

BIG DATA TECHNIQUES FOR ACCELERATOR OPTIMIZATION*

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Abstract

Accelerators and the experiments that they enable are some of the largest, most data intensive, and most complex scientific systems in existence. The interrelations between machine subsystems are complicated and often nonlinear. The system dynamics involve large parameter spaces that evolve over multiple relevant time scales, and accelerator systems. Any accelerator-based experiments and applications are almost always difficult to model. LIV.DAT, the Liverpool Centre for Doctoral Training in Data intensive science, was established in 2017 as a hub for training students in Big Data science. The centre currently has 36 PhD students that are working across nuclear, particle and astrophysics, as well as in accelerator science. This paper presents results from R&D into betatron radiation models and beam parameter reconstruction for plasma acceleration experiments at FACET-II, simulations for MeV energy gain in dielectric structures driven by a CO₂ laser and modelling of seeded self-modulation of long elliptical bunches in plasma. It also gives an overview of the training program offered to the LIV.DAT students.

INTRODUCTION

In 2017 LIV.DAT, the Liverpool Centre for Doctoral Training in Data intensive science was established. LIV.DAT has quickly established itself as a center of excellence in data science, across a significant part of STFC research, including nuclear, particle and astrophysics, as well as accelerator science. The center also acts as a model for training cohorts of student in Big Data science and currently has more than 30 PhD students [1].

Recent years have witnessed a dramatic increase of data in many fields of science and engineering, due to the advancement of sensors, mobile devices, biotechnology, digital communication and internet applications. Very little targeted training is provided internationally to address a growing skills gap in this area. LIV.DAT provides a comprehensive training program to its students to address this problem.

SELECTED RESEARCH RESULTS

The focus of the centre is on addressing current challenges in data science through a structured R&D program across three scientific work packages:

- Monte Carlo (MC) methods as tools to address a wide range of physics problems, from the dynamic behavior of galaxies, cross sections in specific particle interactions to dose delivery planning in ion beam therapy;

- High Performance Computing (HPC) and Machine Learning (ML) using computing clusters to simulate cutting edge physics and engineering problems that cannot be dealt with on desktop computers;
- Data Analysis across the entire spectrum of physics research.

All three work packages are very relevant for accelerator science research. In the following recent research results from three specific projects are presented to exemplify the research progress made across the center.

Betatron Radiation Models

Single shot non-invasive beam emittance diagnostics is highly desirable for characterizing charged particle beams. Betatron radiation emitted by a beam provides an interesting opportunity to measure this important parameter. Research by LIV.DAT student Monika Yadav focuses on the numerical modelling of this radiation by computing the Liénard-Wiechert fields from the trajectories of particles tracked in the quasi-static Particle-in-Cell (PIC) code *QuickPIC* [2] in the specific case of the FACET facility at SLAC National Accelerator Laboratory [3].

Research has focused on the characterization of the radiation for a prototypical parameter set based on typical parameters for plasma wakefield acceleration experiments at FACET-II. To understand the relationship between the beam-plasma interaction and the produced radiation, these parameters were perturbed in a number of ways. As an example, the 1-D angular distribution is shown in the following Fig. 1. It can be seen that the differences in the total radiation are almost negligible and that hence betatron radiation diagnostics is a poor way to distinguish between beams of spot sizes with the same emittance - at least for the parameter set which was considered.

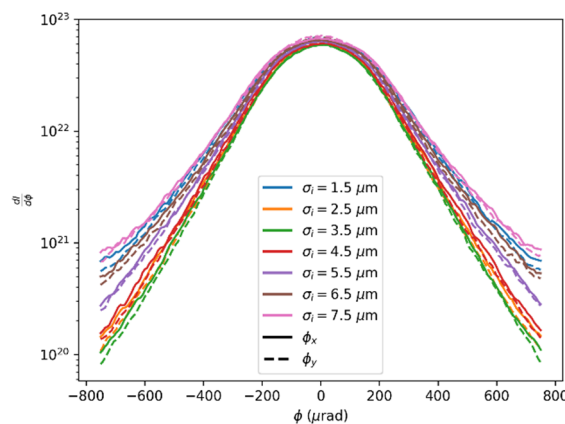


Figure 1: Example of witness beam 1d angular distribution for a range of different initial spot sizes [3].

