# DiracSolver: a tool for solving the Dirac Equation

Ioannis G. Tsoulos<sup>(1)</sup>, O.T. Kosmas<sup>(2)</sup>, V.N. Stavrou<sup>(3)</sup>

- (1) Department of Communications, Informatics and Management, Technological Educational Institute of Epirus, Greece
  - (2) Modeling and Simulation Centre, MACE, University of Manchester, M13 9PL Manchester, UK
  - (3) Military Institutes of University Education (ASEI), Hellenic Naval Academy, 18539 Piraeus, Greece

#### Abstract

Advantageous numerical methods for solving the Dirac equations are derived. They are based on different stochastic optimization techniques, namely the Genetic algorithms, the Particle Swarm Optimization and the Simulated Annealing method, their use of which is favored from intuitive, practical, and theoretical arguments. Towards this end, we optimize appropriate parametric expressions representing the radial Dirac wave functions by employing methods that minimize multi parametric expressions in several physical applications. As a concrete application, we calculate the small (bottom) and large (top) components of the Dirac wave function for a bound muon orbiting around a very heavy (complex) nuclear system (the <sup>208</sup>Pb nucleus), but the new approach may effectively be applied in other complex atomic, nuclear and molecular systems.

**Keywords:** Neural networks, Genetic algorithm, Simulated annealing, Particle swarm optimization, Solutions of the Dirac equations

### 1 Introduction

In many modern physical problems and specifically those related to the structure and evolution of quantum systems, the evaluation of exact predictions for various physical observables is required [1, 2, 3, 4]. These predictions are based on wave functions describing the states of the quantum system in question that come out of accurate solutions of specific type differential equations, like the Schroedinger and Dirac equations, etc. [3, 4, 5]. Because, usually, analytic solutions of such differential equations describing many body quantum systems are not possible, the application of advanced algorithms is required [5, 6].

Concrete examples of the category of physical problems we deal with in the present work are systems of leptons (electron, muon, tau particle, etc.) bound in extended Coulomb fields created by the protons of atomic nuclei [11, 12]. It is well known that, such problems may be solved analytically in special cases and only under the assumption of point-like constituents of the systems, i.e. pointlike nucleons, nuclei etc. (a fairly crude approximation), but the consideration of the finite size of nucleons and nuclei necessitates the use of advantageous numerical techniques [4, 5, 6]. In the first case, the wave functions of e.g. a hydrogenic-type lepton-nucleus system are obtained, and the Schroedinger as well as the Dirac equations may be solved analytically. In the second case, however, for solving these equations, the application of modern numerical methods should be adopted in complete analogy with the 2-body problem where, after removing (or neglecting) the center of mass motion, one rewrites these equations in the relative lepton-nucleus coordinate system (assuming spherical symmetry of the Coulomb field, the differential equations to be solved, are expressed in terms of the relative coordinate r). Then, the main problem is restricted to solving the radial part of the above mentioned 3-Dimensional differential (Schroedinger or Dirac) equations [4, 5, 6].

In recent years, there is intense interest in treating numerical solutions of wave functions for many body problem through the use of the field of machine learning methods [7, 8, 9, 10]. In this work, we make an attempt to derive methods for solving the Dirac differential equations on the basis of the assumptions of stochastic methods. More specifically, we choose the genetic algorithms [13], the particle swarm optimization (PSO) [14] and the simulated annealing method [15] in the context of which, one may optimize appropriate multi-parametric expressions representing the radial part of the wave functions describing a lepton orbiting around a complex nucleus [1, 2, 5].

It is worth noting that, within the context of these methods compact expressions for the radial part of the Schroedinger and Dirac wave functions, in the form of a rather simple summation times an exponential, both functions of the radial coordinate r, are obtained, which afterwards facilitate several physical applications.

In this paper, we applied the algorithms to obtain the ground state wave function describing a muon-nucleus system (muonic <sup>208</sup>Pb atom), however, its application in order to find the wave functions for other quantum states like those of a tau mesic atom [16] or hydrogenic-type electron nucleus systems, etc. [6], is straightforward. From a computational point of view, the training in our method is performed by using the DiracSolver software package that proved to be both convenient and efficient. This offers the possibility for the developed in this work new approach, to be effectively applied in other complex atomic, nuclear and molecular systems.

The rest of the paper is organized as follows. In Section 2, the relativistic mathematical formulation and the construction of the error function of the problem is described. Then, the new minimization methods are presented (in Section 3) and the Software documentation is discussed (Section 4). These methods are applied in concrete physical systems and the obtained results for

example runs are also presented and discussed in Section 5. Finally (Section 6) the main conclusions extracted in this work are summarized.

### 2 Formulation of the mathematical problem

In this section we concentrate on the description, with the sufficient needed detail, of the theoretical formalism of the Dirac equations that refer to the motion of a quantum mechanical system moving in a central force field with relativistic velocity. The 3-Dimensional Dirac equations describing a Dirac particle in a central field are explained in the Appendix where the main ingredients and the required physical quantities are defined [21]. In the next subsection, we focus on the analysis of the radial part of the coupled first order (ordinary) differential Dirac equations.

