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Charged Particle in an Electromagnetic Field Using Variational Integrators

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Abstract. In the present work we extend the discrete Lagrangian integrator method presented in Ref. [1] to derive appropriate numerical maps for the solution of mechanical problems in which the potential energy depends on the velocity of the system. As a representative concrete example and simulated experiment of the method presented here, we examine the motion of a charged particle moving in an electromagnetic field.

Keywords: variational integrators, discrete variational mechanics, charged particle dynamics, numerical integration
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INTRODUCTION

In discrete Lagrangian mechanics one defines the discrete Lagrangian function, $L_d(q_k, q_{k+1}, h)$, q_k corresponds to time t_k and q_{k+1} to time $t_{k+1} = t_k + h$, which approximates the action integral along the curve segment with endpoints q_k and q_{k+1} of the system's trajectory as [2, 3, 4, 5]

$$L_d(q_k, q_{k+1}, h) = \int_{t_k}^{t_{k+1}} L(q, \dot{q}, t)dt. \tag{1}$$

The latter integral, is commonly approximated as $\int_0^h L dt \approx hL$, where h is the time step and L is evaluated by using expressions for q and $\dot{q} = dq/dt$ describing the specific variational integration algorithm, e.g. in the rectangle rule [4] the velocity of the system is calculated by the expression $\dot{q} \approx (q_{k+1} - q_k)/h$. Relying on Eq. (1), one defines the action sum

$$S_d = \sum_{k=0}^{N-1} L_d(q_k, q_{k+1}, h), \tag{2}$$

that corresponds to the discrete trajectory of the particle, with N determining the number of points [3, 4]. Then, the discrete Hamilton's principle, $\delta S_d = 0$, gives the discrete Euler–Lagrange equations.

In the present paper, integration techniques constructed for such purposes are employed in order to determine the trajectory of the motion of a charged particle moving in an electromagnetic field and especially its trajectory in the general case of its motion in a uniform magnetic field.

LAGRANGIAN FORMALISM OF CHARGED PARTICLE IN AN ELECTROMAGNETIC FIELD

A charged particle of charge e and mass m moving in an electric field $\mathbf{E}$ and a magnetic field $\mathbf{B}$, classically is subjected to the force $\mathbf{F}$ acting on the particle which is given by the Lorentz force law, i.e.

$$\mathbf{F} = e\mathbf{E} + e\mathbf{v} \times \mathbf{B}, \tag{3}$$

where $\mathbf{v}$ is the instantaneous velocity of the particle. Since the Lorentz force is velocity dependent, it cannot result as the gradient of some scalar potential. Nevertheless, the classical path of the particle is still given by the principle of the least action with the Lagrangian described below.

From the classical time-dependent electromagnetic theory [7] it is known that if $\mathbf{A}$ is the vector potential and ϕ the scalar potential, then the magnetic field $\mathbf{B}$ and electric field $\mathbf{E}$ are written in terms of $\mathbf{A}$ and ϕ as

$$\mathbf{B} = \nabla \times \mathbf{A}, \tag{4}$$

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$$\mathbf{E} = -\nabla\phi - \frac{\partial \mathbf{A}}{\partial t}. \tag{5}$$

We assume that $\mathbf{A}$ and ϕ are functions of the position vector $\mathbf{r}$ and time t, i.e. $\phi = \phi(\mathbf{r},t)$ and $\mathbf{A} = \mathbf{A}(\mathbf{r},t)$. The Lagrangian of the system is written as

$$L = T - U, \tag{6}$$

where the kinetic energy T and the velocity dependent potential energy U are given by [7]

$$\begin{aligned} T &= \frac{1}{2}m\mathbf{v}^2, \\ U &= e\phi - e\mathbf{v}\cdot\mathbf{A}. \end{aligned} \tag{7}$$

Thus, the Lagrangian L of a charged particle in an electromagnetic field is written as

$$L(x_j, \dot{x}_j, t) = \frac{1}{2}m\mathbf{v}^2 - e\phi + e\mathbf{v}\cdot\mathbf{A}. \tag{8}$$

The latter Lagrangian, by applying Hamilton's principle provides the same type of continuous Euler–Lagrange equations as that of the velocity independent potential, i.e. the common Lagrangian $L = T - V$, where $\mathbf{F} = -\nabla V$. This means that the Euler–Lagrange equations that provide the trajectory of a charged particle moving in a field with electric and magnetic components $\mathbf{E}$ and $\mathbf{B}$, respectively, in cartesian coordinates where $L = L(x_j, \dot{x}_j, t)$, read

$$\frac{d}{dt}\frac{\partial L}{\partial \dot{x}_j} - \frac{\partial L}{\partial x_j} = 0. \tag{9}$$

Notice that in our notation we use the symbol U for the velocity dependent potential and the symbol V for the velocity independent one. In both cases, however, the latter equations have exactly the same form.

