# Summary of WG6: Theory and simulations

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**Abstract.** The presentations of working group 6 ( theory and simulations) of the fourth edition of the European Advanced Accelerator Workshop presented new ideas for experimental schemes, analytical models, and updates on well-known Particle in Cell codes. New schemes for improving electron beam quality, positron acceleration, ion acceleration, and radiation generation were proposed. Recently developed features of several Particle in Cell codes were also reported.

## 1. Introduction

The discussions and presentations in the theory and simulations working group (WG6) were covered mostly simulation codes and propositions of new experimental set ups. Additionally, analytical work supported by Particle in Cell (PIC) simulations and experimental modeling were also presented. This is reflected on our summary, which is organized as it follows:

- New regimes explored with theory and/or simulation and experimental modeling.
- Code updates and numerical schemes.

## 2. New regimes and experimental modeling

After the experimental demonstration of high accelerating gradients, with GeV energy gains in cm scale plasmas of the last two decades, the natural next step of plasma acceleration is the demonstration of high-quality acceleration and the overcoming of the main limitations of its well-established schemes. For example, a new scheme for laser wakefield acceleration (LWFA), called Traveling-Wave Electron Acceleration (TWEAC), was proposed. The scheme is based the interaction of two laser pulses with oblique incidence and tilted wave-front. Particle in Cell simulations showed that with this geometry the depletion and dephasing limits of LWFA can be overcome [1]. An exciting setup that has gained attention in the last few years, the hybrid laser and plasma wakefield acceleration (L|PWFA) has been experimentally demonstrated. In this scheme a first stage of LWFA is used to accelerate an electron beam that is the driver in a second plasma wakefield acceleration (PWFA) stage. Start-to-end 3D simulations of the experiment were presented [2]. This kind of simulation is essential to assess the second stage driver beam parameters, which influence the final quality of the witness electron beam injected by ionization in the second stage.

The external injection of witness beams in plasma wakefields is a promising method to control the properties of the bunch before a subsequent plasma accelerator stage. In this context, it is of paramount importance to understand all the interactions during the external injection process, as it was demonstrated by the analytical calculation of the force exerted on the beam at the plasma-vacuum boundary [3], prompted by the electron injection scheme of the AWAKE experiment [4]. Ongoing work of the effects of transverse instabilities and their role on the maximum injected beam charge and efficiency were discussed [5]. The role of ion motion in the mitigation of the hosing instability was discussed in two talks from different groups. The large force exerted by the tightly focused witness beams, which is a typical case in the blowout regime, can trigger ion motion which helps detuning the oscillations of individual beam slices, effectively mitigating hosing [6, 7]. It was also shown that by using tapered beams, the beam emittance can be preserved [8].

Beam breakup instabilities (BBI), such as the hosing instability, are the major issue for particle acceleration in hollow plasma channel structures. It was shown that a coaxial plasma filament can effectively mitigate BBI and highly efficient acceleration was demonstrated [9]. Modifications of the setup aiming at TeV energies in a single stage were presented [10]. Another crucial topic regards positron acceleration. It was demonstrated that the ion motion following the blowout regime naturally creates a quasi-hollow channel with a ring-like structure near the axis that can focus positrons [11]. High quality acceleration and mitigation of hosing were discussed in this regime, which appears to address both these issues. Another novel setup for positron acceleration that was presented requires a transversely finite plasma column [12]. If the plasma radius is small enough that the electron trajectories in the blowout go outside the plasma region, a detuning of the restoring forces occurs and the returning electrons will extend over a larger region instead of the spike usually associated with the blowout. A region of accelerating and focusing fields for positrons is found if the the plasma column radius and the driver parameters are properly chosen.

The nature of plasma acceleration is such that different parts of the witness beam experience different accelerating fields, therefore an increase in the correlated energy spread is obtained. Optimal beam-loading is usually thought as the way to mitigate this effect. A novel setup that uses staging and the correlated energy spread to its advantage was shown [13]. The beam would pass through a magnetic chicane between stages, which rotates the beam in the phase-space in such a way that the most energetic particles after the first stage will experience the lowest accelerating fields in the second (and vice-versa). After the acceleration in the second stage, the energy chirp gained in the first stage can thus be compensated.

Applications of plasma accelerators to radiation generation were also discussed. PIC simulations helped to understand a high-flux of moderate energy ($\sim 14\,\mathrm{keV}$) X-rays observed in a laser driven experiment [14]. A secondary self-injection of an electron beam with high charge and large oscillating radius after strong laser compression and focusing observed in the simulations is likely to be the explanation for the observed photons in the experimental data. Another interesting radiation generation case was presented, a phenomenon due to the coupling of the electron oscillations and the density gradients at the edges of the plasma column in a tunnel-ionized plasma [15]. At the far-field, the observed spectra is of a single-cycle THz radiation. The role of the gas used, which can lead to sharper or smoother transitions of the plasma column-neutral gas interface, was also discussed. Another foreseen application is the study of non-perturbative quantum electrodynamics (QED) in lepton collisions. The required bunches properties are extremely challenging, but they are under investigation and will be probed at SLAC-FACET II [16].

