

# ACCELERATOR OPTIMIZATION USING BIG DATA TECHNIQUES

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## Abstract

Managing, analyzing and interpreting large, complex datasets and high rates of data flow is a growing challenge for many areas of science and industry. At particle accelerators and light sources, this data flow occurs both, in the experiments as well as the machine itself. The Liverpool Big Data Science Center for Doctoral Training (LIV.DAT) was established in 2017 to tackle the challenges in Monte Carlo modelling, high performance computing, machine learning and data analysis across particle, nuclear and astrophysics, as well as accelerator science. LIV.DAT is currently training 24 PHD students, making it one of the largest initiatives of this type in the world. This paper presents research results obtained to date in projects that focus on the application of big data techniques within accelerator R&D.

## INTRODUCTION

LIV.DAT, the Liverpool Centre for Doctoral Training in Data intensive science, is a hub for training students in Big Data science [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 programme to its students to address this problem.

## RESEARCH

The focus of the centre is on addressing the data challenges presented by research in astronomy, nuclear, particle and accelerator physics. R&D is structured across the following 3 main work packages:

- Monte Carlo (MC) methods as powerful tools for a range of physics problems, from the dynamic behavior of galaxies, cross sections in specific particle interactions to treatment planning in ion beam cancer therapy;
- High Performance Computing (HPC) and Machine Learning (ML) to benefit from the computing power of large clusters to simulate problems that cannot be dealt with on desktop computers;
- Data Analysis across the entire spectrum of physics research.

All three work packages are highly relevant for accelerator science. Beam control and manipulation, beam dynamics studies and analysis of beam diagnostics output data all directly benefit from performance enhancements in the underpinning data handling techniques.

## Comet Assay Image Analysis

In today's digital age, tasks that were previously rudimentary and tedious are becoming automated, creating more efficient, precise and reproducible workflows. The healthcare sector is a prime example where technology is being utilized more and more. Such an example can be seen in image analysis.

Cancer is a disease that has been researched for many years, with a lot of effort being put into finding methods of treatment that successfully destroy cancerous cells whilst sparing as much healthy tissue as possible. Proton therapy is a rapidly growing field as increasing evidence suggests that it induces more complex damage in DNA of cells than do x-ray photons [2]. The cells are less likely to be able to repair this damage, increasing the chance that the cancer is destroyed. A way in which we can determine the level of damage caused to a cell's DNA following irradiation is the Comet Assay [3]. The images produced in the comet assay can be analyzed in various ways, ranging from manual categorization via a number ranking [4] to the use of computer software to automate the measurements. Even when using the currently available software, in some cases a user is still required to identify elements of the images e.g. the overall comet body and comet head. When analyzing a large number of images, this can become time consuming, as well as potentially introduce bias.

LIV.DAT student Selina Dhinsey develops a program which fully automates the analysis of comet assay images as shown in Fig. 1, measuring comet area, tail length and % tail fluorescence (tail DNA), the latter two being widely used in comet assay measurements [5]. The program incorporates Neural Network (NN) architecture, using instance segmentation to identify comet bodies within the image and then perform analysis to measure the bodies. Preliminary results are very promising with segmentation accuracies predicted at over 90% for each identified comet. However, there are still cases where not all comets are being identified so the model requires further tuning. A difficulty in the application of NN here is the lack of data; only a limited number of images are available for training and testing purposes. To counter this, a Monte Carlo model is being developed which will allow the creation of a large amount of simulated data and will also aid the development of a deeper understanding of the physical mechanisms underlying the comet assay.

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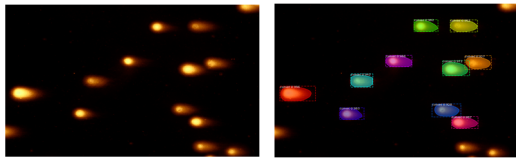


Figure 1: A comet assay image before (left) and after (right) applying instance segmentation.

### Modeling of the AWAKE Experiment

The Advanced Wakefield Experiment (AWAKE) in 2016 became the first every proton-beam-driven plasma wakefield acceleration (PWFA) experiment [6-8]. 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. However, having a sufficiently dense plasma so as to avoid growth of transverse filamentation instabilities in the beam [9] means that the plasma oscillation wavelength is over 100x shorter than the SPS proton beam. Therefore, AWAKE relies on another instability, Seeded Self Modulation (SSM), to transversely modulate the beam into microbunches. However, this SSM process needs to be carefully controlled to saturation such that the microbunch train is then optimally positioned to resonantly enhance the wakefield down the train [10].