Solving analytically the Euler–Lagrange equations (9) in the case of the Lagrangian of Eq. (8), the equations of motions describing the helical orbit of the charged particle (in cartesian coordinates) are [7]

$$\begin{aligned} x_1 &= x(t) = -\frac{vsin(\theta)}{\omega}sin(\omega t) + x_0 \\ x_2 &= y(t) = \frac{vsin(\theta)}{\omega}cos(\omega t) + y_0 \\ x_3 &= z(t) = vcos(\theta)t. \end{aligned} \tag{10}$$

In the latter equations $\mathbf{r}_0 = (x_0, y_0, 0)$ denote the initial point vector of the system, $v = |\mathbf{v}|$ is the magnitude of its initial velocity (we assume that $\mathbf{v}$ forms an angle θ with z-axis) and ω is the frequency of the particle's orbit (see Appendix).

The analytical solutions of Eqs. (11) will provide us a reference scheme for testing the numerical solution of the proposed variational integrator algorithm.

A DISCRETE LAGRANGIAN INTEGRATOR FOR THE VELOCITY DEPENDENT POTENTIAL

As it is well known, from the action sum S_d of Eq. (2) by performing the differentiation, one obtains the discrete Euler–Lagrange equations [4]

$$D_2L_d(q_{k-1}, q_k, h) + D_1L_d(q_k, q_{k+1}, h) = 0, \tag{11}$$

where D_i denotes derivative with respect to the $i-$th argument of L_d.

Considering the discrete Lagrangian $L_d(q_k, q_{k+1}, h)$ and a set of S intermediate points q^j, with $q^j = q(t_k + c^j h)$, we can approximate L_d with the weighted sum [1]

$$L_d = (q_k, q_{k+1}, h) = h\sum_{j=1}^{S} w_j L(q(t_k + c^j h), \dot{q}(t_k + c^j h), c^j h), \tag{12}$$

with $c^1 = 0$ and $c^S = 1$.

Equations (11), for the discrete Lagrangian of the charged particle using the ansatz for the positions q and derivatives $\dot{q}$ described in [1], provide a numerical map $(q_{k-1}, q_k) \rightarrow (q_k, q_{k+1})$ as follows

$$\begin{bmatrix} B_1 & B_2 & 0 \\ -B_2 & B_1 & 0 \\ 0 & 0 & B_1 \end{bmatrix} \begin{pmatrix} q^1_{k+1} \\ q^2_{k+1} \\ q^3_{k+1} \end{pmatrix} = \begin{pmatrix} B_3 q^1_k - B_1 q^1_{k-1} + B_2 q^2_{k-1} \\ B_3 q^2_k - B_2 q^1_{k-1} - B_1 q^2_{k-1} \\ -B_3 q^3_k - B_1 q^3_{k-1} \end{pmatrix}, \tag{13}$$

where the upper indices $1,2,3$ denote the components of vector q_k. For the above discrete Lagrangian integrator, if we adopt the phase fitted coefficients $b, \bar{b}, B$ and $\bar{B}$ described in Ref. [1], we find

$$B_1 = \frac{1}{h^2} \sum_{j=1}^{S} w_j B \bar{B}, \tag{14}$$

$$B_2 = \frac{1}{2h} \sum_{j=1}^{S} w_j \omega (\bar{b} B - b \bar{B}), \tag{15}$$

$$B_3 = \frac{1}{h^2} \sum_{j=1}^{S} w_j (B^2 + \bar{B}^2), \tag{16}$$

where ω denotes the oscillation frequency of the particle's orbital motion (see Appendix).

