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This paper was prepared for submittal to the
16th International Conference on the Numerical Simulation of Plasmas
Santa Barbara, CA
February 9-12, 1998

January 12, 1998

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Toward Higher Order Particle Simulation of Space-Charge-Dominated Beams*

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The intense particle beams to be used as drivers for Heavy Ion Inertial Fusion exhibit dynamics which are dominated by space-charge (abbreviated s-c) forces, rather than by thermal pressure (as in most traditional accelerator applications). Such beams are non-neutral plasmas, and the particle-in-cell technique (with the addition of detailed models for the externally applied fields and the domain geometry) has proven effective in their study.1-3 Typically, the applied focusing, bending, and accelerating fields vary rapidly with axial position, while the s-c fields (which are comparable in strength to the applied fields) vary smoothly; it is desirable to avoid using many steps to resolve the applied field variations while still computing accurate orbits. We are exploring high-order particle advance methods and other techniques to enhance the efficiency of these simulations. The earlier stages of this work 4 included initial studies of: sub-cycling of the particle advance relative to the field solution; higher-order time-advance algorithms; force-averaging by integration along approximate orbits; and orbit-averaging. In this paper we describe further progress: (1) development of prescriptions for “smooth” cutoffs of tabulated fringe-field data so as to preserve the convergence of a high-order advance, studied using the realistic-profile model problem described in [4]; (2) for a high order advance and the model problem, comparison of both “true” and “approximate” (old-data, non-symplectic) every-substep s-c force application to periodic (“operator-split”) s-c force application; and (3) 2-d PIC (WARPxy code) convergence studies of the Candy-Rozmus (C-R) explicit fourth-order symplectic integrator 5 using both “true” (every-substep) s-c and operator-split s-c, and of the leapfrog mover, modeling a transport line with sharp-edged fields.

Symplectic integrators preserve Hamiltonian structure and avoid spurious damping or excitation, but are not energy conserving 6. Defining position “x”, velocity “v”, and acceleration “a”, and letting “:=” denote assignment, the general nonrelativistic explicit algorithm for one timestep is:

\[ x := x + c_i \Delta t \; v; \quad v := v + d_i \Delta t \; a(x); \text{ repeated for substeps } i = 1, \ldots, k. \] (1)

The \( c_i \) and \( d_i \) are chosen so that the final composed mapping satisfies the Taylor series expansion of the solution up to order \( \Delta t^3 \), for an n-th order scheme. The Candy-Rozmus (C-R) scheme has the advantage of offering fourth-order accuracy with three force evaluations per step. The schemes of greatest current interest are:

**Leapfrog:**

\[ c_1 = 0, \quad c_2 = 1, \quad d_1 = d_2 = 1/2 \] (2)

**Candy & Rozmus:**

\[ c_1 = c_4 = 1/[2(2-21/3)], \quad c_2 = c_3 = [1-21/3]/[2(2-21/3)]; \quad d_1 = d_3 = 1/[2-21/3], \quad d_2 = -21/3/[2-21/3], \quad d_4 = 0 \] (3)

We have employed a model problem which captures much of the key physics of transport through a pair of permanent-magnet quadrupole lenses of alternating polarity, tracking a particle on the principal plane \( y = 0 \). (For algorithm development we actually employ an electric field of equivalent strength.) Linear fringe fields \((< x)\) are included, but higher multipoles and pseudo-multipoles are not included. Several models of the force profile as a function of the axial coordinate z are used in our studies [4]; here we concentrate on the effective use of tabulated data, in this case the output of an analytic calculation.

Our tabulated data is discontinuous at the ends of the record, at the 0.00188 level relative to the peak of unity, due to abrupt termination of the list of 300 tabulated values describing each quadrupole. Various prescriptions can be employed to handle the transition: (1) one can ignore the discontinuity; (2) one can subtract the last value from all the values of the record, then rescale the function to preserve either the value of the peak or the integral, yielding continuity of the function but not its derivatives; (3) one can multiply the data near the end of the record by a “fillet function”; and (4) one can append a smooth continuation of the function which matches on to zero, using e.g. cubic polynomials (this has the undesirable effect of lengthening the record and does not offer continuity of all derivatives). One attractive fillet function \( h(\eta) \) is:

\[ h(\eta) = \frac{1 - \tanh \text{ cot} kh(\eta)}{2} \] (4)

Here, \( \eta \) ranges from zero to one. One selects the set of abscissa points over which the transition is to occur, in our case the last \( n_f \) points of the record, and computes \( F_{\text{smoothed}} = h(\eta(i)) \; F_\text{true} \), where \( \eta(i) = (i-1)/n_f \) for \( i = 1, \ldots, n_f \). The function \( h \) has the desirable property that it approaches the ends of the unit interval with all derivatives zero, so that there is never a discontinuity in \( F_{\text{smoothed}} \) or any of its derivatives. It has the curious property that the left and right limits of \( h \) and any of its derivatives approaching zero from both above and below are equal, but it is formally undefined at zero, and no power series about zero can describe its behavior. Figure 1 shows the application of this function to our tabulated dataset using various values of \( n_f \). Figure 2 shows the model problem domain, including the force profile made up of two quadrupoles and the “drift” spaces between them (the test is carried out over a section of a periodically repeating system), as well as a typical trajectory. In these tests a simple linear variation of the space charge force is used.
In a PIC code with bilinear or trilinear interpolation (such as WARPxy or WARP3d), the pairwise interparticle force is continuous as a function of interparticle separation, but its derivative is “almost always” discontinuous [7], and we must determine empirically whether such multilinear interpolation is “smooth enough” in practice. As a test problem, we consider a simple transport lattice with hard-edged quadrupoles. The half-lattice period length is 50 cm, the quad occupancy factor is 50%, the boundary is a square metal pipe at ±3.2 cm, and a 64x64 grid represents one quadrant (two-axis symmetry is assumed). We initiate a space-charge-dominated beam with a semi-Gaussian distribution and semi-axes of 2.07 and 1.17 cm, using 20,000 particles. The undepressed “phase advance per lattice period” of the quasi-harmonic motion in the applied field is 73.8°, depressed to 15° by the space charge defocusing.

