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Symplectic integration of magnetic systems

Stephen D. Webb

RadiaSoft LLC, 1348 Redwood Ave., Boulder, CO 80304, United States

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ABSTRACT

Simulation of the long time behavior of systems requires more than just numerical stability to return dependable results – it must preserve the underlying geometric structure of the continuous equations. Symplectic integrators are the most common form of geometric integrator, and are therefore of interest in simulating plasmas for many plasma periods, for example. We present here results on generating symplectic integrators for magnetic systems, and in particular show that the algorithms due to Boris and Vay are symplectic.

1. Introduction

Symplectic integration [1–5] has become a staple of accelerator physics and astrophysics simulations, as it provides unconditional stability, if not the short term accuracy of Runge–Kutta type schemes. While numerical solutions for systems such as magnetized plasmas are not derived directly from Hamiltonian systems, the canonical method due to Boris [6–8] shows many of the properties of a symplectic integrator.

The primary difficulty in developing symplectic integrators for magnetic systems, as was pointed out by Ruth [1], is the $\vec{p} \cdot \vec{A}$ term that leads to implicit forms and which is not separable into an exactly integrable Hamiltonian. Even worse is for relativistic systems, where no clear expansion parameter for the radical in the Hamiltonian exists. In this case, the kinetic energy is not even close to separable. This problem does not appear in Lagrangian mechanics, where the vector potential appears in a $\dot{q} \cdot \vec{A}$ form outside the radical. However, Lagrangian mechanics lacks the canonical transformation formalism used in deriving symplectic integrators.

To obtain geometric integrators from a Lagrangian formalism, it is best to approach the problem using a discretized action integral. This method, described in [9] and the citations therein, obtains recursion relations for the q_k in configuration space that conserve the symplectic two-form.

In this paper, we present the formalism necessary to show that the Boris method is a symplectic integrator. An overview of discrete Lagrangian mechanics based on the work of Marsden and West [9] is first presented. This method is then applied to Lagrangians with vector potentials, first the nonrelativistic limit, where this is shown to be the Boris update. For the relativistic dynamics of particles in magnetic fields, we find that the generalization of the Boris update developed by Vay is symplectic.

2. Discretized Lagrangian mechanics

As discussed by Marsden and West ([9], and citations therein), the Lagrangian action integral may be approximated by some discretization scheme by

E-mail address: sdavis.webb@gmail.com.

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$$\int_0^t L(q,\dot{q},t')\,dt' \approx \sum_{k=0}^{N-1} L_D(q_{k+1},q_k,t_k) \tag{1}$$

where $t_k = t_0 + kh$ for a time step h. Thus, under this derivation, each L_D has the units of action, or $[L] \times [dt]$. Minimizing this action against variations δq_k of the physical trajectory, with $\delta q_0 = \delta q_N = 0$ to fix the endpoints, gives a variation of the discrete action

$$\begin{aligned}\delta S_D = \sum_{k=1}^{N-1}&\left(\frac{\partial}{\partial q_{k+1}} L_D(q_{k+1},q_k,t_k)\delta q_{k+1} + \frac{\partial}{\partial q_k} L_D(q_{k+1},q_k,t_k)\delta q_k\right)\\ &+ \partial_{q_0} L_D(q_0,q_1)\delta q_0 + \partial_{q_N} L_D(q_N,q_{N-1})\delta q_N = 0\end{aligned} \tag{2}$$

By shifting the summations to match the indices of the variations, this gives the discrete Euler–Lagrange (DEL) equations

$$D_2 L_D(q_{k+1},q_k) + D_1 L_D(q_k,q_{k-1}) = 0 \tag{3}$$

where D_n is the derivative with respect to the nth variable.

In the continuous Lagrangian limit, the symplectic two-form

$$\Omega_L(q,\dot{q}) = \frac{\partial^2 L}{\partial q_i \partial \dot{q}_j}\mathbf{d}q^i \wedge \mathbf{d}q^j + \frac{\partial^2 L}{\partial \dot{q}_i \partial \dot{q}_j}\mathbf{d}\dot{q}^i \wedge \mathbf{d}q^j \tag{4}$$

is conserved under the Euler–Lagrange equations. For the discretized Lagrangian, the tangent bundle $T\mathbb{Q}$ does not include $\dot{q}$, as the time derivatives do not appear in the Lagrangian. The discretized symplectic two-form that is conserved is given by

$$\Omega_{L_D}(q_0,q_1) = \frac{\partial^2 L}{\partial q_0^i \partial q_1^j}\mathbf{d}q_0^i \wedge \mathbf{d}q_1^j \tag{5}$$

Because $\Omega_{L_D} = \mathbf{d}\Theta_L$ is an exterior derivative, and $\mathbf{d}^2 = 0$, this symplectic two-form is conserved for all solutions of the DEL equations. This proof is provided in detail in Marsden and West.