For the calculation of the initial positions q_k needed in the procedure, the discrete equations of motion in position-momentum coordinates must be used, i.e. [1, 4]

$$\begin{aligned} p_k &= -D_1 L_d(q_k, q_{k+1}, h), \\ p_{k+1} &= D_2 L_d(q_k, q_{k+1}, h). \end{aligned} \tag{17}$$

Subsequently, the application of the integration steps of the method proceeds normally [4].

NUMERICAL RESULTS

In the present work we restrict ourselves in the study of the motion of the charged particle in a uniform magnetic field $\mathbf{B} = B_0 \hat{z}$, where $B_0 =$const. The corresponding vector potential is then given by the expression

$$\mathbf{A} = -\frac{1}{2}(\mathbf{r} \times \mathbf{B}). \tag{18}$$

It can, then, be readily proved that the latter vector potential satisfies Eq. (4).

In the case when the motion of a charged particle takes part along the magnetic field, $\mathbf{v} // \mathbf{B}$, two cases must be distinguished, i.e. those for which the enclosed angle θ is either 0 or π. In both cases the magnetic force is zero and the motion of the particle remains unaffected (assuming that there is no other force field present). In the present paper we assume that none of these cases occurs.

Motion of the charged particle perpendicular to a uniform magnetic field

As a first application of our present method we examine the simple case of the motion of a charged particle e moving perpendicular to a uniform magnetic field $\mathbf{B} = B_0 \hat{z}$. In this case the angle θ between $\mathbf{v}$ and $\mathbf{B}$ is taken to be $\theta = \frac{\pi}{2}$ (similar results can be obtained for the case when $\theta = \frac{3\pi}{2}$).

Under the above assumptions, the trajectory of the particle is planar. From a simulation performance point of view the particle's trajectory by applying our present method, has been rather easily obtained and it is shown in Fig. 1(left).

Furthermore, in the right subfigure of Fig. 1 we tested the step β of the trajectory by considering the circular orbit as a special case of the general helical orbit for which we have [7]

$$\beta = v_p T = \frac{2\pi}{\omega} v cos(\theta), \tag{19}$$

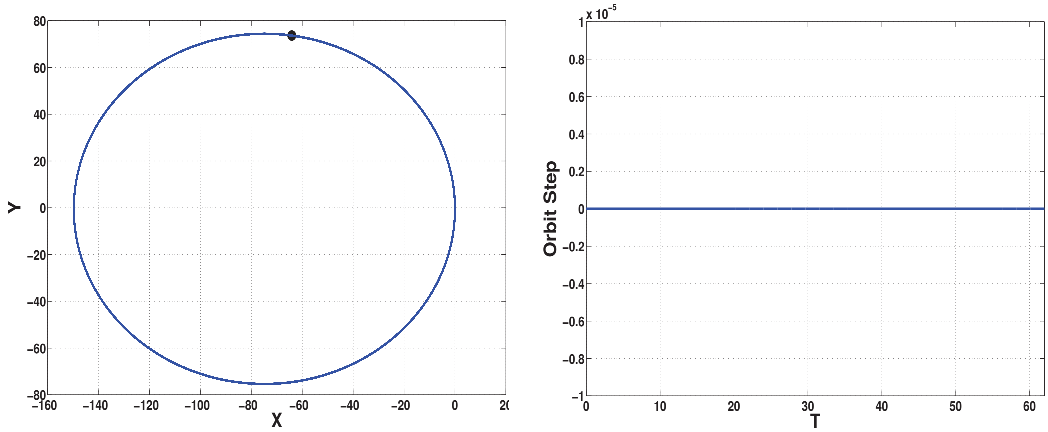

FIGURE 1. (Left) Circular orbit using the phase fitted discrete Lagrangian method of order $S = 5$ for a charged particle moving perpendicular to the magnetic field. Velocity and magnetic field vectors are at an angle $\theta = \frac{\pi}{2}$. (Right) The step of the orbit considered as a spacial case of the helical orbit (see the text).

where T represents the period of the orbit and $v = |\mathbf{v}|$. As it is clear from Fig. 1, the calculated step of the orbit is zero (as expected) for the velocity of the particle perpendicular to magnetic field.

From an algorithmic point of view, here we use the phase fitted discrete Lagrangian integrator method [1] of algebraic order $S = 5$.

