A POSTERIORI ERROR ESTIMATION FOR SIMULATIONS OF CHARGED PARTICLE BEAMS

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Abstract

An exact invariant I has been shown to exist for general three-dimensional Hamiltonian systems of N particles confined within a general velocity-independent potential. Since the invariant depends on the explicitly known trajectories of the particle ensemble, it can only be obtained *after* the solutions of the equations of motion have been calculated. If the time evolution of the particle ensemble is obtained from a computer simulation, the invariant can no longer be expected to be strictly constant because of the generally limited accuracy of numerical methods. The deviation of a numerically obtained "invariant" from a strict constant of motion may thus be used as *a posteriori* error estimation for the respective simulation.

1 EXPLICITLY TIME-DEPENDENT HAMILTONIANS

We consider a system of a non-relativistic ensemble of N particles of the same species moving in an explicitly time-dependent potential, whose Hamiltonian H takes the form

$$H = \sum_{i=1}^{N} \left[\tfrac{1}{2}\dot{x}_i^2 + \tfrac{1}{2}\dot{y}_i^2 + \tfrac{1}{2}\dot{z}_i^2 \right] + V(\vec{x}, \vec{y}, \vec{z}, t) \,, \qquad (1)$$

with $\vec{x}$, $\vec{y}$, and $\vec{z}$ the N component vectors of the spatial coordinates of all particles. From the canonical equations, we derive for each particle i the equation of motion

$$\ddot{x}_i + \frac{\partial V(\vec{x}, \vec{y}, \vec{z}, t)}{\partial x_i} = 0 \,, \qquad (2)$$

and likewise for the y and z degree of freedom. The functions $x_i(t)$ and $\dot{x}_i(t)$ denote the i-th particle trajectory in the x-direction and its time derivative that follow from the integration of the equation of motion (2). A quantity

$$I = I\left(\vec{x}(t), \dot{\vec{x}}(t), \vec{y}(t), \dot{\vec{y}}(t), \vec{z}(t), \dot{\vec{z}}(t), t \right) \qquad (3)$$

constitutes an invariant of the particle motion if its total time derivative vanishes, i.e. if $dI/dt = 0$ along the phase-space path representing the system's time evolution.

2 THE INVARIANT

The invariant I as defined by (3) for the Hamiltonian (1) follows as [1]

$$I = 2f_2(t)\, H - \dot{f}_2(t) \sum_{i=1}^{N} \left(x_i \dot{x}_i + y_i \dot{y}_i + z_i \dot{z}_i \right) + \ddot{f}_2(t) \sum_{i=1}^{N} \tfrac{1}{2}\left(x_i^2 + y_i^2 + z_i^2 \right) , \qquad (4)$$

with $f_2(t)$ representing a solution of

$$\dot{f}_2(t) \left(2V + \sum_{i=1}^{N} \left[x_i \frac{\partial V}{\partial x_i} + y_i \frac{\partial V}{\partial y_i} + z_i \frac{\partial V}{\partial z_i} \right] \right) + 2f_2(t)\, \frac{\partial V}{\partial t} + \dddot{f}_2(t) \sum_{i=1}^{N} \tfrac{1}{2}\left(x_i^2 + y_i^2 + z_i^2 \right) = 0 \,. \qquad (5)$$

The domain of (3), and hence the physical significance of the subsequent equation (5), is restricted to the actual phase-space path, defined as the one-parameter subset of the $6N$-dimensional phase-space on which the equations of motion (2) are fulfilled.

Along the phase-space path, all terms of Eq. (5) that depend on the particle trajectories are in fact functions of the parameter time t only. Accordingly, the potential $V(\vec{x}(t), \vec{y}(t), \vec{z}(t), t)$ and its derivatives are time-dependent coefficients of an ordinary differential equation for $f_2(t)$. The invariant (4) is easily shown to provide a time integral of Eq. (5) by calculating the total time derivative of (4), and inserting the single particle equations of motion (2). Hence, Eq. (4) embodies a time integral of Eq. (5) if and only if the system's evolution is *strictly* consistent with the equations of motion (2).

3 EXAMPLE

As a simple example, we investigate the one-dimensional Hamiltonian system of an "asymmetric spring", defined by

$$H = \tfrac{1}{2}\dot{x}^2 + \tfrac{1}{2}\omega^2(t)\, x^2 + a(t)\, x^3 \,. \qquad (6)$$

The related equation of motion follows as

$$\ddot{x} + \omega^2(t)\, x + 3a(t)\, x^2 = 0 \,. \qquad (7)$$

The invariant I is immediately found writing down the general invariant (4) for one dimension and one particle with the Hamiltonian H given by (6)

$$I = f_2 \left(\dot{x}^2 + \omega^2 x^2 + 2ax^3 \right) - \dot{f}_2 x \dot{x} + \tfrac{1}{2}\ddot{f}_2 x^2 \,. \qquad (8)$$

According to (5), the function $f_2(t)$ for this particular case is given as a solution of the third order differential equation

$$\dddot{f}_2 + 4\dot{f}_2\omega^2 + 4f_2\omega\dot{\omega} + x(t)\left(4f_2\dot{a} + 10\dot{f}_2 a \right) = 0 \,. \qquad (9)$$

Since the particle trajectory $x = x(t)$ is explicitly contained in Eq. (9), we must know it prior to integrating Eq. (9). The trajectory is obtained integrating the equation of motion (7).

