Nuclear Instruments and Methods in Physics Research A 740 (2014) 250–256

Contents lists available at ScienceDirect

Nuclear Instruments and Methods in Physics Research A

journal homepage: www.elsevier.com/locate/nima

How to test and verify radiation diagnostics simulations within particle-in-cell frameworks

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ARTICLE INFO

Available online 13 November 2013

Keywords:
Liénard–Wiechert potentials
Thomson scattering
Laser wakefield acceleration
Particle-in-cell codes
Radiation
Synthetic diagnostics

ABSTRACT

The particle-in-cell code PIConGPU provides the feature of calculating angular resolved radiation spectra in the far field based on Liénard–Wiechert potentials for all macroparticles of a plasma simulation. In order to verify the physics of our code we present a series of physics test scenarios, which compare numerical results to analytic solutions of nonlinear Thomson scattering at relativistic electrons. These scenarios range from single particle and electron bunch tests to full-scale laser-plasma simulations that include the collective effects of a plasma, as well as coherent and incoherent superposition of radiation of many particles. For the calculated test cases good agreement to the theoretical results with respect to absolute spectral intensities was found in all observation directions. In an electron density scan of a laser-plasma scenario, we reproduce a second-harmonic intensity scaling also observed in experiment.

1. Electromagnetic radiation as a diagnostic tool

Particle-in-cell (PIC) codes [1,2] have been very successful in modeling the particle dynamics of laser plasma interactions such as LWFA [3], PWFA [4] or TNSA [5]. A whole range of predictions by PIC simulations could be observed experimentally [6–9]. Recently, even time-resolved density structures could be measured and compared against PIC simulations [10].

Such models of experimentally observable quantities by simulations are also called synthetic diagnostics. They are indispensable tools to compare simulated and experimental results and allow insights into physics that neither simulations nor experiments alone could give.

Another common diagnostic method in laser plasma experiments is the observation of electromagnetic radiation emitted from the plasma electrons [11,12]. Although there exist theoretical predictions for a few specific electron dynamics occurring in laser particle interactions [13–16], one has to rely on extensive simulations to describe the emitted radiation once the laser plasma interactions become more complex.

The state-of-the-art of synthetic radiation diagnostics within PIC simulations is that one selects a number of particles and then stores their trajectories either on disk or in memory [17–20]. The spectrally resolved intensity is then computed using these trajectories. Due to memory constraints, the number of trajectories is limited to around $N_p \sim 10^3$–10^6. This directly limits the sampling of the electron phase space.

In addition, these codes are either limited to compute the radiation of many particles for only a few observation directions ($N_\theta \sim 1$) [17,19] or to calculate the emissions for many directions ($N_\theta \sim 10^2$–10^3) for only a small number of particle trajectories ($N_p \sim 1$–10^2) [21–23]. This renders quantitative comparison of simulation data to spatially varying intensities as measured by cameras or array detectors impossible, especially if the radiation observed is partially coherent.

In contrast to that, PIConGPU [24] computes the far field radiation directly in the PIC cycle and thereby avoids storing electron trajectories. Since this approach is only compute bound, we can calculate the radiation of all macro-particles provided by the PIC code ($N_p \sim 10^8$–10^{10}). This leads to orders of magnitude finer sampling of the phase space allowing to reproduce radiation emitted by only a small fraction of all particles, which due to a high degree of coherence or directionality of its radiation can result in a larger fraction of the resulting spectrum.

Due to the use of graphic cards as hardware accelerators, PIConGPU can compute the far field radiation for considerably more observation directions ($N_\theta \sim 10^2$–10^3) and allows computing the reciprocal phase space in unprecedented detail. By trading computations for memory, the synthetic radiation diagnostic in PIConGPU avoids the memory wall [25] and will perform well even on the next generation super computers.

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http://dx.doi.org/10.1016/j.nima.2013.10.073

Only such computationally demanding approaches are able to reduce the risks of misidentifying spectral signals due to the particle or directional sampling and enable quantitative predictions on spectral signatures in plasmas with both coherent and incoherent radiation.

In this paper, we emphasize the physics verification of our synthetic diagnostics of angularly and spectrally resolved far field radiation and present first comparisons with experimental results. First we show in single particle tests that these test particles quantitatively radiate according to analytical solutions of nonlinear Thomson scattering, hence verifying the correct modeling of numerically challenging relativistic effects for both longitudinal and transverse electron motion. Then in many-particle tests, the incoherent nature of radiation emerging from the superposition over all (macro) particles is examined. Finally, nonlinear Thomson scattering scenarios within a plasma include the influence of space-charge forces on the calculated spectra, thus testing the integration between the PIC code and the radiation code.

The technical details on the actual implementation of the radiation diagnostics in PIConGPU, as well as the requirements on the phase space sampling for the far field radiation are beyond the scope of this work. These will be addressed in a future paper.

