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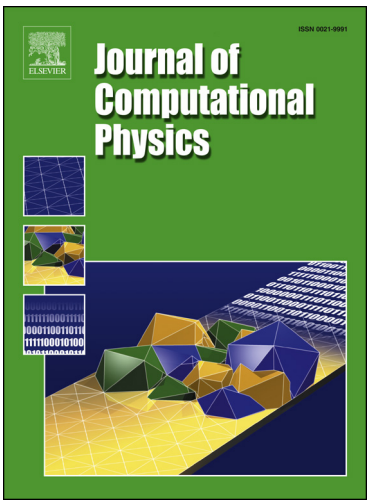

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A split-step method to include electron-electron collisions via Monte Carlo in Multiple Rate Equation simulations

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Abstract

A split-step numerical method for calculating ultrafast free-electron dynamics in dielectrics is introduced. The two split steps, independently programmed in `C++11` and `FORTRAN` 2003, are interfaced via the presented open source wrapper. The first step solves a deterministic extended multi-rate equation for the ionization, electron-phonon collisions, and single photon absorption by free-carriers. The second step is stochastic and models electron-electron collisions using Monte-Carlo techniques. This combination of deterministic and stochastic approaches is a unique and efficient method of calculating the nonlinear dynamics of 3D materials exposed to high intensity ultrashort pulses. Results from simulations solving the proposed model demonstrate how electron-electron scattering relaxes the non-equilibrium electron distribution on the femtosecond time scale.

Keywords:
Split-step method, Operator splitting, Laser-induced ionization, Free electron dynamics, Monte Carlo, Electron-electron collisions, `C++11`, `FORTRAN` 2003, interface, `OpenMP`

1. Introduction

Ultrafast laser-material interactions play a critical role for many modern laser applications. In particular, a detailed understanding of laser-induced ionization and many-body effects in dielectrics is necessary for progress in laser machining and ablation [1], laser surgery [2], and laser-induced breakdown spectroscopy [3]. The physics of these applications is strongly nonlinear, and there are few, if any, analytical solutions to problems of general interest [4]. Simulations therefore provide the primary method of theoretical testing for new models for ultrafast laser-material dynamics, as well as for closely related experimental research involving high intensity ultrashort pulse propagation [5–7].

The research areas of laser-material dynamics and pulse propagation are rich in nonlinear physics and can require considerable computational effort to perform comprehensive simulations [6, 8]. This issue is compounded when modeling pulse propagation at high intensities, since the laser field is sufficiently high to ionize the medium through which it propagates. This fact should necessitate a simultaneous and detailed modeling of pulse propagation and free-carrier dynamics, but this is rarely done because of computational constraints. What is typically done instead are calculations of reduced dimensionality [9], or fully 3D models using a highly detailed model of pulse propagation coupled with a greatly simplified model of laser-material dynamics [10], or vice versa [11]. To couple these research areas frequently requires the collaboration of theorists with differing expertise and who program their calculations using different code languages. The occasional need to interface two programming languages for a research collaboration can also have additional

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