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Computational performance of simple and efficient sequential and parallel Dirac equation solvers

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ABSTRACT

This paper is dedicated to the study of the computational performance of basic and efficient pseudo-spectral methods (Braun et al. (1999), Grant (2006) [1], Mocken and Keitel (2004) [2], Mocken and Keitel (2008) [3]) and of a Quantum Lattice Boltzmann-like approach (Fillion-Gourdeau et al. (2012), Fillion-Gourdeau et al. (2014), Lorin and Bandrauk (2011), Salomonson and Öster (1989), Succi and Benzi (1993)) for solving the Time Dependent Dirac Equation (TDDE) modeling the interaction of classical electromagnetic fields with quantum relativistic particles.

1. Introduction

In this work, we are interested in the simulation of the relativistic dynamics of an electron of mass m coupled to an external classical electromagnetic field. The time-dependent Dirac equation reads [4]

$$\mathrm{i}\partial_t \psi(t,\mathbf{x}) = H\psi(t,\mathbf{x}) \tag{1}$$

where $\psi(t,\mathbf{x})$ is the time and coordinate dependent four-spinor, and H is the Hamiltonian operator. The latter is given by

$$H = \boldsymbol{\alpha}\cdot[c\mathbf{p} - e\mathbf{A}(t,\mathbf{x})] + \beta mc^2 + \mathbb{I}_4 V(t,\mathbf{x}), \tag{2}$$

where the momentum operator is $\mathbf{p} = -\mathrm{i}\nabla$. More specifically, the Dirac equation under consideration reads [4]

$$\begin{aligned}\mathrm{i}\partial_t \psi(t,\mathbf{x}) = \Big\{&\alpha_x\Big[-\mathrm{i}c\partial_x - eA_x(t,\mathbf{x})\Big] + \alpha_y\Big[-\mathrm{i}c\partial_y - eA_y(t,\mathbf{x})\Big]\\ &+\alpha_z\Big[-\mathrm{i}c\partial_z - eA_z(t,\mathbf{x})\Big] + \beta mc^2 + \mathbb{I}_4 V(t,\mathbf{x})\Big\}\psi(t,\mathbf{x}),\end{aligned} \tag{3}$$

where $\psi(t,\mathbf{x}) \in L^2(\mathbb{R}^3)\otimes\mathbb{C}^4$ is the time and coordinate ($\mathbf{x} = (x,y,z)$) dependent four-spinor. In (3), $\mathbf{A}(t,\mathbf{x})$ represents the three space components of the electromagnetic vector potential, $V(t,\mathbf{x}) = eA_0(t,\mathbf{x}) + V_{\text{nuc.}}(\mathbf{x})$ is the sum of the scalar and interaction potentials, e is the electric charge (with $e = -|e|$ for an electron), $\mathbb{I}_4$ is the 4×4 unit matrix and $\boldsymbol{\alpha} = (\alpha_\gamma)_{\gamma=1,\dots,4}$, β are the Dirac matrices. In this work, the Dirac representation is used, where

$$\alpha_\gamma = \begin{bmatrix} 0 & \sigma_\gamma \\ \sigma_\gamma & 0\end{bmatrix}, \quad \beta = \begin{bmatrix}\mathbb{I}_2 & 0\\ 0 & -\mathbb{I}_2\end{bmatrix}. \tag{4}$$

The σ_γ are the usual 2×2 Pauli matrices defined as

$$\sigma_x = \begin{bmatrix}0 & 1\\ 1 & 0\end{bmatrix}, \ \sigma_y = \begin{bmatrix}0 & -\mathrm{i}\\ \mathrm{i} & 0\end{bmatrix} \text{ and } \sigma_z = \begin{bmatrix}1 & 0\\ 0 & -1\end{bmatrix}, \tag{5}$$

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while $\mathbb{I}_2$ is the 2×2 unit matrix. Note that the light velocity c and fermion mass m are kept explicit in Eq. (2), allowing to adapt the method easily to natural or atomic units (a.u.).