Because $\dot{q}$ is replaced by a finite difference in the discrete Lagrangian, it is important to note that any velocity-like variables are auxiliary and do not play a role in the underlying geometric structure. This is an important distinction with Hamiltonian symplectic integrators, where the p and q both play a role in the geometry – the Hamiltonian symplectic two form explicitly involves the momentum.

As an example of how this yields a symplectic integrator, consider the Lagrangian for a one dimensional particle in a potential

$$L(q,\dot{q},t) = \frac{1}{2}\dot{q}^2 - V(q,t) \tag{6}$$

The discretization is non-unique – indeed choosing $q \mapsto {}^{(q_k+q_{k+1})}/_2$ yields an implicit integration scheme for general V, while choosing $q \mapsto q_{k+1}$ will yield the explicit integrator below. Because we are interested in explicit integrators, we will consider the discrete Lagrangian

$$L_D(q_{k+1},q_k) = \frac{1}{2}\frac{(q_{k+1}-q_k)^2}{h} - V\big(q_{k+1},(k+1)h\big)h \tag{7}$$

for a discrete time step t. Applying the DEL equations to this discrete Lagrangian yields

$$q_{k+1} - 2q_k + q_{k-1} = -\frac{\partial V}{\partial q_k}(q_k,kh)h \tag{8}$$

which we recognize immediately as $F = m\ddot{q}$ in the form of a central differencing. If we define the velocity vector to be

$$v_{k+1} = \frac{q_{k+1}-q_k}{h} \tag{9}$$

then this yields the first order symplectic integrator

$$v_{k+1} = v_k - \frac{\partial V}{\partial q_k}(q_k,kt)h \tag{10}$$

$$q_{k+1} = q_k + v_{k+1}h \tag{11}$$

which has the usual first order leapfrog scheme.

Unlike in Hamiltonian symplectic integration schemes, where the generating function defines the p and q update sequences explicitly, we were forced here to introduce the velocity as an auxiliary variable, turning our N second order recursion relations into $2N$ first order recursion relations. This is because, in Lagrangian mechanics, the q and $\dot{q}$ variables are not independent – the same reason there are no useful canonical transformations to generate symplectic integrators. This will become a useful construct when we consider the relativistic Lagrangian in Section 4.

To obtain a higher order integrator, it is necessary to sum two or more Lagrangians per time step, in the form

$$S_D = \sum_{k=0}^{N} \sum_{i=1}^{M} L_D^{i,k}\left(q_k^{i+1}, q_k^i, \gamma^i h\right) \tag{12}$$

where the individual L_D^i are for a substep of a single time step. From here on, we will drop the k indexing of the discretized Lagrangian as we are only concerned with a single time step linking k to $k+1$. By carrying out the same variational calculation, the resulting DEL equations for this decomposed system are given by

$$D_2 L_D^i\left(q_k^{i-1}, q_k^i, \gamma^i h\right) + D_1 L_D^{i+1}\left(q_k^i, q_k^{i+1}, \gamma^{i+1} h\right) = 0 \tag{13a}$$

$$D_2 L_D^M\left(q_k^{M-1}, q_k^M, \gamma^M h\right) + D_1 L_D^1\left(q_{k+1}^0, q_{k+1}^1, \gamma^1 h\right) = 0 \tag{13b}$$

where the γ^i index the time sub-steps and the steps are joined by $q_k^M = q_{k+1}^0$. The second equation gives the linkage between the last step of one time step, and the first step of the next one – in practice this frequently manifests as the final velocity of one time step equaling the initial velocity of the next.

If $L_D(q_0, q_1, h) = \sum_i L_D^i$ is the discrete Lagrangian, then the adjoint of the Lagrangian is defined as

$$L_D^*(q_0, q_1, h) \equiv -L_D(q_0, q_1, -h) \tag{14}$$

It is straightforward to show that a self-adjoint discrete Lagrangian $L_D^* = L_D$ only contains odd order corrections to the action integral, and therefore any self-adjoint discrete Lagrangian is automatically second order. We will therefore consider only self-adjoint Lagrangians in this paper.