### 2.1 The coupled radial Dirac equations

In order to figure out the mathematical problem we face in this paper, we start with the description of the quantum system we deal with, that consists of a lepton of mass  $m_{\ell}$  ( $\ell = e, \mu, \tau$ , for electron, muon, tau particle, respectively) bound in the electrostatic field created by an atomic nucleus. The latter contains a number of A nucleons (Z of them are protons with mass  $m_p$  and N are neutrons with mass  $m_n$ , so as A = Z + N) having total mass  $M = Nm_n + Zm_p - B(Z, N)$ , where B(Z, N) denotes the binding energy of the nuclear system [22] (for convenience, B(Z,N) may initially be neglected). The reduced mass, m, of the bound, in such a system, lepton is given by

$$m = \frac{m_{\ell}}{1 + m_{\ell}/M}.\tag{1}$$

In our investigation, we consider the two reduced radial wave functions of the Dirac equation for central force fields (see Appendix), i.e. the large (top), f(r), and the small (bottom), g(r), components that satisfy the differential equations (see for example [11, 6])

$$\frac{d}{dr}f(r) + \frac{1}{r}f(r) = \frac{1}{\hbar c}(mc^2 - E + V(r))g(r)$$
(2)

$$\frac{d}{dr}g(r) - \frac{1}{r}g(r) = \frac{1}{\hbar c}(mc^2 + E - V(r))f(r). \tag{3}$$

In this work, for simplicity we restrict ourselves in the ground state (1s state) of the bound lepton-nucleus system and the quantum number  $\kappa$  (see Appendix) takes the value  $\kappa = -1$  [6]. In Eqs. (2) and (3), E denotes the total energy of the lepton, c is the speed of light and  $\hbar c = 197.327$  MeV fm.

For the description of the central force nuclear field, as mentioned in the Introduction, we take into account the finite size of the studied nucleus by deriving the potential V(r) from a realistic charge density distribution of the atomic nucleus (see Sect. 5).

In order to deduce the error function to be minimized, we use the following parameterized solutions for the small and large components of the Dirac wave function

$$f(r) = re^{-\beta r} N(r, \mathbf{u_f}, \mathbf{v_f}, \mathbf{w_f})$$
(4)

and

$$g(r) = re^{-\beta r} N\left(r, \mathbf{u_g}, \mathbf{v_g}, \mathbf{w_g}\right) \tag{5}$$

with  $\beta > 0$ . The parameters  $\mathbf{u_g}$ ,  $\mathbf{v_g}$ ,  $\mathbf{w_g}$  may be assumed to be the parameters of a feed-forward artificial neural network  $N\left(r,\mathbf{u_g},\mathbf{v_g},\mathbf{w_g}\right)$  [5, 23]. From the aforementioned parameters  $\beta$  is more or less related to the wave number  $k = \sqrt{(2m_\ell E)}$  of the free particle wave function.  $u_g, v_g, w_g$  essentially they have no physical meaning which means that the smaller the value of n in the summation of Eq. 7 the larger the reliability of method.

The normalization of these wave functions is defined as

$$N = \int_0^\infty [g^2(r) + f^2(r)]dr = 1.$$
 (6)

Other authors use alternatively computational techniques based on expansions of the corresponding wave function into classical polynomials such as Laguerre, Legendre etc. [17, 18, 19]. The proposed method, however, utilizes Neural Networks that can easily approximate every type of function and provide accurate solutions compared to other methods[20]. Moreover, they are reliable even in environments with error fluctuations.

After the above, in order to find f(r) and g(r), one has to minimize an error function  $\mathcal{F}(\mathbf{u}, \mathbf{v}, \mathbf{w})$  of the form [1, 2]

$$\mathcal{F} = N^{-1} \sum_{i=1}^{n} \left\{ \left[ \frac{df(r_i)}{dr} + \frac{f(r_i)}{r_i} - \frac{mc^2 - E + V(r_i)}{\hbar c} g(r_i) \right]^2 + \left[ \frac{dg(r_i)}{dr} - \frac{g(r_i)}{r_i} - \frac{mc^2 + E - V(r_i)}{\hbar c} f(r_i) \right]^2 \right\}.$$
 (7)

The minimization provides the values of the set of parameters  $\mathbf{u}, \mathbf{v}, \mathbf{w}$  and the binding energy  $\epsilon_b$  of the lepton in the Coulomb field of the nucleus [24, 25] given by

$$\epsilon_b = E - mc^2 \tag{8}$$

where the total energy of the lepton E is given by

$$E = \frac{mc^2 \int_0^\infty [g^2(r) + f^2(r)]dr + \int_0^\infty V(r)[g^2(r) - f^2(r)]dr}{\int_0^\infty [g^2(r) - f^2(r)]dr}.$$
 (9)

In the present work, we have derived efficient algorithms in order to solve the above quantum mechanical eigenvalue problem through the optimization of  $\mathcal{F}$  (for a great number of n in Eq. (7)) as presented below.