In order to prove that Eq. (8) is indeed an invariant of the particle motion, we may calculate the total time derivative of Eq. (8). Inserting the equation of motion (7), we end up with Eq. (9), which is fulfilled by definition of $f_2(t)$ along the given trajectory $x = x(t)$.

Substituting $\rho_x^2(t) \equiv f_2(t)$, Eq. (9) may be converted into the alternative form of an "envelope equation"

$$\ddot{\rho}_x(t) + \omega^2(t)\rho_x(t) - \frac{g_x(t)}{\rho_x^3} = 0\,. \qquad (10)$$

Eq. (10) is equivalent to (9), provided that the time derivative of the function $g_x(t)$, introduced in (10), is given by

$$\dot{g}_x(t) = -x(t)\left(2\dot{a}\rho_x^4 + 10a\rho_x^3\dot{\rho}_x\right)\,. \qquad (11)$$

Expressing the invariant (8) in terms of $\rho_x(t)$, and inserting the auxiliary equation (10), we get

$$I = \rho_x^2\dot{x}^2 - 2\rho_x\dot{\rho}_x x\dot{x} + x^2\left(\dot{\rho}_x^2 + \frac{g_x(t)}{\rho_x^2}\right) + 2a(t)\rho_x^2 x^3\,. \qquad (12)$$

With regard to the definition of $g_x(t)$ given by Eq. (11), we observe that the invariant (12) reduces to the well-known Lewis invariant [2] for the time-dependent harmonic oscillator if $a(t) \equiv 0$, which means that $g_x(t) = \mathrm{const.}$

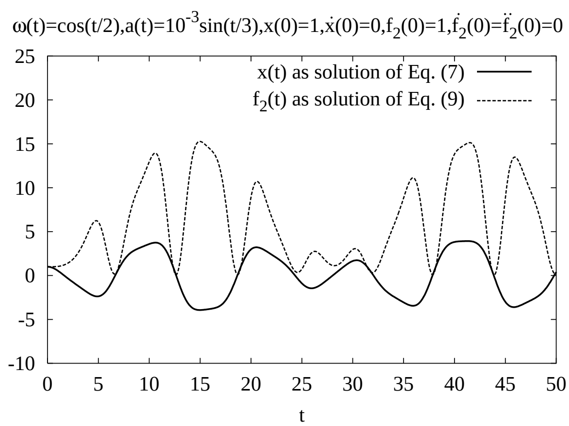

Figure 1: Example of a numerical integration of Eq. (7) and the subsequent numerical integration of Eq. (9).

Fig. 1 shows a special case of a numerical integration of the equation of motion (7). Included in this figure, we see the result of a subsequent numerical integration of Eq. (9). Knowing both results, we are able to calculate the invariant I given by Eq. (8), or, equivalently, by Eq. (12). Fig. 2 displays the relative deviation of the numerically obtained invariant I from an exact invariant, thereby providing a measure for the accuracy of the numerical method.

4 SYSTEM OF COULOMB INTERACTING PARTICLES

A more challenging example is defined by an ensemble of N Coulomb interacting particles of the same species moving in a time-dependent quadratic external potential, as typically given in the co-moving frame for charged particle

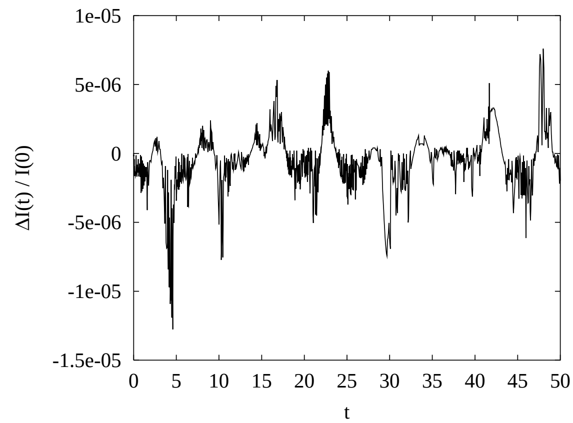

Figure 2: Relative deviation of the numerically calculated invariant (12) from the exact invariant $I(0)$.

beams that propagate through linear external focusing devices. The potential function V of this system is given by

$$V(\vec{x},\vec{y},\vec{z},t) = \sum_{i=1}^{N}\Big[\tfrac{1}{2}\omega_x^2(t)\,x_i^2 + \tfrac{1}{2}\omega_y^2(t)\,y_i^2 + \tfrac{1}{2}\omega_z^2(t)\,z_i^2 + \tfrac{1}{2}\sum_{j\neq i}\frac{c_1}{r_{ij}}\Big]\,, \qquad (13)$$

with $r_{ij}^2 = (x_i - x_j)^2 + (y_i - y_j)^2 + (z_i - z_j)^2$ and $c_1 = q^2/4\pi\epsilon_0 m$, q and m denoting the particles' charge and mass, respectively. The equations of motion that follow from (2) with (13) are

$$\ddot{x}_i + \omega_x^2(t)\,x_i - c_1\sum_{j\neq i}\frac{x_i - x_j}{r_{ij}^3} = 0\,, \qquad (14)$$

and likewise for the y and z degrees of freedom. We note that the factor $1/2$ in front of the Coulomb interaction term in (13) disappears since each term occurs twice in the symmetric form of the double sum.