The study will next be expanded to understand the full potential of the method to diagnose the parameters of a

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beam from the spectral and angular distribution of the betatron radiation.

Optimization of Dielectric Laser Accelerators

In recent years there has been a growing interest in dielectric laser accelerators (DLA) [4, 5] as a promising candidate for future endoscopy and cancer treatment due to its compactness and very narrow output beam [6]. To optimize this novel type of accelerator, it is essential to incorporate real experimental parameters, including higher order effects and nonlinearities to get a better agreement between theory and experiments and hence understanding of the underlying physics processes. High resolution, full 3-dimensional, PIC simulations are an essential tool for investigating charged particle dynamics in electromagnetic field excitations [7-9].

Recent studies by LIV.DAT student Gyandra Yadav focused on numerical studies into the optimization of dielectric structures that are being excited by a CO₂ laser with a wavelength of 10.6 μm [10]. Their work focused on studies incorporating the main parameters from the BNL-ATF facility [11] in VSim [12] with the aim to optimize a rectangular dual period grating structure with 100 pillars.

The code was executed on the Shaheen-II supercomputing cluster in Saudi Arabia. Finite difference time domain (FDTD) simulations considered grating structures, illuminated by the CO₂ laser with a pulse duration of 1.6 ps and an intensity of the order of 10¹⁶ W/m². In this case, they demonstrated that the electron beam travelling through the channel between the dual pillars of the grating gains around 2 MeV in energy from an initial energy of 50 MeV [10].

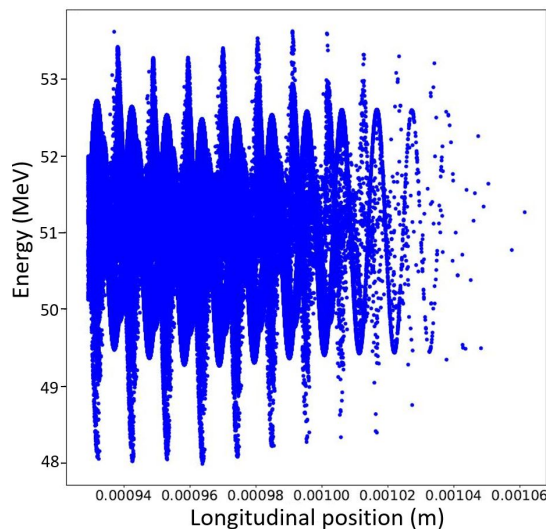


Figure 2: Energy gain of electrons with their longitudinal position close to the end of the grating structures [10].

The above Fig. 2 illustrates the energy gain of the electrons as a function of their longitudinal position. The energy gain corresponds to an average acceleration gradient of around 2 GeV/m.

The simulation framework that has been established allows the study and optimization of dielectric laser accelerators for specific applications with a current focus on an

improvement of six-dimensional phase space preservation. This gives a powerful basis to plan and support future experimental studies.

Seeded Self-Modulation of Long Elliptical Bunches in Plasma

The Advanced Wakefield Experiment (AWAKE) in 2016 became the first every proton-beam-driven plasma wakefield acceleration (PWFA) experiment [13-15]. Proton-beam-driven PWFA (PDPWFA) works by driving an electrostatic Langmuir wave in a plasma channel, using a relativistic beam of charged particles. The electromagnetic fields of the proton beam leads to transverse attraction of plasma electrons towards the beam's propagation axis, setting up an oscillation. The finite speed of the beam hence sets up a series of high and low electron density regions near the axis in its wake, at a characteristic 'plasma wavelength', between which the longitudinal electric field can reach up to 50 GV/m - three orders of magnitude higher than a conventional RF accelerator. A relativistic witness beam injected at the right position into this wakefield can, in principle, continuously gain energy from the plasma wakefield. Using the SPS proton beam as a driver as in AWAKE allows limitations on acceleration length due to energy depletion as with an electron beam driver to be overcome.