### 3 Description of the minimization methods

The proposed software, utilizes three different optimization methods: a genetic algorithm, a particle swarm optimization method and a simulated annealing method, to solve the Dirac equation. The binding energy  $\epsilon_b$  of the Dirac particle (lepton) orbiting a chosen atomic orbit is determined from the minimum energy,  $E_{min} = \epsilon_b$ , satisfying the eigenvalue problem, Eqs. (2) and (3). In the following each, of these methods is described in detail.

### 3.1 Genetic algorithm

Genetic algorithms are methods based on the so called genetic operations of natural selection, reproduction and mutation. They have been used successfully in many areas such as combinatorial problems [26], neural network training [27, 28], electromagnetic [29], design of water distribution networks [30] etc. The main steps of the used genetic algorithm are shortly described in [31] and they have:

- Step 1 (initialization):
  - Generate N uniformly distributed random points (chromosomes) and store them to the set S.
  - Set iter=0
  - Set  $p_s$  the selection rate
  - Set  $p_m$  the mutation rate
  - Set IMAX the maximum number of allowed iterations.
- Step 2 (evaluation): Evaluate the function value of each chromosome.
- Step 3 (termination check): If termination criteria are hold terminate. The termination criteria of the used algorithm are based on asymptotic considerations. At every generation denoted by iter, the variance  $\sigma^{(\text{iter})}$  of the best located value is recorded. If there is not any improvement for a number of generations, it is highly possible that the global minimum is already found and hence the algorithm should terminate. Also if iter >= IMAX then terminate.
- Step 4 (genetic operations):
  - **Selection**: Select  $m \leq N$  parents from S. The selection is performed using the tournament selection technique.
  - **Crossover**: Create m new points (offsprings) from the previously selected parents.
  - **Mutation**: Mutate the offsprings produced in the crossover step with probability  $p_m$ .

- Step 5 (**replacement**): Replace the *m* worst chromosomes in the population with the previously generated offsprings.
- Step 6
  - **Set** iter=iter+1
  - goto step 2

### 3.2 Particle swarm optimization

The swarm optimization algorithm (PSO) was initially suggested by Kennedy and Eberhart [14] and it is an evolutionary type algorithm based on population of candidate solutions (swarm of particles) which move in an n-dimensional search space. Every particle i is assigned its current position  $\mathbf{x}_i$  and the corresponding velocity  $\mathbf{u}_i$ . These two vectors are repeatedly updated, until a predefined convergence criterion is met. The PSO method has been applied to a wide range of problems [32, 33, 34, 35] and here we use a variant of the original method described in [36]. The main steps are:

#### 1. Initialization.

- (a) **Set** k = 1 (iteration counter).
- (b) **Set** the number of particles m.
- (c) Set the maximum number of iterations  $k_{\text{max}}$
- (d) **Initialize** randomly the positions of the m particles  $x_1, x_2, \ldots, x_m$
- (e) **Initialize** randomly the velocities of the m particles  $u_1, u_2, \ldots, u_m$
- (f) For i = 1, ..., m do  $p_i = x_i$ .
- (g) Set  $p_{\text{best}} = \arg\min_{i \in 1,...,m} f(x_i)$
- (h) Set  $p_{\text{old}} = p_{\text{best}}$
- $2. \ \mathbf{For} \ i=1, \ldots, m \ \mathbf{Do}$ 
  - (a) **Update** the velocity  $u_i$  with the equation

$$u_i = \psi_1 r_1 (p_i - x_i) + \psi_2 r_2 (p_{\text{best}} - x_i)$$
 (10)

where  $\psi_1$  and  $\psi_2$  are positive constants.

(b) **Update** the position  $x_i$  as and  $p_{best}$ 

$$x_i = x_u + u_i \tag{11}$$

- (c) Calculate the objective function for particle  $i, f(x_i)$
- (d) If  $f(x_i) \leq f(p_i)$  then  $p_i = x_i$
- 3. End For

- 4. **Termination** Check Step
  - (a) Set  $p_{\text{best}} = \arg\min_{i \in 1,...,m} f(x_i)$
  - (b) Calculate the variance  $\sigma^{(k)}$  of the best located value (as in Genetic Algorithm case)
  - (c) If there is not any improvement for a number of generations, terminate and report  $p_{\mathrm{best}}$  as the discovered minimum.
- 5. Set k = k + 1. If  $k \ge k_{\text{max}}$  then terminate.
- 6. Goto Step 2.

### 3.3 Simulated Annealing

Simulated annealing [15] mimics the annealing process to solve an optimization problem. The temperature parameter T controls the search which typically starts off high and is slowly "cooled" or lowered in every iteration. At each iteration a series of new points are generated. If the new point has a better function value it replaces the current point and iteration counter is incremented. It is possible, however, to accept and move forward with a worse point, but the probability of doing so is directly dependent on the temperature T (this step, sometimes, helps identify a new search region in hope of finding a better minimum and protects the algorithm from being trapped in local minima).

