires a symbiotic relation between the electromagnetic solver and HPC. The linac is being developed by Ion Linac Systems to produce a low-energy, high-current, proton beam. We use VSim, an electromagnetic solver and PIC software developed by Tech-X to determine the electromagnetic fundamental mode of operation of the accelerating structures and discuss its implementation at the THETA supercomputer in the Argonne Leadership Computing Facility.

INTRODUCTION

In recent years, there has been an increased need for compact accelerators to drive a diverse range applications, in particular those requiring high intensity ion beams in the low and medium energy regimes, such as in the industry, medical and security areas [1]. Making these technologies cost effective and widely accessible requires highly efficient and low cost accelerators.

One such compact ion beam accelerator is being developed by our collaborators at Ion Linac Systems (ILS) to drive a medical application called Boron Neutron Capture Therapy (BNCT) [2]. BNCT is a non-invasive therapy for locally invasive malignant tumors, where the tumor is first tagged with a Boron-based tracer, and then irradiated with a beam of epithermal neutrons. Boron efficiently absorbs the epithermal neutrons and the resulting nuclear reaction releases the energy dose in the micro-meter range, well within the cancerous cell, thus suppressing unnecessary dose to healthy cells, making BNCT a very targeted therapy. BNCT has traditionally been done with neutrons released in nuclear reactors, which have a wide energy spectrum. In an accelerator driven approach, the linac produces a high intensity proton beam, the beam is then directed towards a target for neutron production through spallation. The resulting neutron beam has a narrow band energy spectrum, making it a more efficient therapy [2].

Besides the infrastructure costs associated with the accelerator footprint, the operational costs of the machine also impact the widely use of this technology. We are looking into integrating both optimization and Artificial Intelligence (AI) algorithms into the linac controllers as a way to reduce operational costs [3]. The idea is that some control tasks during beam during set-up or operation, can be addressed by an AI controller, resulting in increased linac efficiency with minimum supervision from the operator.

An advanced controller we are developing is based on the use of a surrogate model of the linac. A surrogate model is a fast executing representation of an otherwise slow, high-resolution simulation model [4]. Because this model has been trained offline, it becomes practical for real-time operation. Training of a NN consists on showing different case examples of what normal operation looks like. Experimental data may be scarce because dedicated machine runs for are expensive, similarly using a detailed simulation of the system may be computationally expensive to produce. An AI-model approach thus becomes important, as it can learn the characteristics of the available data, experimental and simulated, and learn how to react multiple scenarios that were not part of the original training set. Of course the AI-model is only as good as the data used during the training phase. This is the motivation to have as detailed model of the system as possible, but there is a caveat, as more computation time may be required with increased resolution. This contribution discusses general characteristics of such a detailed simulation specific for the ILS linac and optimizing High Performance Computing (HPC) resources for these simulations towards advanced controllers.

Accelerating Structures

The linac discussed in this contribution was designed and built by ILS, it is formed by an ECR ion source, a Radio Frequency Quadrupole (RFQ) and a proprietary Radio Frequency Focused Interdigital (RFI) [5]. Figure 1 shows a side view of the RFQ. The RFQ is an accelerating structure well

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Figure 1: Side view of the ILS RFQ with power coupler, vacuum and diagnostic ports.

suited for ions at low energy, where the velocity of the beam is low enough that the beam can be focused using transverse electric fields. At the core of the RFQ design are four electrodes, or veins, that help focus the electromagnetic fields to provide focusing to the beam. Tapering the veins introduce a longitudinal component of the electric field that provides acceleration to the beam. An RFQ is a very versatile device as it provides different functions within the same structure: beam capture, focusing, bunching and acceleration [6]. The RFQ becomes less efficient as the beam energy increases and it is usually the first accelerating stage in a system of different accelerating structures, usually delivery the beam into a Drift Tube Linac (DTL). The ILS linac uses an RFI, an optimized version of the RFQ that allows to reach the proton beam energy required for BNCT in a shorter distance than using a DTL. The RFI alone has been found to be four times more efficient than equivalent RFQ or DTL linacs [2]. The length of the full ILS proton linac is quite compact at about 2.8 m.

EM SIMULATIONS WITH VSim

We use VSim [7, 8], an electromagnetic and particle-in-cell (PIC) code, to model the ILS linac: both the RFQ and RFI structures. We use VSim to calculate the TE_{210} mode of operation given the existing geometry files. These are found to be in good agreement with bead-pull measurements and with previous simulations [9]. Table 1 shows the frequency for both structures as calculated with VSim and compared against measurements.

Figure 2 shows the longitudinal electric field in the TE_{210} mode for the RFQ, where it can be noted that the fields are concentrated near the beam axis.