3. Symplectic integrators for magnetic systems

We will now use this formalism to compute an explicit symplectic integration scheme for Lagrangians with vector potentials, beginning in the non-relativistic regime with a Lagrangian

$$L(q, \dot{q}, t) = \frac{1}{2} m \dot{q}^2 + \dot{q} \cdot \frac{e}{c} \vec{A}(q, t) - e\phi(q, t) \tag{15}$$

The dynamics are unchanged by the addition of a total derivative, or by dividing the Lagrangian by a constant. Thus, dividing through by the mass and defining

$$\vec{a} = \frac{e}{mc} \vec{A} \tag{16}$$

$$\varphi = \frac{e}{m} \phi \tag{17}$$

yields the normalized Lagrangian

$$L(q, \dot{q}, t) = \frac{1}{2} \dot{q}^2 + \dot{q} \cdot \vec{a}(q, t) - \varphi(q, t) \tag{18}$$

Given the close relationship between symplectic integration schemes and Trotter splitting for the Schrödinger equation, it is perhaps fruitful to take inspiration from path integration. It is well-known (for a discussion of this, see [10]) that, in evaluating a path integral with gauge fields, it is necessary to evaluate the gauge field either as

$$\vec{A}(q) \mapsto \frac{1}{2}\left(\vec{A}(q_k, 0) + \vec{A}(q_{k+1}, h)\right) \tag{19}$$

or

$$\vec{A}(q) \mapsto \vec{A}\left(\frac{q_{k+1} + q_k}{2}, {}^{h}\!/_{2}\right) \tag{20}$$

to preserve the gauge invariance of the equations of motion. We will consider the former first, and then consider the latter, as well as a third alternative which also proves to be useful, although its gauge properties are likely not as well-behaved.

Consider the discretized splitting into two Lagrangians given by

$$L_D^1\big(q_k^0, q_k^1, t\big) = \frac{1}{2}\frac{(q_k^1 - q_k^0)^2}{h/2} + \cdots + \big(q_k^1 - q_k^0\big)\cdot\frac{1}{2}\big(\vec{a}\big(q_k^0, 0\big) + \vec{a}\big(q_k^1, h/2\big)\big) - \frac{h}{2}\varphi\big(q_k^1, h/2\big) \tag{21a}$$

$$L_D^2\big(q_k^1, q_k^2, t\big) = \frac{1}{2}\frac{(q_k^2 - q_k^1)^2}{h/2} + \cdots + \big(q_k^2 - q_k^1\big)\cdot\frac{1}{2}\big(\vec{a}\big(q_k^1, h/2\big) + \vec{a}\big(q_k^2, h\big)\big) - \frac{h}{2}\varphi\big(q_k^1, h/2\big) \tag{21b}$$

Because this two-step discrete Lagrangian is the composition of a half step with its adjoint, the resulting Lagrangian is self-adjoint and, hence, 2nd order by construction. Taking the DEL equations on these Lagrangians obtains the relations

$$v_k^1 = \frac{q_k^1 - q_k^0}{h/2} \tag{22}$$

$$v_k^1 - v_k^2 + \frac{1}{2}\big(a\big(q_k^0, 0\big) - a\big(q_k^2, h\big)\big) - \cdots - \frac{1}{2}\nabla_{q_k^1}\big[\big(v_k^2 + v_k^1\big)\cdot a\big(q_k^1, h/2\big)\big]h - \nabla\varphi\big(q_k^1, h/2\big)h = 0 \tag{23}$$

$$v_k^2 = \frac{q_k^2 - q_k^1}{h/2} \tag{24}$$

Here, we note that $q_k^0 = q_k^1 - v_k^1 h/2$ and $q_k^2 = q_k^1 + v_k^2 h/2$, and by Taylor expanding the vector potential, we obtain that

$$\frac{1}{2}\big(a\big(q_k^0, 0\big) - a\big(q_k^2, h\big)\big) \approx -\frac{1}{2}\big[\big(v_k^1 + v_k^2\big)\cdot\nabla\big]a\big(q_k^1, h/2\big)h - \frac{\partial a}{\partial t}\big(q_k^1, h/2\big)h + \mathcal{O}\big(h^3\big) \tag{25}$$

The higher order terms are corrections at the precision of the Lagrangian integral, and therefore do not reduce the order of the integrator scheme. Furthermore, in most electromagnetic particle-in-cell codes, the fields are only second order accurate in the time step anyway. Thus, this approximation does not reduce the precision of the integrator.