A typical description of SA algorithm is as follows [37, 38, 39]:

- 1. Set k = 0,  $T_0 > 0$ . Sample  $x_0$  as the initial point.
- 2. Set  $N_{eps} > 0$ , a positive integer
- 3. Set  $\epsilon > 0$ , a small positive double precision value.
- 4. Set  $r_T > 0$ ,  $r_T < 1$ , a positive double precision value.
- 5. For  $i = 1, ... N_{eps}$ 
  - (a) Sample a point y
  - (b) If  $f(y) \leq f(x_k)$  then  $x_{k+1} = y$
  - (c) Else Set  $x_{k+1} = y$  with probability min  $\left\{1, \exp\left(-\frac{f(y) f(x_k)}{T_k}\right)\right\}$
- 6. EndFor
- 7. Set  $T_{k+1} = T_k r_T$
- 8. **Set** k = k + 1.
- 9. If  $T_k \leq \epsilon$  terminate
- 10. **Goto** step 2.

#### 4 Software documentation

Although this method is complete, it requires many calculation steps for each matrix element. In order to verify the method, we have used it for calculating the ground state of atomic and nuclear systems by solving the Dirac equations. We have solved these problems analytically for any excitation and for an arbitrary value of the total angular momentum. These solutions are the only examples of general analytic solution of the Dirac equation in three dimensional space for the study of nuclear systems composed of N nucleons.

In order to carry out our algorithm systematically, we choose some maximum value  $k_{max}$  for the maximum number of iterations allowed [36]. A computer code implementing the formalism described above for one row states was developed. The code starts from one coordinate states with a given value for  $k_{max}$ .

#### 4.1 Installation

The user should issue the following commands to build the program Dirac Solver (under some Unix machine):

- 1. Download the code DiracSolver.tar.gz
- 2. gunzip DiracSolver.tar.gz
- 3. tar xfv DiracSolver.tar
- 4. cd DiracSolver
- 5. qmake.
- 6. make

The main executable is called DiracSolver

#### 4.2 User interface

The graphical interface of the program is written entirely in Qt and it contains the following tabs:

- 1. Settings tab. A screenshot of this tab is show in Fig 4. The user can select the desired global optimization method (Genetic algorithm, Pso or Simulated Annealing) and subsequently he can alter some default parameters of the selected method such as the number of chromosomes in genetic algorithm, the initial temperature in Simulated Annealing etc. Also, under the section Equation Settings the user can change the number of hidden nodes used by the neural network for the Dirac equation and he can select the desired material for the equation. This list contains 9 materials.
- 2. Run tab. A typical screenshot of this tab is outlined in Fig 5. The user can start or terminate the optimization process through two buttons located here.

3. **Graph tab.** The final outcome of the procedure is displayed in this tab. A typical screenshot is demonstrated in Fig 6. The user can save the plot for the material either in png format or in text format ideal for programs such as Gnuplot. Also in this tab the user can save the parameters of the optimization method as well as the parameters of the neural network in a text file using the button entitled SAVE PARAMETERS.

## 5 Application of the method in a physical system

In this section, we apply the new algorithms to find the ground state (1s state) wave functions f(r) and g(r) of Eqs. (2) and (3), i.e. large and small component, respectively, of the Dirac equations (4) and (5), that describe the motion of a muon bound in the Coulomb field created by the  $^{208}Pb$  nucleus, a system known as "the mu-mesic  $^{208}Pb$  atom". We stress that the application of the new methods, to find the basis (or excited) states Dirac wave functions of other quantum systems like hydrogenic-type electron-nucleus systems, the tau-mesic atoms [16], etc., is straightforward.

The potential energy  $V(\mathbf{r})$  entering Eqs. (2) and (3), for the nuclear Coulomb field originating from an extended nuclear charge density distribution  $\rho(\mathbf{r})$ , is calculated by [5]

$$V(\mathbf{r}) = -e^2 \int \frac{\rho(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} d^3 \mathbf{r}'.$$
 (12)

The nuclear charge density  $\rho(\mathbf{r})$  in this work is obtained from model independent analysis of the electron scattering experimental data of Ref. [40]. For the chosen nuclear systems (we assume their charge distribution is spherically symmetric) the radial charge density distribution entering Eq. (12) is described by a two-parameter Fermi distributions [40, 41] of the form

$$\rho(r) = \frac{\rho_0}{1 + e^{(r-c)/z}}. (13)$$

For the parameters c and z (known as radius and thickness parameter, respectively), in the case of  $^{208}Pb$  nucleus, we adopted the values of Ref. [40]. The parameter  $\rho_0$  is determined from the normalization of  $\rho(\mathbf{r})$  [40]. The root mean square charge radius of this nuclear isotope (representing the extension of the nuclear finite size), is  $R_{ms} \approx 5.5$  fm. It should be noted that, for both the Schroedinger and Dirac solutions one has to take into account some (may be significant) corrections to the potential V(r) such as the nuclear polarization [5], the vacuum polarization [6, 24], etc. In the present work, we have taken into account an effective potential  $V_{vp}$  due to the vacuum polarization corrections described by an effective potential as in Refs. [1, 5].