The timesteps in WARPxy were chosen to be “commensurate,” that is, such that quadrupole edges are always encountered at an integer number of steps; this effectively restarts the problem at each discontinuity, so that the high-order integrator is not reduced to first order. Tests were also carried out using the “residence correction” algorithm in WARP’s leapfrog mover using “non-commensurate” steps; that algorithm succeeds in preserving second order accuracy even when integrating over discontinuities, but it is not readily generalized to higher order.

Fig. 4. Results for WARPxy tests using sharp-edged applied fields (see text).
In addition to establishing smooth ends of the record, it is necessary to employ a smooth interpolant if the full fourth-order convergence of the C-R scheme is to be preserved; a cubic-spline is sufficient. Results from the model problem are shown in Figure 3, for two different force prescriptions: (a) linear interpolation into a table with the last value subtracted (option 2 above), and (b) cubic spline interpolation with 50-point fillet smoothing (option 3 above). The convergence of four integrators is compared: (A) standard leapfrog; (B) the Candy-Rozmus integrator, using the currently evaluated space charge force (i.e., based on the instantaneous \( x \)) at each substep of the cycle; (C) the Candy-Rozmus scheme, using the "old" value of the space charge (saved from the beginning of the cycle) at each substep; and (D) an operator-split variation of the Candy-Rozmus scheme, whereby a space-charge "half-kick" is applied at the beginning and at the end of the cycle, space charge being ignored during the substepping.

From the figure it can be seen that, on the model problem, the high order schemes offers significantly greater accuracy than leapfrog. The latter two schemes (C,D) require less computation in a particle code than the full scheme (B), but (as can be seen) are less accurate. The "saved space charge force" algorithm (C) is more accurate than the operator split scheme (D), but unlike that scheme it is not reversible, and hence not symplectic. The full scheme (B) requires about three times the computational effort per cycle of leapfrog, but for errors in the range of one part in \( 10^4 \) or better, a step size eight times larger can be employed, leading to a net gain of order 2.5. The gain may be even larger for the schemes (C,D) if very high accuracy is not required. We now proceed to describe our tests using the full 2-D particle code WARPxy.
Figure 4 shows the results of a series of WARPxy runs. Both the beam's rms width in x and the final position of a single particle are used as error measures. Symbols in a large font denote a positive error, those in a small font a negative error. In each case the reference result is obtained by use of the Candy-Rozmus integrator with a number of steps per lattice period twice the largest shown in the figure. At early time, e.g., \( 1/16 \) lattice period (not shown), the full C-R integrator yields clean fourth-order convergence of \( x_{\text{rms}} \) but not of individual particle orbits. At two periods, the fourth-order convergence is observed at large step sizes, but at the smallest step sizes small second-order errors (presumably from grid crossings) are evident. By 20 periods, convergence has degraded to second order, but the errors in \( x_{\text{rms}} \) and other moments are enough smaller than those of leapfrog that there is a net advantage to the C-R schemes. The error in \( x_{\text{rms}} \) is oscillatory with a period of about 3.5 lattice periods. These results suggest that, for bilinear interpolation, operator splitting may be a good choice.

Longer runs (out to 200 periods) show that, for this sharp-edged system, the C-R integrator retains a fourfold advantage out to \( \sim 50 \) periods in accuracy of moments, but ultimately does no better than leapfrog (and is more expensive). We find that the error in an orbit (as measured by comparing leapfrog runs using 256 and 512 leapfrog steps per lattice period) increases nonuniformly but roughly exponentially. This appears to be the divergence of neighboring orbits in a chaotic system. Roundoff differences are enough of an initial separation to trigger the effect, though a truncation error can give a larger seed. Those orbits visibly diverge after about 20 l.p.'s on a linear scale, but are in fact diverging from the beginning. We conjecture that use of higher precision may afford convergence of the individual orbits for a somewhat longer time.

The moments remain well-behaved after 200 lattice periods, in the sense that e.g. the emittance growth rate seems roughly invariant (though the curves don't overlay), even with 32 steps per period. We conjecture that this is because, when the particles deviate from their "ideal" orbits, they simply move onto a neighboring orbit, which they might just as well have been initialized onto at the start, if the integrator were perfect and there were no roundoff. Note that this WARPxy problem does not fully exploit the high order integrator, which may also aid in capturing extended fringe field effects using a minimal number of steps (as in the model problem above). To obtain true fourth-order accuracy, a smooth, higher-order spatial interpolant (particle shape) could be used, incurring an increased cost of the gather/scatter steps. Since use of a finer grid would be undesirable in 3-D, one should probably avoid enlarging the effective particle size, perhaps by using "sharpening" operators to offset any spreading. [8] Of course, discrete particle effects (such as artificial collisionality) also introduce errors, and one must be realistic about the accuracy that is ultimately achievable in any particular application. The usual validations (varying timestep size, zoning, and number of particles) remain essential.

* Work performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under contract W-7405-ENG-48 and by the Naval Research laboratory under contracts DE-AI02-93ER40799 and DE-AI02-94ER54232.


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