Computer Physics Communications 192 (2015) 313–321

Contents lists available at ScienceDirect

Computer Physics Communications

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

SIMLA: Simulating particle dynamics in intense laser and other electromagnetic fields via classical and quantum electrodynamics ☆

D.G. Green [1], C.N. Harvey *

Centre for Plasma Physics, School of Mathematics and Physics, Queen's University Belfast, Belfast, Northern Ireland, BT7 1NN, United Kingdom

ARTICLE INFO

Article history:
Received 3 December 2014
Received in revised form
22 February 2015
Accepted 23 February 2015
Available online 14 March 2015

Keywords:
Intense laser–electron interactions
Strong-field quantum electrodynamics
Radiation reaction

ABSTRACT

We present the Fortran program SIMLA, which is designed for the study of charged particle dynamics in laser and other background fields. The dynamics can be determined classically via the Lorentz force and Landau–Lifshitz equations or, alternatively, via the simulation of photon emission events determined by strong-field quantum-electrodynamics amplitudes and implemented using Monte-Carlo routines. Multiple background fields can be included in the simulation and, where applicable, the propagation direction, field type (plane wave, focussed paraxial, constant crossed, or constant magnetic), and time envelope of each can be independently specified.

Program summary

Program title: SIMLA

Catalogue identifier: AEWD_v1_0

Program summary URL: http://cpc.cs.qub.ac.uk/summaries/AEWD_v1_0.html

Program obtainable from: CPC Program Library, Queen's University, Belfast, N. Ireland

Licensing provisions: Standard CPC licence, http://cpc.cs.qub.ac.uk/licence/licence.html

No. of lines in distributed program, including test data, etc.: 4536

No. of bytes in distributed program, including test data, etc.: 38351

Distribution format: tar.gz

Programming language: Fortran.

Computer: Home and office-spec desktop and laptop machines, networked or stand alone.

Operating system: Linux, Mac OS, Windows, with Fortran compiler. Matlab required to exploit full post-processing features.

RAM: Varies greatly depending on calculation to be performed.

Supplementary material: A SIMLA manual with tutorial type examples is available.

Classification: 15.

Nature of problem: Calculation of dynamics and emission spectra of charged particles in multiple (intense) laser and other background fields, including effects of classical and quantum radiation reaction.

Solution method: Solution of the Landau–Lifshitz equation (or simply Lorentz equation for weak fields), or alternatively, via the simulation of photon emission events determined by strong-field quantum-electrodynamics amplitudes and implemented using Monte-Carlo type routines.

☆ This paper and its associated computer program are available via the Computer Physics Communication homepage on ScienceDirect (http://www.sciencedirect.com/science/journal/00104655).

* Correspondence to: Department of Applied Physics, Chalmers University of Technology, SE-41296 Gothenburg, Sweden.
E-mail addresses: dermot.green@balliol.oxon.org (D.G. Green), cnharvey@physics.org (C.N. Harvey).

[1] Present address: Joint Quantum Centre (JQC), Durham/Newcastle, Department of Chemistry, Durham University, South Road, Durham, DH1 3LE, United Kingdom.

http://dx.doi.org/10.1016/j.cpc.2015.02.030

Restrictions: As a single particle code, the parameters are restricted to a regime in which pair production does not occur. The program will abort with an explicit error message if such a parameter regime does occur in a given simulation.

Additional comments: Classical spectra calculated separately in independent Matlab program 'spectrum.m'. Manual included with tutorial style examples

Running time: Varies greatly depending on calculation requested, from seconds to hours.

1. Introduction

Recent technological advances have led to the development of lasers of unprecedented powers and intensities. The current record of 2×10^{22} W cm^{-2} was set by the HERCULES laser in 2008 [1]. It is expected that this will be routinely surpassed when a number of new facilities come online, such as the European 'Extreme Light Infrastructure' (ELI) [2] and the Russian ExaWatt Centre for Extreme Light Studies (XCELS) [3]. These facilities aim to reach intensities of the range 10^{23}–10^{25} W cm^{-2}, allowing the probing of fundamental physics in the ultra-high intensity regime. In particular, these lasers will enable an investigation of intensity effects in strong field quantum electrodynamics (QED) (see, e.g., [4,5]).