We furthermore note that, in other similar works (e.g. Ref. [4, 3]), authors employ a phenomenological description for the V(r) corresponding to a uniform distribution of the nuclear charge within the mean charge radius  $R_{ms} = R_c$  of

the form

$$V(r) = \begin{cases} \frac{(Z-1)e^2}{2R_c} \left[ 3 - \left(\frac{r}{R_c}\right)^2 \right] &, & r \leq R_c, \\ \frac{(Z-1)e^2}{r} &, & r > R_c. \end{cases}$$

It must be mentioned that, for large distances the matching of the wave functions f(r) and g(r) to their asymptotic behavior was done as in [41, 24, 25]. For light nuclei this matching is achieved at  $r \approx 60-70$  fm and for heavy and very heavy nuclear isotopes at  $r \approx 40-50$  fm.

The default values for the parameters of the Genetic algorithm, the PSO method and the Simulated Annealing method are displayed in Table 1. A typical outcome for the three optimization procedures is shown in Figures 1, 2 and 3. Example values obtained through the optimization techniques examined here, for the muon binding energy of Eq. (8) are listed in Table 2. For comparison with the experimental values of  $\varepsilon_b$  the reader is referred to Refs. [5, 6].

We should mention that, in realistic nuclear structure calculations, integrals of the form of Eq. (11) of Ref. [5] (see also Ref. [12]) may be explicitly obtained without the need to utilize approximation adopting an average muon wave function  $\langle \Phi_{\mu} \rangle$  at r=0. This, of course, implies that the evaluation of the required nuclear matrix elements becomes, in general, more complicated and time consuming. However, the obtained analytic-type expressions for the solution of the Dirac wave functions given by Eqs. (4) and (5) facilitates the calculations of the necessary physical observables.

Before closing this section it is worth making the following remarks: the advantages of utilizing Eqs. (4) and (5) for the muon wave functions become more evident when one calculates the incoherent rate in a muonic process like e.g in the ordinary muon capture, the muon to electron conversion ( $\mu^- \rightarrow e^-$ ), the muon to positron conversion ( $\mu^- \rightarrow e^+$ ), etc., where one has to face a large number of (double or multiple) numerical integrations corresponding to transition integrals from the initial (ground) to a final state of the chosen system. In addition, due to the fact that in our method the muon wave functions are available in a convenient way, i.e. as linear combinations of well-behaved (sigmoid) functions, the use of extrapolation and/or interpolation techniques required in other methods [12] is avoided and the accuracy of the results obtained this way is very high.

# 6 Summary and Conclusions

In many physical problems, one needs to describe accurately the motion of bound leptons (e,  $\mu$ ,  $\tau$ , etc.) in atomic orbits. Because this motion is relativistic, one must go beyond the usual calculation of the lepton density at the site of the atomic nucleus obtained through the use of the Schroedinger wave function. This means that one should solve numerically the Dirac equation in the field of the finite size nuclei. Specifically, for high Z values of the atomic nuclei, the motion of a muon, tau leptons, etc. is relativistic, and the small component g(r) of their wave functions is non-negligible. Therefore, for such calculations

one requires the additional contribution associated with that component of the Dirac equation.

In this paper, we have constructed three independent algorithms, based on three different stochastic optimization methods, for solving numerically the Dirac equation. These methods used a relativistic formalism to evaluate the radial part of these wave functions.

We applied the algorithm to find the ground state Dirac wave functions of a lepton-nucleus system, however, it is straightforward to apply these algorithms to obtain the basis states of other quantum systems like the tau mesic atoms. Also, they could be easily used for finding the wave functions that describe states of lepton-nucleus systems in which the lepton is orbiting in higher states (excited states).

The comparison of the algorithms presented above with the state of the art symmetrization algorithms, proves the computational advantages of our present algorithms.

### 7 Acknowledgements

Dr. Odysseas Kosmas wishes to acknowledge the support of EPSRC, United Kingdom, via grand  $\rm EP/N026136/1$  "Geometric Mechanics of Solids".

# 8 Appendix A

The general form of the 3-dimensional relativistic bound-state wave function  $\psi$  describing the motion of a Dirac particle in central force system is written as [21]

$$E\psi = \left[ -i\gamma_5 \sigma_r \left( \frac{\partial}{\partial r} + \frac{1}{r} - \frac{1}{r} \beta K \right) + V(r) + m_i \beta \right] \psi$$
 (14)

where  $\gamma_5$ ,  $\beta$ ,  $\sigma_r$  and K are the (4x4) matrices

$$\gamma_5 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \beta = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{15}$$

$$\sigma_r = \begin{pmatrix} \sigma \cdot \mathbf{r} & 0 \\ 0 & \sigma \cdot \mathbf{r} \end{pmatrix}, \qquad K = \begin{pmatrix} \sigma \cdot \ell + 1 & 0 \\ 0 & -(\sigma \cdot \ell + 1) \end{pmatrix}$$
 (16)

(in the above matrices the unit stands for the unit matrix) where  $\sigma = (\sigma_1, \sigma_2, \sigma_3)$ , with  $\sigma_i, i = 1, 2, 3$ , being the well known Pauli matrices [22]. The symbols E and V(r) denote the total energy and potential energy, respectively, and  $\ell$  represents the orbital angular momentum of the Dirac particle. The latter operator is defined by  $\ell = i\mathbf{r} \times \nabla$ . Also,  $m_i$  is the reduced mass of the lepton (e,  $\mu$ ,  $\tau$ ), etc. given in Eq. (1).