By noting that $\nabla(v\cdot\vec{A}) - (v\cdot\nabla)\vec{A} = v\times\vec{B}$, and defining the normalized magnetic $\vec{b} = (e/mc)\vec{B}$ and electric $\vec{e} = (e/m)\vec{E}$ fields, the update sequence for an explicit magnetic Lagrangian is given by

$$q_k^1 = q_k^0 + v_k^1(h/2) \tag{26}$$

$$v_k^2 = v_k^1 + \left(\frac{1}{2}\big(v_k^1 + v_k^2\big)\times\vec{b}\big(q_k^1, t/2\big) + \vec{e}\big(q_k^1, t/2\big)\right)h \tag{27}$$

$$q_k^2 = q_k^1 + v_k^2(h/2) \tag{28}$$

This is equivalent to the update sequence proposed by Boris. This proves that the update derived by Boris in 1970 is, in fact, a symplectic integrator.

The reader may note that this Taylor expansion does not necessarily guarantee symplecticity – could it be possible that we have broken the symplectic two-form by taking an implicit algorithm and making it explicit? This is not the case, as we will now argue. The approximation made earlier may be used as a definition of the electric and magnetic fields, and in fact is invertible. That is to say, we could rewrite the Lagrangian in terms of the electric and magnetic fields to the same order of accuracy as the Lagrangian itself, and re-derive the equations of motion in terms of the fields instead of the potentials. We have included the forward case because it is constructive – it shows how the fields arise from the potentials in much the same way that they arise from the continuous Lagrangian.

Now we consider the relativistic Lagrangian

$$L(q, \dot{q}, t) = mc^2\sqrt{1 - \dot{q}^2/c^2} + \dot{q}\cdot\frac{e}{c}\vec{A}(q, t) - e\phi(q, t) \tag{29}$$

As with the nonrelativistic limit, we consider a split of the form

$$L_D^1\big(q_k^0, q_k^1, t\big) = -mc^2\frac{h}{2}\sqrt{1 - \left(\frac{q_k^1 - q_k^0}{h/2}/c\right)^2} + \cdots + \big(q_k^1 - q_k^0\big)\cdot\frac{1}{2}\big(\vec{a}\big(q_k^0, 0\big) + \vec{a}\big(q_k^1, h/2\big)\big) - \frac{h}{2}\varphi\big(q_k^1, h/2\big) \tag{30a}$$

$$L_D^2(q_k^1, q_k^2, t) = -mc^2 \frac{h}{2}\sqrt{1 - \left(\frac{q_k^2 - q_k^1}{h/2}/c\right)^2}$$
$$+ \cdots + (q_k^2 - q_k^1) \cdot \frac{1}{2}\left(\vec{a}(q_k^1, h/2) + \vec{a}(q_k^2, h)\right) - \frac{h}{2}\varphi(q_k^1, h/2) \tag{30b}$$

Employing the same minimization as in the previous section, we obtain the recursion relations

$$q_k^1 = q_k^0 + v_k^1(h/2) \tag{31}$$
$$\gamma_k^2 v_k^2 = \gamma_k^1 v_k^1 + \left(\frac{1}{2}(v_k^1 + v_k^2) \times \vec{b}(q_k^1, t/2) + \vec{e}(q_k^1, t/2)\right)h \tag{32}$$
$$q_k^2 = q_k^1 + v_k^2(h/2) \tag{33}$$

It is necessary to invert Eq. (32) for both v_k^2 and γ_k^2 to obtain the explicit update sequence. This is equivalent to the update method derived by J.-L. Vay [11], illustrating that the Vay integrator is also symplectic.