Table 1: Frequency of the RFQ and RFI Calculated with VSim and Compared to Measurement

	RFQ		**RFI**	
	VSim	**Meas.**	**VSim**	**Meas.**
Freq. [MHz]	201.487	200.87	201.527	200.915

Considerations for a Surrogate Model

For a surrogate model, we want to have a very detailed model of the ILS linac, as accurate as possible. From the simulation side, this can be accomplished by having an extensive hexahedral mesh, large enough to resolve the linac geometry, the electromagnetic fields at the corresponding frequency and the particle dynamics. One can note the RFQ and RFI have a large volume but the fields and the beam are concentrated near the beam axis.

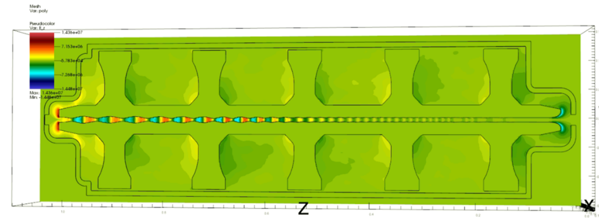

Figure 2: Longitudinal electric field on the RFQ calculated with VSim and using an hexahedral mesh with 37M cells.

The simulations over a few RF periods can be computationally demanding, we exploit the power of HPC to expedite the simulations. This becomes particularly important when building a big training data set for a surrogate model, where each of the data points is an independent simulation under different initial conditions and saving as little time per simulation as possible will increase our computing performance. We use the supercomputer THETA at ALCF, a petaflop class system with more than 2.8×10^5 computing cores. Figure 3 shows the computing time as a function of the number of cores assigned to the RFQ simulation on THETA.

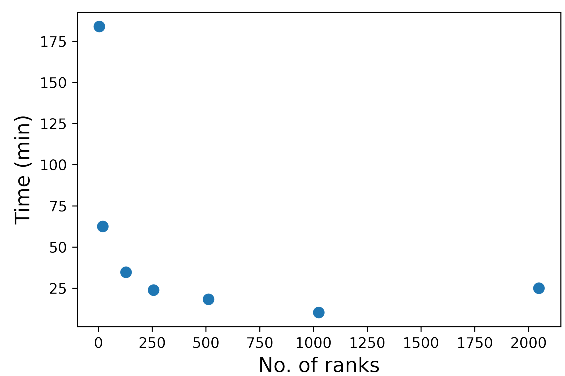

Figure 3: Computation time as a number of ranks or processes.

COMMENTS

We are developing advanced AI-based controllers for the ILS linac as a way to reduce the costs associated with accelerator operations. In particular we are looking into building surrogate models of the RFQ and RFI, where both experimental and simulated data to train the surrogate model is required. We are using the electromagnetic and plasma code VSim to model the electrodynamics and beam dynamics of both the RFQ and RFI. However, the simulated data becomes time consuming to produce when we have a very

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detailed model of the system. We are using the THETA supercomputer at ALCF to expedite the detailed simulations of the ILS linac using VSim and have optimized hardware resources to this particular simulation. Use of HPC enables us to run several simulations in a reasonable amount of time towards a surrogate model of the ILS linac.

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REFERENCES

[1] M. Fazio *et al.*, “Basic Research Needs Workshop on Compact Accelerators for Security and Medicine”, DOE Office of Science, SC, USA, Rep. OSTI-1631121, May 2019.

[2] D. A. Swenson, “CW proton LINAC for the BNCT application”, in *Proc. 24th Linear Accelerator Conf. (LINAC’08)*, Victoria, Canada, Sep.-Oct. 2008, paper MOP062, pp. 220-222.

[3] S. G. Biedron, “Adding data science and more intelligence to our accelerator toolbox”, in *Proc. 10th Int. Particle Accelerator Conf. (IPAC’19)*, Melbourne, Australia, May 2019, pp. 1191-1197. doi:10.18429/JACoW-IPAC2019-TUZPLM1

[4] A. L. Edelen, S. G. Biedron, B. E. Chase, D. Edstrom, S. V. Milton, and P. Stabile, “Neural networks for modeling and control of particle accelerators”, *IEEE Transactions on Nuclear Science*, vol. 63, no. 2, pp. 878-897, 2016. doi:10.1109/TNS.2016.2543203

[5] D. A. Swenson, “An RF focused interdigital ion accelerating structure”, in *AIP Conference Proceedings*, vol. 680, no. 1, pp. 1013-1016, 2003. doi:10.1063/1.1619880

[6] T. P. Wangler, *RF Linear Accelerators 2nd ed*, Weinheim, Wiley, 2008.

[7] C. Nieter and J. R. Cary, “Vorpal: A versatile plasma simulation code”, *J. Comput. Phys.*, vol. 196, pp. 448-473, 2004. doi:10.1016/j.jcp.2003.11.004

[8] Tech-X Corporation, ”VSim”, https://txcorp.com/vsim/ .

[9] S. J. Smith *et al.*, “2D-3D PIC Code Benchmarking/Anchoring Comparisons For a Novel RFQ/RFI LINAC Design”, in *Proc. 9th Int. Particle Accelerator Conf. (IPAC’18)*, Vancouver, Canada, Apr.-May 2018, pp. 1194-1197. doi:10.18429/JACoW-IPAC2018-TUPAL077