Finally, new ion acceleration results were discussed during WG6 as well. Results of ion acceleration in near-critical and underdense targets were shown [17], demonstrating optimal regimes and profiles to optimize ion acceleration in those scenarios [18]. Another exciting, and perhaps counter-intuitive result that was presented is the positive effects of non-ideal laser contrast in the ion acceleration of overdense targets. The role of non-ideal contrast in obtaining higher energy ions was discussed [19].

## 3. Code updates and numerical schemes

Most of the presentations regarding simulation codes were about the implementation of known models to different Particle-in-Cell codes, the development of new data analysis tools, or preparation of codes for the next generation of supercomputers.

Perhaps the main exception to this trend was the presentation of a new finite differences time domain (FDTD) Maxwell solver which is free of numerical dispersion along one direction [20]. As shown in several benchmarks, this allowed to significantly reduce if not eliminate numerical Cherenkov instability (NCI) without using spectral solvers.

Updates and future plans for many of the most used PIC codes were also presented. The preparation of the open source PIC code WarpX [21] to exascale machines were displayed, as well as its features such as mesh refinement, and its ongoing progress in the plan on simulating several GeV accelerator stages. Updates on VSim preparation for the exascale and the code adaptation to run in graphics processing units (GPUs) were also detailed [22].

The preparation towards exascale computing was also highlighted by a presentation on the open source PIC code PIConGPU [23], with increasing levels of abstractions to program of different computing architectures. It was also shown progress on *in-situ* live data visualization [24] and progress on making PIConGPU user friendly by adopting Jupyter notebooks and graphical user interface as both simulation input and data analysis tool. The code speed has allowed to perform challenging realistic 3D PIC simulations of the L|PWFA experiment and of ion acceleration experiments in the near-critical density.

The main features of the quasi-3D spectral open source PIC code FBPIC [25] were also presented. The code was born to gather many numerical schemes and techniques optimized for plasma acceleration and the possibility to run simulations GPU. In particular, the combination of boosted frame and a Galilean transformation was shown to eliminate NCI from plasma acceleration simulations [26]. Convergence studies with FBPIC for the accurate simulations of LWFA were also presented, highlighting the need of higher resolutions than those normally used and numerical artifacts that can decrease the simulation accuracy [27].

Ongoing studies on the azimuthal modes decomposition of experimentally-measured laser intensity profiles from Apollon and future realistic LWFA simulations with the open source PIC code Smilei were presented [28]. The implementation of adaptive vectorisation [29] and of the Single Domain Multiple Decomposition (SDMD) [30] in Smilei were reported as well. The latter technique decouples the decomposition based on the load balancing (based on the number of particles in a sub-domain) and the decomposition of the field grid, speeding up the field operations and being suitable for decompositions adapted to spectral solvers.

The implementation of envelope or ponderomotive guiding center models in three different PIC codes was also described. These models only need to describe the laser envelope, so one needs to solve the plasma scales instead of the laser wavelength, hence reducing the simulation cost. Applications of the ponderomotive guiding center model developed in the PIC code OSIRIS [31] to density downramp injection [32] and to the AWAKE experiment were presented [33]. The description of the kinetic and hybrid fluid-kinetic envelope model in the open source PIC code ALaDyn [34] was presented, as well as its application to the resonant multi-pulse ionization injection (REMPI) scheme [35]. The application of the kinetic envelope model presented in [34], developed also in the code Smilei , to the design of single stage and multi-stage LWFA Apollon experiments was presented [36].

A powerful approximation used to speedup PIC simulations is the quasi-static approximation

[37]. Recent developments of the quasi-static open source PIC code QuickPIC [38] were presented, including ongoing work on the first quasi-static PIC code with azimuthal Fourier decomposition QPAD (QuickPIC with Azimuthal Fourier Decompostion).

The multi-physics code FLASH [39] was presented as well. The code is used to simulate capillary discharges, used for example to create deeper guiding channels [40] or for active plasma lenses [41, 42].

## 4. Conclusions

The presentations and discussion of the WG6 covered analytical models, the proposition of new experimental set ups and updates on PIC codes like the implementation of new numerical models and solvers.

Despite the difficulties in finding general solutions to the equations describing plasma acceleration, considerable efforts have been shown to develp analytical models, benchmarked with PIC simulations, to describe specific aspect of the phenomena of interest. The proposed new experimental setups aim at overcoming intrinsic difficulties of plasma acceleration schemes and improving the beam quality for different applications. Reduced models that considerably reduce the computing resources needed by PIC simulations are reaching a high level of maturity and benchmarked on increasingly more challenging plasma acceleration simulations. PIC codes are also evolving and adapting to the next generation computing architectures, such as GPU supercomputers and exascale machines.

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