Motion of the charged particle oblique to the magnetic field

In the general case, the velocity $\mathbf{v}$ of the charged particle forms an arbitrary angle with the magnetic field $\mathbf{B}$ and here we assume that the vectors $\mathbf{v}$ and $\mathbf{B}$ are at an acute angle θ, $0 < \theta < \frac{\pi}{2}$. In order to study this motion, we analyze the velocity vector such that one of the components to be parallel and other vertical to the magnetic field $\mathbf{B}$, i.e.

$$v_p = vcos(\theta), \qquad v_v = vsin(\theta). \tag{20}$$

The velocity component perpendicular to the magnetic field creates a magnetic force which provides the centripetal force for the particle to move along a circular path (as in the previous example).

On the other hand, as has been discussed at the beginning of this section, the velocity component parallel to magnetic field does not derive magnetic force and the charged particle moves in this direction with the constant velocity v_p without being accelerated.

For the case when the angle of the initial velocity with $z-$axis is $\theta = \frac{\pi}{4}$, the behavior of the proposed algorithm, Eq. (13), is implied from the particle's trajectory illustrated in Fig. 2. This has been obtained using the assumptions of the phase fitted discrete Lagrangian integrator method of Ref. [1] with algebraic order $S = 5$.

SUMMARY, CONCLUSIONS AND FUTURE WORK

In the present work, variational integrator techniques [4, 5] were employed for mechanical problems in which the potential component of the Lagrangian depends on the velocity of the system. For such cases, an extension of the phase fitted discrete Lagrangian integrators [1] is proposed. As an example the special case of a charged particle in electromagnetic field was studied.

Although preliminary simulation results illustrate the excellent behavior of the proposed technique compared to the integrators of Ref. [4], the comparison with energy-conserving methods [6] and numerical methods like those of Refs. [8, 9] remains to be carried out.

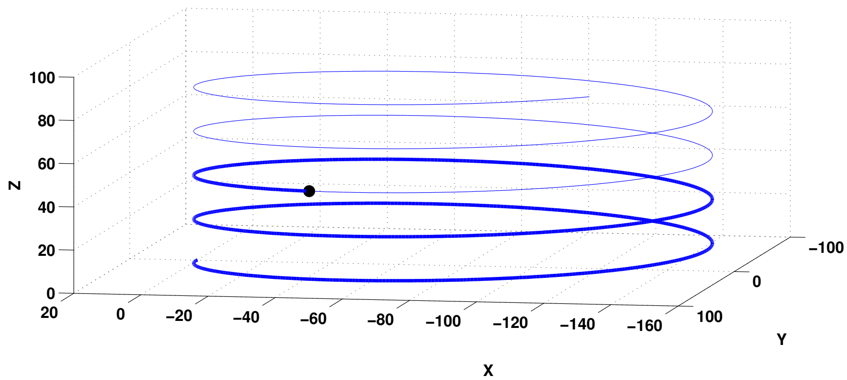

FIGURE 2. The calculated orbit for the particle oblique to magnetic field when velocity and magnetic field vectors are at an angle $\theta = \pi/4$ using the phase fitted discrete Lagrangian integrator method of order $S = 5$.

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APPENDIX

If $\mathbf{r}(t)$ is a parametrized (with respect to time) representation of the curve, its curvature is defined as

$$k(t) = \frac{\dot{\mathbf{r}}(t) \times \ddot{\mathbf{r}}(t)}{|\dot{\mathbf{r}}(t)|^3}. \tag{21}$$

The magnitude of the velocity of the particle at a point $\mathbf{r}(t)$ is $|\dot{\mathbf{r}}(t)|$. After a short time step h, the angular displacement of the particle will be $h|\dot{\mathbf{r}}(t) \times \ddot{\mathbf{r}}(t)|/|\dot{\mathbf{r}}(t)|^2$, which gives the following expression for the frequency

$$\omega(t) = \frac{|\dot{\mathbf{r}}(t) \times \ddot{\mathbf{r}}(t)|}{|\dot{\mathbf{r}}(t)|^2}. \tag{22}$$

From Eqs. (21) and (22) the well known relation $\omega(t) = k(t)|\mathbf{r}(t)|$ holds. For more details see Ref. [1]

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