4. Two more integrators

An alternative second order Lagrangian is given by

$$L_D^1 = \frac{1}{2}\frac{(q_k^1 - q_k^0)^2}{h/2} + (q_k^1 - q_k^0) \cdot a(q_k^1) - \frac{h}{2}\varphi(q_k^1, h/2) \tag{34a}$$
$$L_D^2 = \frac{1}{2}\frac{(q_k^2 - q_k^1)^2}{h/2} + (q_k^2 - q_k^1) \cdot a(q_k^1) - \frac{h}{2}\varphi(q_k^1, h/2) \tag{34b}$$

Again, this is the concatenation of a discrete Lagrangian with its adjoint, and hence is second order. This gives the second order update sequence

$$q_k^1 = q_k^0 + v_k^1 \frac{h}{2} \tag{35a}$$
$$v_k^2 = v_k^1 + \frac{h}{2}\nabla\left[(v_k^1 + v_k^2) \cdot a(q_k^1)\right] - \nabla\varphi(q_k^1, h/2)h \tag{35b}$$
$$q_k^2 = q_k^1 + v_k^2 \frac{h}{2} \tag{35c}$$

This Lagrangian has the advantage of being second order and directly invertible, but cannot be rewritten in terms of the electric and magnetic fields. Because this may be directly inverted for v_k^2 in terms of a matrix inverse, without any sort of root solving, this algorithm can be made explicit through a matrix inversion. We will refer to this as the explicit midpoint integrator.

Another Lagrangian that is possible is the implicit midpoint Lagrangian

$$L_D(q_{k+1}, q_k, h) = \frac{1}{2}\frac{(q_{k+1} - q_k)^2}{h}$$
$$+ \cdots + (q_{k+1} - q_k) \cdot a\left(\frac{q_{k+1} + q_k}{2}, h/2\right) - h\varphi\left(\frac{q_{k+1} + q_k}{2}, h/2\right) \tag{36}$$

The resulting integration scheme, which is second order by virtue of being self-adjoint, is given by

$$q_k = q_{k-1} + v_k h \tag{37a}$$

$$v_{k+1} = v_k + a\left(\frac{q_k + q_{k-1}}{2}, -h/2\right) - a\left(\frac{q_{k+1} + q_k}{2}, h/2\right)$$
$$+ \cdots + h\nabla_{q_k}\left\{v_k \cdot a\left(\frac{q_k + q_{k-1}}{2}, -h/2\right) + v_{k+1} \cdot a\left(\frac{q_{k+1} + q_k}{2}, h/2\right)\right.$$
$$\left. + \cdots - \varphi\left(\frac{q_{k+1} + q_k}{2}, h/2\right) - \varphi\left(\frac{q_k + q_{k-1}}{2}, -h/2\right)\right\} \tag{37b}$$

$$q_{k+1} = q_k + v_{k+1} h \tag{37c}$$

where the implicit dependence on the coordinates can be replaced with velocity by substituting Eq. (37c) and Eq. (37a) into Eq. (37b). We will consider this update sequence further in the next section.

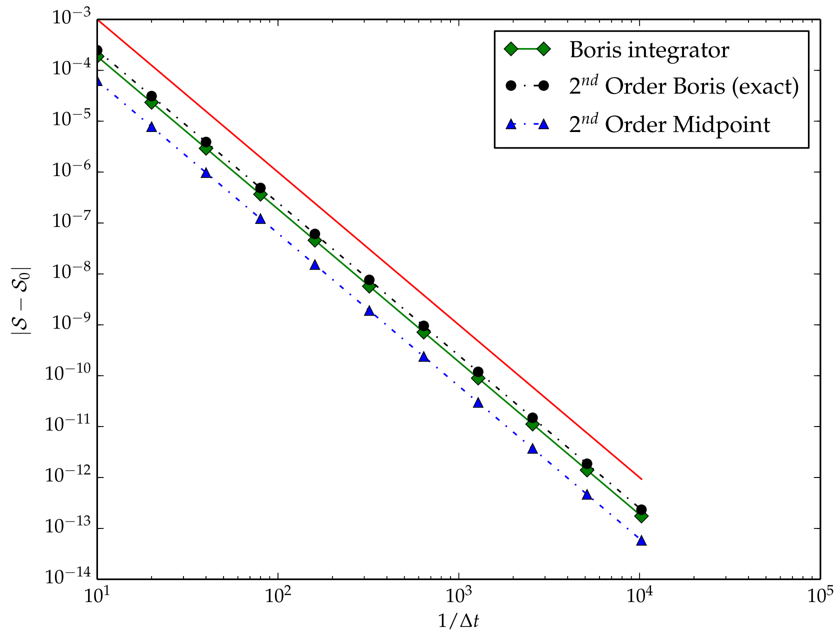

Fig. 1. A comparison of the order of convergence of the action integral for this system. The red line is Δt^{-3}. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