Throughout this work, we consider the single particle Dirac equation which is relevant for calculations describing Quantum Electrodynamics (QED) processes coupled to strong classical fields (e.g. particle–antiparticle pair creation from very high intensity electromagnetic classical fields [5]). *The purpose of this paper is not to derive original numerical solvers for the Dirac equation, or to provide simulations of specific quantum relativistic problems, but to compare the efficiency of two existing simple but accurate methods for solving the Dirac equation*. Although *pseudo-spectral methods* are used for decades for solving the Dirac equation, for instance for Graphene or pair production simulations [1–3,6–13], recently a real space method [14–17] was established to address these physical questions. This real space method, which has closed connection with the Quantum Lattice Boltzmann method [18,19] is simply a finite-difference method at CFL $= 1$ [20], for solving a first order linear hyperbolic system with eigenvalues of equal magnitude. This method which is based on the Method of Characteristics (MC) will be referred in this paper to as a *MC-based method*. Thanks to its simplicity, the MC-based method is shown to be highly scalable and much more efficient sequentially and in parallel than pseudo-spectral methods for a fixed number of degrees of freedom (dof). Its main weakness is however the strict condition which is imposed on the space step. In comparison, the pseudo-spectral methods are much more flexible regarding the choice of the spatial discretization step, that is the number of dof. In summary, for physical problems involving very small space scales, the MC-based will be shown to be much more efficient than pseudo-spectral methods. This will be the case for instance for problems involving heavy ions, or for intense and short laser–molecule interactions. In the opposite, when a fine spatial resolution is not required pseudo-spectral methods will be shown to be more efficient thanks to the possibility to select much coarser meshes, while keeping a very good accuracy (spectral convergence). The strength of the QLB method is two fold: the linear computational complexity with a very small prefactor and the hyperbolicity of the Dirac equation which allows for very efficient domain decomposition (without iteration) on straight interfaces. However, the main negative feature is the constraint of the space step (CFL condition), imposed by the speed of light and the physical timescale (zeitterbewegung [21]). We show in the paper, that the parallelization of the QLB (or MC-based scheme) can be extremely efficient.

Naturally, other types of methods exist for solving the Dirac equation, such as variational methods [22–27] or Krylov-type methods [28], but these are not discussed in this paper, which focuses on simple and efficient techniques.

The paper is organized as follows. In Section 2 (resp. Section 3), we recall the basics of the MC-based (resp. basic pseudo-spectral) method for the Dirac equation modeling the interaction of an electron with and external electromagnetic field. We next present in Section 4, an overview of the parallel computing aspects. In Section 5 (resp. Section 6), a series of sequential and parallel experiments is presented to illustrate the strengths and weaknesses of each method in the one-dimensional (resp. multi-dimensional) case. We conclude in Section 7.

2. Method of characteristic-based TDDE solver in cartesian coordinates

2.1. Operator splitting (first order)

We here recall the principle of operator splitting for the computation of an approximate solution to Eqs. (1) and (2) at time t_{n+1}, and denoted by $\psi^{n+1}(\mathbf{x})$. The initial condition at time t_n is assumed given by

$$\psi(t_n, \mathbf{x}) = \psi^n(\mathbf{x}). \tag{6}$$

As previously discussed in [16], this can be done [14,15] with an operator splitting scheme. We first define the operators

$$A = -\mathtt{i}c\alpha_x\partial_x \tag{7}$$

$$B = -\mathtt{i}c\alpha_y\partial_y \tag{8}$$

$$C = -\mathtt{i}c\alpha_z\partial_z \tag{9}$$

$$D = \beta mc^2 + \mathbb{I}_4 V(t, \mathbf{x}) - e\boldsymbol{\alpha} \cdot \mathbf{A}(t, \mathbf{x}). \tag{10}$$

The following splitting in Cartesian coordinates is considered [16] (the $\mathbf{x}$-dependence in the wavefunction argument for notational convenience):

$$\mathtt{i}\partial_t \psi^{(1)}(t) = A\psi^{(1)}(t), \ \ \psi^{(1)}(t_n) = \psi^n, \qquad t \in [t_n, t_{n+1}) \tag{11}$$

$$\mathtt{i}\partial_t \psi^{(2)}(t) = B\psi^{(2)}(t), \ \ \psi^{(2)}(t_n) = \psi^{(1)}(t_{n+1}), \ \ t \in [t_n, t_{n+1}) \tag{12}$$

$$\mathtt{i}\partial_t \psi^{(3)}(t) = C\psi^{(3)}(t), \ \ \psi^{(3)}(t_n) = \psi^{(2)}(t_{n+1}), \ \ t \in [t_n, t_{n+1}) \tag{13}$$

$$\mathtt{i}\partial_t \psi^{(4)}(t) = D\psi^{(4)}(t), \ \ \psi^{(4)}(t_n) = \psi^{(3)}(t_{n+1}), \ \ t \in [t_n, t_{n+1}) \tag{14}$$

$$\text{and} \ \ \psi^{n+1} = \psi^{(4)}(t_{n+1}) \tag{15}$$

where the upper subscript in parenthesis on the wavefunction denotes the splitting step number. Note that this simple splitting scheme leads to an error that scales in $O(\Delta t^2)$, corresponding to a first-order numerical scheme (for more details on the analysis of the method, see [16]). The method consists of solving each equation independently with an initial condition given by the solution of the previous step. Note also that for every step, the time increment is identical, i.e. $\Delta t \equiv t_{n+1} - t_n$. This splitting approach will be used in this paper with both the MC-based and pseudo-spectral-methods.

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