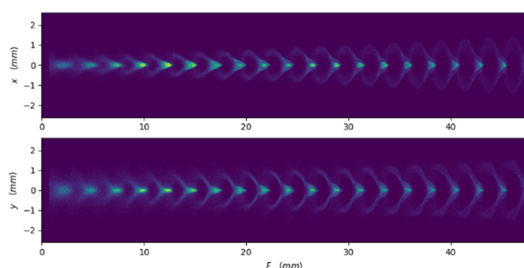


Figure 2: Charge density (arb. units) on the  $y=0$  (top) and  $x=0$  (bottom) plane of an elliptical cross-section beam (1:2 aspect ratio) after undergoing seeded self-modulation through 5.5 m of plasma, simulated with the 3D Particle-in-Cell code OSIRIS [11].

A preliminary analysis of experimental data from AWAKE Run 1 shows that the  $x$ - and  $y$ - final focusses of the proton beam may not in fact coincide, leading to

different phase space distributions at the plasma entrance. It is likely that this is the cause of severe transversely asymmetric shot-to-shot variation observed in integrated post-modulation beam profiles. Such spatial asymmetry has been shown through theory and simulation [12] to enhance the growth of the transverse beam hosing instability. The project of Aravinda Perera aims to explore the effect of non-circular aspect ratio and transverse correlated momentum spread on the efficiency of the SSM process and other instabilities, which ultimately dictates the achievable gradient for accelerating the witness electron beam, Fig. 2. This is being done through massively parallel 3D PIC simulations on thousands of CPU cores that perform first-principles electromagnetic calculations using millions of pseudo-particles to represent plasma and proton beam.

### Optics Modelling for HL-LHC

To extend the discovery potential of the LHC, the machine will get a major upgrade in the 2020s to increase its luminosity by a factor of five beyond its design value and the integrated luminosity by a factor of ten. The LHC has demonstrated an unprecedented optics control for high energy colliders, down to the 1% level in  $\beta$ -beating and  $|C| = 2 \cdot 10^4$  in coupling. However, the High Luminosity (HL) upgrade represents a new challenge for optics measurement and correction algorithms in both, the linear and non-linear regimes. The extreme squeezing of the beam at IP1 and IP5 will lead to immense  $\beta$ -functions in the IRs, enhancing the impact of magnet tilts, alignments and field errors and feed-down effect. As  $\beta^*$  is reduced, non-linear errors will pose severe challenges in experimental regions even for the linear optics commissioning via their feed-down to  $\beta$ -beating and linear coupling, by distortion of tune footprints, and by reducing the available dynamic aperture, thus becoming a serious operational challenge [13, 14].

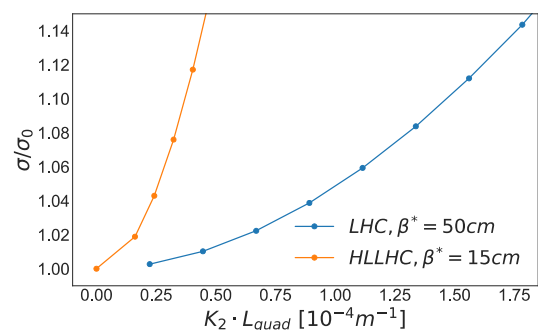


Figure 3: Relative increase in IP beam size from powering the right and left IP skew quadrupoles for LHC and HLLHC. A faster beam blow-up and a lower tolerance to local coupling bumps was found.

Felix Soubelet works on the computation of optics for HLLHC and the development of measurement techniques and correction algorithms to address the above challenges. He plans to build a beam-based/online model that can reproduce all measurements, including misalignments,

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magnetic field errors, orbit and  $\beta$ -beating. The first stage of his project consists of performing studies of the beamline focusing properties and tolerances in the interaction regions with a focus on the impact of linear and non-linear errors, and a comparative analysis of existing correction models and their viability in HLLHC, see Fig. 3. In a next step, new correction methods for the interaction region  $\beta$ -function will be developed with a focus on non-linear optics and tested during 2021 LHC commissioning. Additionally, the possibility of developing machine learning techniques to enhance measurement accuracy and correction algorithm effectiveness will be investigated.