Even though  $\psi$  is not an eigenstate of  $\ell^2$ , however, the upper and lower components of  $\psi$ ,  $\psi_{\alpha}$  and  $\psi_{\beta}$  respectively, are separately eigenstates (they have

fixed total angular momentum j and spin s quantum numbers), so that  $\psi$  is written as

 $\psi = \begin{pmatrix} \psi_{\alpha} \\ \psi_{\beta} \end{pmatrix}. \tag{17}$ 

Then, the solutions of the 3-Dimensional Dirac equation (14), describing a Dirac particle in a central force field, in spherical coordinates take the form [6]

$$\psi = \psi_{\kappa}^{\mu} = \frac{1}{r} \begin{pmatrix} f(r)_{\kappa} \Phi_{\kappa\mu}(\theta, \phi) \\ ig(r)_{\kappa} \Phi_{-\kappa\mu}(\theta, \phi) \end{pmatrix}.$$
 (18)

The quantum numbers  $\kappa$  and  $\mu$  describing the above wave functions, are eigenvalues of the operators -K and the projection  $\mathbf{j}_z$  of the total angular momentum operator  $\mathbf{j} = \ell + \mathbf{s}$  (s denotes the spin operator of the Dirac particle for which we assume s = 1/2) [6].

In Eq. (18), the radial wave functions g(r) and f(r) are determined through the two coupled first-order differential equations, Eqs. (2) and (3), and  $\Phi_{\kappa\mu}(\theta,\phi)$ is a spherical spinor in the direction  $(\theta,\phi)$  (the known spin spherical harmonics) defined by the equation

$$\Phi_{\kappa\mu} = \sum_{m_{\ell}m_{s}} \langle \ell m_{\ell} \frac{1}{2} m_{s} | (\ell \frac{1}{2}) j m \rangle Y_{\ell m_{\ell}}(\theta, \phi) \chi_{\frac{1}{2}m_{s}}$$
(19)

 $(Y_{\ell m_{\ell}} \text{ represent a spherical harmonic})$  where  $j = |\kappa| - \frac{1}{2}$  which gives  $\kappa = \mp (j + 1/2)$  with  $j = \ell \pm 1/2$ . The symbol  $\langle | \rangle$  in Eq. (19) denotes the well known Clebsch-Gordan coefficients which are numbers arising in angular momentum couplings in quantum mechanics [22].

Table 1: The default parameters for the Algorithms used.

Genetic Algorithm		PSO method		Simulated Annealing	
PARAMETER	VALUE	PARAMETER	VALUE	PARAMETER	VALUE
N	200	m	200	$T_0$	80.0
IMAX	200	$k_{ ext{max}}$	200	$N_{ m eps}$	200
$p_s$	0.1	$\psi_1$	1.0	$\epsilon$	$8 \times 10^{-5}$
$p_m$	0.05	$\psi_2$	1.0	$r_T$	0.9

Table 2: Muon binding energies obtained for each of the algorithmic methods for a set of interesting muonic atoms (see the text).

	· · · · · · · · · · · · · · · · · · ·		/
MATERIAL	GENETIC	PSO	ANNEALING
<sup>28</sup> Si	0.604	0.581	0.575
<sup>48</sup> Ti	1.585	1.510	1.504
$^{64}\mathrm{Zn}$ $^{98}\mathrm{Mo}$	2.443	2.490	2.415
124Sn	4.093 5.319	4.089 5.319	4.059 $5.318$
$^{156}\mathrm{Gd}$	7.625	7.627	7.624
186W	9.222	9.224	9.210
<sup>208</sup> Pd <sup>238</sup> II	10.599 $12.363$	10.599 12.363	10.545 $12.433$
U	12.505	12.505	12.400

# 9 Appendix B: PROGRAM SUMMARY

Title of program: DiracSolver Catalogue identifier:

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

Computer for which the program is designed and others on which it has been tested: The tool has been tested on Linux, Android and Windows. The tool is designed to be portable in all systems running the GNU C++ compiler using the QT programming library.

Licensing provisions: GPLv3

Installation: Technological Educational Institute of Epirus, Greece.

Programming language used: GNU-C++

Memory required to execute with typical data: 200KB.

No. of bits in a word: 64 No. of processors used: many

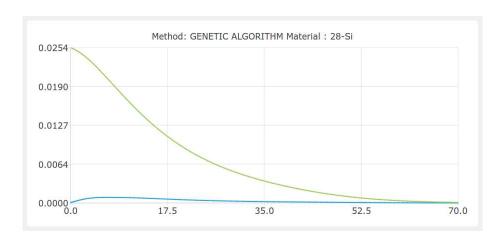


Figure 1: The output for material  $^{28}\mathrm{Si}$  using Genetic Algorithm.

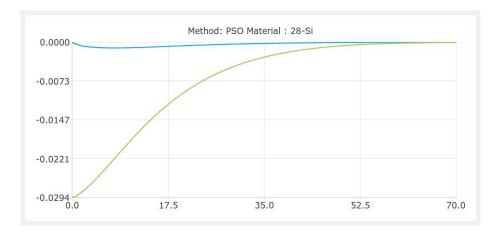


Figure 2: The output for material <sup>28</sup>Si using Particle Swarm Optimization.