In Fig. 1 we consider the order of convergence of the action integral for a system with a constant magnetic field. As per Marsden and West [9], the order of an integrator is given by the order of the correction to the exact integral

$$\int_0^h L(\dot{q}, q, t)\,dt = \sum_i L_D^i\left(q_k^i, q_k^{i+1}, \gamma_i h\right) + \mathcal{O}\left(h^{n+1}\right) \tag{38}$$

for an order-n symplectic integrator.

In Fig. 1, we consider the order of three of the integration schemes: the Boris integrator, the exact Boris Lagrangian (action computed using the same Lagrangian), and the implicit midpoint. As is clear, all of the integrators are second order symplectic integrators which give comparable approximations to the action integral. The choice of integrator will depend upon the specific application.

For self-consistent electromagnetic algorithms, the Boris or Vay integrators have become a staple due to their nice stability properties. We have here shown that these properties derive from symplecticity, and furthermore that they may be used in parallel with solutions of the electric and magnetic fields directly. This has found application with, for example, solutions of Maxwell's equations using the curl equations on a staggered Yee mesh [12] with Esirkepov deposition [13].

Of the other two integrators, the explicit midpoint integrator does not promise any advantages over the Boris/Vay integrators. The implicit midpoint integrator, on the other hand, has the advantage of being unconditionally stable, and is immune to the ω_p–Δt instability described in, for example, Chapter 9 of [7]. One must weigh the implicit nature of this algorithm, along with the more intensive computational requirements, against the ability to take fewer time steps for a fixed period of time without loss of stability.

5. Conclusion

We have seen four second order symplectic integrators for systems with magnetic fields, and shown that the Boris and Vay integrators are symplectic. This assures us that the trajectories of the particles are exact solutions to a Hamiltonian which converges to the exact Hamiltonian as the time step vanishes, and by the KAM theorem and other associated results these results preserve most of the phase space structure of the original Hamiltonian.

The results presented in this paper apply purely to the particle motion, assuming the fields are known exactly everywhere and at all times. To obtain a totally stable self-consistent treatment of a plasma would also require that the field solve, whatever it may be, also be symplectic. This suggests a future course in obtaining electromagnetic particle-in-cell algorithms entirely from a discretized Lagrangian.

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References

[1] R.D. Ruth, A canonical integration technique, IEEE Trans. Nucl. Sci. NS-30 (4) (1983) 2669–2671.
[2] E. Forest, R.D. Ruth, Fourth-order symplectic integration, Physica D 43 (1) (1989) 105–117.
[3] H. Yoshida, Construction of higher order symplectic integrators, Phys. Lett. A 150 (5–7) (1990) 262–268.
[4] J.M. Sanz-Serna, Runge–Kutta schemes for Hamiltonian systems, BIT Numer. Math. 28 (4) (1988) 877–883.
[5] E. Forest, Geometric integration for particle accelerators, J. Phys. A, Math. Gen. 39 (2006) 5321–5377.
[6] J.P. Boris, Relativistic plasma simulation–optimization of a hybrid code, in: Proceeding of the Fourth Conference on Numerical Simulations of Plasmas, 1970.
[7] C.K. Birdsall, A.B. Langdon, Plasma Physics via Computer Simulation, McGraw-Hill, New York, 1985.
[8] R.W. Hockney, J.W. Eastwood, Computer Simulation Using Particles, Taylor & Francis, 1989.
[9] J.E. Marsden, M. West, Discrete mechanics and variational integrators, Acta Numer. 10 (2001) 357–514.
[10] L. Schulman, Techniques and Applications of Path Integration, Dover Publications, 2005.
[11] J.-L. Vay, Simulation of beams or plasmas crossing at relativistic velocity, Phys. Plasmas 15 (2008) 056701.
[12] K.S. Yee, Numerical solution of initial boundary value problems involving Maxwell's equations in isotropic media, IEEE Trans. Antennas Propag. 14 (3) (1966) 302–307.
[13] T. Esirkepov, Exact charge conservation scheme for Particle-in-Cell simulation with an arbitrary form-factor, Comput. Phys. Commun. 135 (2) (2001) 144–153.