The stability of particle bunches undergoing seeded selfmodulation (SSM) over tens or hundreds of meters is crucial to the generation of GV/m wakefields that can accelerate electron beams. LIV.DAT student Aravinda Perera used 3D particle-in-cell simulations in *QuickPIC* [2] and compared the results to an analytical model of seeded self-modulation (SSM) of elliptical beam envelopes using linear wakefield theory [16].

Figure 3 gives the example of a comparison between the growth rate predicted for aspect ratios between $h = 1.0$ and $h = 0.5$ under the constraint $R_0 = 1.0$ between an analytical expression and PIC simulations. A good agreement was found in the decrease in growth rate due to unequal aspect ratio.

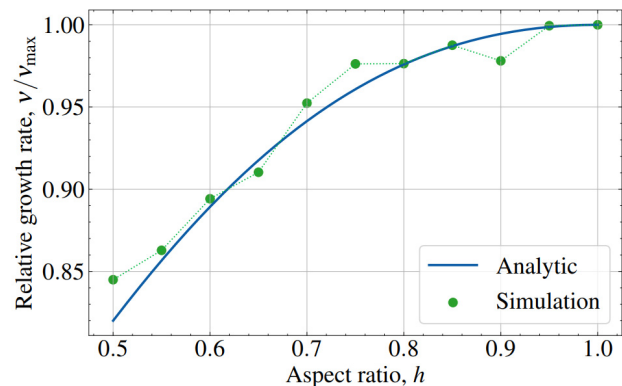


Figure 3: Comparison of analytic and simulated values for peak growth rates of the maximum wakefield potential with beam aspect ratio up to SSM saturation, relative to that for a symmetric beam where $h = 1.0$ [16].

Further studies will focus on a reduction of the divergence between predicted and simulated beam envelopes, as well as further investigations into the validity of the model for highly perturbed beam parameters.

RESEARCHER TRAINING

The training program in LIV.DAT builds on existing modules drawn from the University of Liverpool's MSc in Big Data Science. All students undertake 45 credits from this MSc program in their first year, including mandatory courses on data mining and data analysis.

In addition, the center is offering a wide-ranging training program in close collaboration with other major training initiatives. To date, this has included an international school on Monte Carlo Simulations [17], researcher skills training with researchers from the innovative training networks AVA [18] and OMA [19], an HPC training week hosted by Tech-X in spring 2019, as well as an STFC Summer School on Data Science in 2020 [20]. LIV.DAT has also co-organized a major Symposium on Accelerators for Science and Society in summer 2019 with contributions made by all of its students and talks now available via the event website [21].

The center currently develops a new Massive Open Online Course (MOOC) on Data Science which will take full advantage of Liverpool's virtual learning environment *Canvas*. It shall be launched later this year and will be open to researchers around the world, providing a basic training in data science and connecting this to cutting edge research in Liverpool and its collaboration partners. A seminar program that covers R&D outside of the center complements the above activities and is open to anyone interested with registration via a dedicated indico page [22].

Finally, each student in the center undertakes an industry placement for a minimum of six months, working on a topic outside of their core PhD project. This helps broaden their skills and expertise and boost their employability.

SUMMARY AND OUTLOOK

The LIV.DAT CDT started in October 2017 and is currently training more than 30 PhD students in data science techniques across a wide range of fundamental and applied research. The importance of these techniques for accelerator optimization was illustrated in this paper on the example of three accelerator science R&D projects which rely on high performance computing techniques. A brief overview of the broad training program that the center is offering was also given.

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