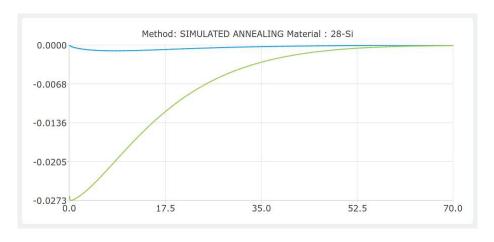


Figure 3: The output for material <sup>28</sup>Si using Simulated Annealing

Figure 4: The tab Settings of the application. The user can choose the optimization method and the running material.

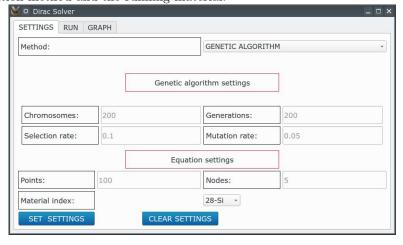


Figure 5: The tab Run of the application. The user can initiate the execution of the optimization method or he can terminate it.

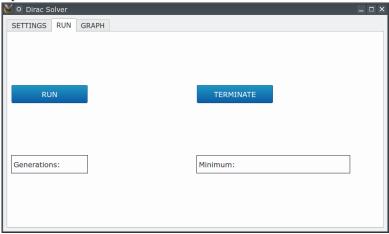


Figure 6: The tab Graph of the application. The user can save the plot in png format or he can save the plot in column format ideal for programs such as gnuplot or he can save the parameters of the execution.



Has the code been vectorized or parallelized?: No.

No. of bytes in distributed program, including test data etc.: 100 Kbytes.

Distribution format: gzipped tar file.

Keywords: Global optimization, stochastic methods, genetic algorithms Nature of physical problem: .

 $Solution\ method:$  .

Typical running time: Depending on number of processing nodes and the used optimization function. Nature of the problem: The software tackle the problem of solving the Dirac equation using stochastic optimization methods.

Solution method: The software utilizes three stochastic optimization methods for the solution of Dirac equation in the form of neural networks. The used methods are: genetic algorithm, particle swarm optimization and simmulated annealing.

### References

- [1] D.G. Papageorgiou, I.N. Demetropoulos, and I.E. Lagaris. Merlin-3.0 a multidimensional optimization environment. *Computer Physics Communications*, 109(2):227–249, 1998.
- [2] D.G. Papageorgiou, I.N. Demetropoulos, and I.E. Lagaris. The merlin control language for strategic optimization. *Computer Physics Communications*, 109(2):250–275, 1998.
- [3] S. Sabin and M. Mihail. New calculations for phase space factors involved in double- $\beta$  decay. *Phys. Rev. C*, 88:037303, Sep 2013.
- [4] S. Sabin, M. Mihail, O. Nitescu, J. Nabi, and M. Ishfaq. New phase space calculations for  $\beta$ -decay half-lives. Advances in High Energy Physics, 2016, 2016.
- [5] T.S. Kosmas and I.E. Lagaris. On the muon-nucleus integrals entering the neutrinoless  $\mu^- \to e^-$  conversion rates. Journal of Physics G: Nuclear and Particle Physics, 28(12):2907, 2002.
- [6] K. Ryuichiro, K. Masafumi, and O. Yasuhiro. Detailed calculation of lepton flavor violating muon-electron conversion rate for various nuclei. *Phys. Rev.* D, 66:096002, Nov 2002.
- [7] Giuseppe Carleo and Matthias Troyer, Solving the quantum many-body problem with artificial neural networks, Science 10, pp. 602-606, 2017.
- [8] John C. Snyder, Matthias Rupp, Katja Hansen, Klaus-Robert MAŒller, and Kieron Burke, Finding Density Functionals with Machine Learning, Phys. Rev. Lett. 108, 2012.
- [9] Louis-François Arsenault, Alejandro Lopez-Bezanilla, O. Anatole von Lilienfeld, and Andrew J. Millis, Machine learning for many-body physics: The case of the Anderson impurity model, Phys. Rev. B 90, 2014.