2. Spectrally resolved far field radiation using Liénard-Wiechert potentials

If charged particles undergo acceleration, they emit electromagnetic radiation. This is due to the retardation of the electric field surrounding the charge. For point like particles, Liénard–Wiechert potentials describe the resulting electromagnetic fields [26]. Using these potentials, the spectrally resolved energy emitted by a single point like charge can be calculated from the particle's trajectory $\vec{r}(t)$ and velocity $\vec{\beta}(t)$ (Fig. 1). The energy $\mathrm{d}^2I/\mathrm{d}\Omega\,\mathrm{d}\omega$ per unit solid angle Ω and unit frequency ω emitted in the direction of the unit vector $\vec{n}$ depends on the electric charge q and the acceleration $\dot{\vec{\beta}}(t)$ of the particle

$$\frac{\mathrm{d}^2I}{\mathrm{d}\Omega\,\mathrm{d}\omega}=\frac{q^2}{16\pi^2\varepsilon_0 c}\left|\int_{-\infty}^{+\infty}\frac{\vec{n}\times\left[(\vec{n}-\vec{\beta})\times\dot{\vec{\beta}}\right]}{(1-\vec{\beta}\cdot\vec{n})^2}\cdot \mathrm{e}^{\mathrm{i}\omega(t-\vec{n}\cdot\vec{r}(t)/c)}\,\mathrm{d}t\right|^2 \quad (1)$$

This equation assumes an observer far away from the charge [26]. Such a far field approximation is feasible because the source of radiation, the laser plasma interaction, is small compared to the experimental setup of detectors.

Eq. (1) describes the far field radiation spectra $\mathrm{d}^2I/\mathrm{d}\omega\,\mathrm{d}\Omega$ in the most general form [27]. The results are valid for arbitrary particle trajectories. In contrast to a synchrotron-like radiation approach as used by [28–30], we do not make any assumption on the particle trajectories or on the spectral distribution of the radiation. A synchrotron-like radiation approach assumes a negligible acceleration parallel to the velocity and is only valid for an arbitrary and highly relativistic $\gamma \gg 1$ particle motion [26].

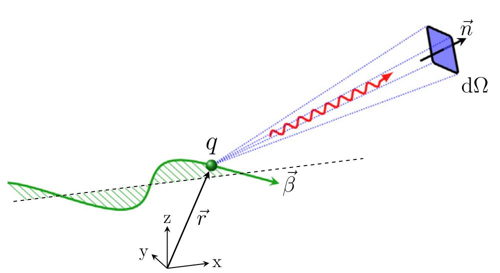

Fig. 1. Schematic diagram illustrating the radiation of a single point like charge q.

When considering N particles, the phase relations between the charges need to be considered. This requires a coherent sum of the Fourier transforms over retarded time

$$\frac{\mathrm{d}^2I}{\mathrm{d}\Omega\,\mathrm{d}\omega}\sim\left|\sum_{t=t_{\mathrm{start}}}^{t_{\mathrm{end}}}\sum_{k=1}^{N} q_k\frac{\vec{n}\times\left[(\vec{n}-\vec{\beta}_k)\times\dot{\vec{\beta}}_k\right]}{(1-\vec{\beta}_k\cdot\vec{n})^2}\cdot \mathrm{e}^{\mathrm{i}\omega(t-\vec{n}\cdot\vec{r}_k(t)/c)}\Delta t\right|^2 \quad (2)$$

In Eq. (2), we already applied the changes required for a numerical solution. The sum over all time steps is a non-equidistant Fourier transform for each particle. By summing over all particles in each time step, trajectories do not need to be stored. This makes our code compute-bounded and not memory-bounded. Solving this equation for millions of particles and thousands of frequencies is computationally expensive and can only be handled efficiently when massively parallelized. The sheer size that would be required to store the particle trajectories on disk makes an algorithmically faster Fast Fourier Transform approach not practicable.

The equation describes both coherent and incoherent radiation correctly. In the approximation of incoherent radiation, the phase relation can be neglected and the emitted energy scales only linearly with the total charge.

Since the absolute intensities emitted depend on the acceleration and velocity the charged particles undergo, the radiation carries information on the dynamics of the plasma electrons and therefore gives insight into their phase space distribution. Due to the ion's three orders of magnitude larger rest mass, they are not accelerated as strongly as electrons. Therefore, mainly electrons contribute to the electromagnetic emissions of laser plasma interactions.

Currently, PIConGPU does not include recoil effects caused by the emitted radiation. This limits the regime of validity to scenarios where the total loss of energy due to radiation is small compared to the total energy of the electron [23]. These effects could be included in PIConGPU by treating the radiation recoil as a mean force on the macro-particles as described in [23,27]. As the radiation calculation discussed in this paper allows for calculating the total energy radiated by each macro-particle for the full solid angle and arbitrary frequencies at each time step, another option of calculating radiation reaction becomes available. In principle, with the techniques discussed here, classical radiation reaction can be accounted for by changing the momentum of each macro-particle according to its energy loss due to radiation. This requires integrating the radiated energy lost over the full solid angle and all relevant frequencies, carefully avoiding double-counting the fields solved in the particle-in-cell cycle. For all following tests, the radiation recoil can be neglected.

3. Test and verification of radiation diagnostics simulations

When an electromagnetic wave interacts with an electron, the electron starts to oscillate. Due to this acceleration, it emits electromagnetic radiation called Thomson scattering. In high field physics, the strength of electromagnetic waves is described by a dimensionless parameter [31]

$$a_0=\frac{eE_0}{m\omega_0 c}. \quad (3)$$

When a_0 is on the order of unity or larger, the motion of the electron due to the electromagnetic wave becomes nonlinear. This leads to radiation with characteristic higher harmonic spectral signatures called nonlinear Thomson scattering. Since today's laser plasma experiments reach $a_0 \geq 1$, the nonlinear particle motion and the resulting radiation needs to be reproduced correctly by simulations. Therefore, we not only checked our results for the