These new facilities will, in part, achieve such intensities by strongly focussing their beams. In such fields the particle dynamics, and resulting emission spectra, are very difficult to determine analytically. In addition, multiple photon emissions can take place during the interaction which also causes the analytical expressions to become unwieldy. In the case of simple fields, the photon spectra for electrons have recently been calculated numerically [6,7]. For arbitrary fields this becomes more difficult (although some progress has been made towards calculating QED processes in structured fields, see [8]) and one is forced to resort to more general numerical schemes in order to simulate the interactions. Recently there have been a number of publications presenting modifications to particle-in-cell (PIC) programs to include QED processes (see, e.g., [7,9–11]). While having the particle–particle capability of a PIC based programs is certainly important for many applications, there are also many situations where the mutual interactions between particles in the field is not of interest and can be neglected. In the case of experiment, a typical example might be a beam of high-energy particles colliding with a laser pulse. Moreover, the dynamics of single isolated particles are of theoretical interest, both to better understand the fundamental physics of particles in these background fields (see for example [12–14]) and in order to test and refine the numerical models used (see [15]). Although PIC schemes can still be used in such cases, we believe it is beneficial to have a dedicated single-particle program that can run on an ordinary desktop computer, and used by a wider audience without reliance on the specialist knowledge and super-computing infrastructure required to run a PIC program. In addition, such a dedicated single-particle program can also be made more efficient than its PIC counterpart, since it is possible to dynamically change the grid spacing during a run.

In this paper we present our single-particle program SIMLA. It is written in modular Fortran and can be run on a modest desktop computer to calculate the dynamics of a charge in laser and other background fields. SIMLA accounts for the effects of radiation reaction via either numerical solution of e.g., the Landau–Lifshitz equation (for classical particles), or via Monte-Carlo simulation using QED emission amplitudes (for quantum particles). Multiple background fields can be included in the simulation and the propagation direction, form of the field (plane wave, focussed paraxial, constant crossed, or constant magnetic), and time envelope of each can be independently specified.[2]

The structure of the paper is as follows. In Section 2 we present a brief overview of the theory of charged particles in electromagnetic fields (including intense laser fields), and its specific implementation in the SIMLA code. We consider the motion of non-radiating classical particles, radiating classical particles, and the stochastic effects of photon emission from quantum particles. In Section 3 a number of test problems are outlined that provide a tutorial introduction to the basic functionality of the code. We conclude with a summary in Section 4.

2. Theory of charged particles in laser fields and its implementation in SIMLA: radiation reaction and stochastic dynamics

2.1. Classical theory

2.1.1. Non-radiating classical motion

In the classical case where radiation damping effects are neglected, the motion of a charged particle in an electromagnetic background field is described by the Lorentz-force equation,

$$\frac{d\mathbf{p}}{dt} = q\left(\mathbf{E} + \mathbf{v} \times \mathbf{B}\right), \tag{1}$$

where $\mathbf{p} = \gamma m \mathbf{v}$ is the relativistic momentum expressed in terms of the γ-factor, velocity $\mathbf{v}$, charge of the particle q and the particle rest mass m (and we are working in units such that $\hbar = c = 1$). The electric and magnetic field components $\mathbf{E}$ and $\mathbf{B}$ can be arbitrary functions of space and time. In this non-radiating classical case, the SIMLA program propagates the particle throughout the field by solving Eq. (1) to determine the acceleration. Although (1) is only expressed in terms of three-vectors, the code maintains covariance by enforcing the mass-shell condition $p^2 = m^2$ when calculating γ (for an alternative solution to this problem we refer the reader to [16]).

In the case of a time-dependent field, such as a laser pulse, it is conventional to specify the field strength using a dimensionless parameter defined with reference to a probe particle. This is $a_0 \equiv qE/\omega m$, where ω is the central frequency of the background field and E is the *maximum* strength of the electric field.

2.1.2. Radiation reaction

Both classical and quantum electrodynamics dictate that a particle in the presence of a background field will radiate. If the acceleration is strong, this radiation can lead to a significant reduction in the energy and momentum of the particle. In the classical case the radiation is emitted continuously (the quantum case, where the radiation is emitted discontinuously, as quanta, is

[2] In the current version up to nine independent background fields can be specified. The code could easily be adapted to handle a larger number, if required.