- [10] Giacomo Torlai, Guglielmo Mazzola, Juan Carrasquilla, Matthias Troyer, Roger Melko, Giuseppe Carleo, Neural-network quantum state tomography, Nature Physics 14, pp. 447-451, 2018.
- [11] N.T. Zinner, K. Langanke, and P. Vogel. Muon capture on nuclei: Random phase approximation evaluation versus data for  $6 \le Z \le 94$  nuclei. *Phys. Rev. C*, 74:024326, Aug 2006.
- [12] P.G. Giannaka and T.S. Kosmas. Detailed description of exclusive muon capture rates using realistic two-body forces. *Phys. Rev. C*, 92:014606, Jul 2015.
- [13] Z. Michalewicz. Genetic Algorithms + Data Structures = Evolution Programs (3rd Ed.). Springer-Verlag, London, UK, 1996.
- [14] J. Kennedy and R.C. Eberhart. New Ideas in Optimization: The Particle Swarm: Social Adaptation in Information-processing Systems. McGraw-Hill Ltd., UK, 1999.
- [15] S. Kirkpatrick, C.D. Gelatt, and M.P. Vecchi. Optimization by simulated annealing. *Science*, 220(4598):671–680, 1983.
- [16] C.H. Ching and E. Oset.  $\tau^-$  capture in nuclei. *Physics Letters B*, 259(3):239–242, 1991.
- [17] V. Alan KosteleckÜ and Michael Martin Nieto, Analytical wave functions for atomic quantum-defect theory, Phys. Rev. A 32, 1985.
- [18] E. M. Wright, J. Arlt, and K. Dholakia, Toroidal optical dipole traps for atomic Bose-Einstein condensates using Laguerre-Gaussian beams, Phys. Rev. A 63, 2000.
- [19] Young-Seek Chung, T.K. Sarkar, Baek Ho Jung, M. Salazar-Palma, Zhong Ji, Seongman Jang, Kyungjung Kim, Solution of time domain electric field Integral equation using the Laguerre polynomials, IEEE Transactions on Antennas and Propagation 52, 2004.
- [20] Kurt Hornik, Approximation capabilities of multilayer feedforward networks, Neural Networks 4, pp. 251-257, 1991.
- [21] M.E. Rose. Relativistic Electron Theory. John Wiley, 1961.
- [22] A. Shalit and H. Feshbach. *Theoretical Nuclear Physics: Nuclear structure*. Theoretical Nuclear Physics. Wiley, 1974.
- [23] C.M. Bishop. Neural Networks for Pattern Recognition. Oxford University Press, Inc., New York, NY, USA, 1995.
- [24] J.C. Sens. Capture of negative muons by nuclei. Phys. Rev., 113:679–687, Jan 1959.

- [25] K.W. Ford and J.G. Wills. Calculated properties of  $\mu$ -mesonic atoms. Nuclear Physics, 35:295–302, 1962.
- [26] JJ. Grefenstette, R. Gopal, B.J. Rosmaita, and D.V. Gucht. Genetic algorithms for the traveling salesman problem. In *Proceedings of the 1st International Conference on Genetic Algorithms*, pages 160–168, Hillsdale, NJ, USA, 1985. L. Erlbaum Associates Inc.
- [27] G.F. Miller, P.M. Todd, and S.U Hegde. Designing neural networks using genetic algorithms. In *Proceedings of the Third International Conference* on Genetic Algorithms, pages 379–384, San Francisco, CA, USA, 1989. Morgan Kaufmann Publishers Inc.
- [28] D. Whitley, T. Starkweather, and C. Bogart. Genetic algorithms and neural networks: optimizing connections and connectivity. *Parallel Computing*, 14(3):347–361, 1990.
- [29] R.L. Haupt. An introduction to genetic algorithms for electromagnetics. *IEEE Antennas and Propagation Magazine*, 37:7–15, apr 1995.
- [30] D.A. Savic and G.A. Walters. Genetic algorithms for least-cost design of water distribution networks. *Journal of Water Resources Planning and Management*, 123:67–77, 1997.
- [31] I.G. Tsoulos. Modifications of real code genetic algorithm for global optimization. *Applied Mathematics and Computation*, 203:598–607, 2008.
- [32] H. Yoshida, K. Kawata, Y. Fukuyama, S. Takayama, and Y. Nakanishi. A particle swarm optimization for reactive power and voltage control considering voltage security assessment. *IEEE Transactions on Power Systems*, 15(4):1232–1239, Nov 2000.
- [33] J. Robinson and Y. Rahmat-Samii. Particle swarm optimization in electromagnetics. *IEEE Transactions on Antennas and Propagation*, 52(2):397– 407, Feb 2004.
- [34] M.A. Abido. Optimal power flow using particle swarm optimization. *International Journal of Electrical Power & Energy Systems*, 24(7):563–571, 2002.
- [35] Z.L. Gaing. Particle swarm optimization to solving the economic dispatch considering the generator constraints. *IEEE Transactions on Power Systems*, 18(3):1187–1195, Aug 2003.
- [36] I.G. Tsoulos and A. Stavrakoudis. Enhancing pso methods for global optimization. Applied Mathematics and Computation, 216(10):2988–3001, 2010.
- [37] O.T. Kosmas and D.S. Vlachos. Simulated annealing for optimal ship routing. Computers & Operations Research, 39(3):576–581, 2012.

- [38] O.T. Kosmas, and D.S. Vlachos. Local path fitting: A new approach to variational integrators. *Journal of Computational and Applied Mathematics*, 236(10):2632–2642, 2012.
- [39] O.T. Kosmas and S. Leyendecker. Analysis of higher order phase fitted variational integrators Advances in Computational Mathematics, 42(3):605–619, 2016.
- [40] H. De Vries, C.W. De Jager, and C. De Vries. Nuclear charge-density-distribution parameters from elastic electron scattering. *Atomic Data and Nuclear Data Tables*, 36(3):495–536, 1987.
- [41] O. Shanker. z dependence of coherent  $\mu e$  conversion rate in anomalous neutrinoless muon capture. *Phys. Rev. D*, 20:1608–1615, Oct 1979.