### Geometry Optimization of DLAs

In recent years there has been a growing interest in dielectric laser accelerators (DLA) [15, 16]. The DLA is a promising candidate for future endoscopy and cancer treatment due to its compactness and very narrow output beam [17]. Many studies have been conducted in the past to optimize the geometry of the dielectric microstructures but experimental values for the acceleration gradient and energy gain is far from the prediction of simulations [18, 19]. Thus, 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 [20]. A comparative study of the energy gain and acceleration gradient for two different geometries is shown in Fig. 4.

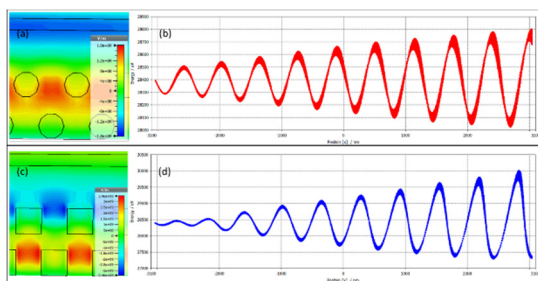


Figure 4: DLA from dual pillar silicon gratings and 4 Bragg reflectors (BR), grating period ( $\lambda_p$ ) is 640 nm, shift in upper layer is  $\lambda_p/2$ , incident plane wave with Gaussian envelope, peaked at 1,930 nm, energy 1 GeV, initial energy of electron beam is 28.4 keV, spot size is 20 nm, energy spread is 0.5 eV, BR is 145 nm thick and has vacuum spacing of 640 nm. (a) and (b): Electric field distribution and energy versus position for cylindrical microstructures. (c) and (d): Same for cuboid microstructures.

Simulation have been performed by Gyanendra Yadav using CST Particle Studio [21] and parameters from [22]. The results suggest that a maximum energy gain for cylindrical microstructures is 400 eV, while it is 1,600 eV for cuboid structures. This shows the significance and enormous scope of geometry optimization.

### Betatron Radiation from Under-Dense Plasma

Plasma wake field accelerators (PWFA) provide unique opportunities for the generation of high quality, short-pulse electrons beams and ultrashort X-ray radiation [23]. A relativistic beam of charged particles or intense laser-pulse is driven into a plasma cell followed by another beam called witness beam. The drive beam expels out electrons and a bubble regime is formed, leaving behind a net positively charged region of ions which are assumed to be immobile and provide a restoring force on the out-going electrons [24]. The high-quality X-rays generated in this process find application in a number of research areas [25]. Monika Yadav has been carrying out studies into the development of a new type of very high brightness betatron radiation source. Using the EPOCH code to simulate double beam dynamics in a plasma channel with different plasma/beam parameters [26], she investigates the underpinning physics principles.

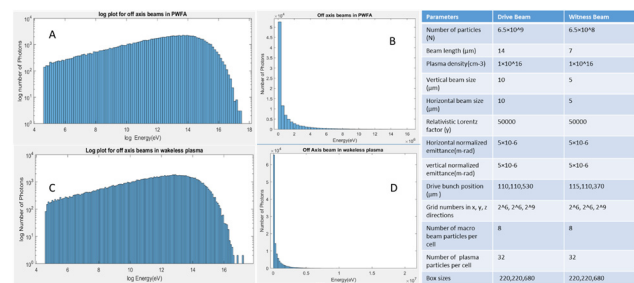


Figure 5: EPOCH simulations [A] Radiation spectrum on log scale [B] and normal scale. [C] Radiation spectrum on log scale [D] and normal scale in wakeless plasma; parameters are for SLAC's 25.5 GeV beam.

When an off-axis witness beam is oscillating, betatron radiation is generated in the range of keV to MeV, Fig. 5. More in-depth simulations towards a less broad radiation spectrum are being done. In future, betatron radiation generation in a wakeless plasma will be experimentally studied at the FACET-II beamline.

### TRAINING

The training program in LIV.DAT builds on existing modules drawn from the University of Liverpool's MSc in Big Data and HPC. All students undertake 45 credits from this MSc program in their first year, including mandatory courses on data mining and data analysis. In addition, they have already followed on international school on MC Simulations [27], a researcher skills training with researchers from the innovative training network AVA [28], and a dedicated HPC training week which was hosted by Tech-X in spring 2019. Each student also undertakes an industry placement for six months, working on a topic outside of their PhD project to broaden their skills and expertise and boost their employability. All students will also contribute to an outreach Symposium on Accelerators for Science and Society on 28 June 2019 [29].

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