With the effective potential (13), Eq. (5) specializes to

$$\begin{aligned}&\langle x^2\rangle\left(\dddot{f}_2 + 4\dot{f}_2\omega_x^2 + 4f_2\omega_x\dot{\omega}_x\right) + \\ &\langle y^2\rangle\left(\dddot{f}_2 + 4\dot{f}_2\omega_y^2 + 4f_2\omega_y\dot{\omega}_y\right) + \\ &\langle z^2\rangle\left(\dddot{f}_2 + 4\dot{f}_2\omega_z^2 + 4f_2\omega_z\dot{\omega}_z\right) + \frac{2W(t)}{mN}\dot{f}_2 = 0\,. \qquad (15)\end{aligned}$$

Herein, the sums over the particle coordinates are written in terms of "second beam moments", denoted as $\langle x^2\rangle$ for the x-direction. Furthermore, $W(t)$ stands for the electrostatic field energy constituted by all particles

$$\langle x^2\rangle(t) = \frac{1}{N}\sum_i x_i^2(t)\,, \qquad W(t) = \frac{m}{2}\sum_i\sum_{j\neq i}\frac{c_1}{r_{ij}}\,.$$

The invariant I for this system is given by (4), provided that $f_2(t)$ is a solution of (15). Again, we may directly prove that Eq. (4) with (1) and (13) is a time integral of Eq. (15)

by calculating the total time derivative of (4) and inserting the single particle equations of motion Eq. (14).

Substituting $\rho^2(t) \equiv f_2(t)$ and defining the function $g(t)$ according to

$$g(t) = \langle x^2 \rangle \rho^3 \left(\ddot\rho + \omega_x^2(t)\rho\right) + \langle y^2 \rangle \rho^3 \left(\ddot\rho + \omega_y^2(t)\rho\right) + \langle z^2 \rangle \rho^3 \left(\ddot\rho + \omega_z^2(t)\rho\right) \,, \tag{16}$$

the third order equation (15) can be transformed into an equivalent system of a first and a second order equation for $\rho(t)$, thereby eliminating the derivatives $\dot\omega_{x,y,z}(t)$ of the lattice functions. Similar to the previous example, solving (16) for $\ddot\rho(t)$ means to express it in the form of an "envelope equation"

$$\ddot\rho + \omega^2(t)\,\rho - \frac{g(t)}{\rho^3\left(\langle x^2\rangle + \langle y^2\rangle + \langle z^2\rangle\right)} = 0\,, \tag{17}$$

with the "average focusing function" $\omega^2(t)$ defined as

$$\omega^2(t) = \frac{\omega_x^2 \langle x^2\rangle + \omega_y^2 \langle y^2\rangle + \omega_z^2 \langle z^2\rangle}{\langle x^2\rangle + \langle y^2\rangle + \langle z^2\rangle}\,.$$

It may easily be shown that Eq. (17) is equivalent to (15) if the time derivative of $g(t)$ satisfies

$$\dot g(t) = 2\rho^3 \Bigg(\langle x\dot x\rangle \left(\ddot\rho + \omega_x^2\rho\right) + \langle y\dot y\rangle \left(\ddot\rho + \omega_y^2\rho\right) + \langle z\dot z\rangle \left(\ddot\rho + \omega_z^2\rho\right) - \frac{W}{mN}\dot\rho \Bigg)\,. \tag{18}$$

We may apply these findings to test the results of a numerical simulation of a system governed by (14). As stated above, Eq. (4) embodies a time integral of (15) — or equivalently a time integral of the set (17) and (18) — if the system's time evolution is *strictly* consistent with the equations of motion (14). On the other hand, a strict consistency can never be accomplished if the evolution of the particle ensemble is obtained from a computer simulation. Under these circumstances, the quantity I as given by Eq. (4) — with $f_2(t)$, $\dot f_2(t)$, and $\ddot f_2(t)$ following from (15) — can no longer be expected to be exactly constant.

Fig. 3 displays the function $f_2(t)$ resulting from a numerical integration of Eq. (15). Its coefficients $\langle x^2\rangle$, $\langle y^2\rangle$, $\langle z^2\rangle$, and $W(t)$ have been calculated from a three-dimensional simulation of a charged particle beam propagating through an isotropic periodic focusing lattice with non-negligible Coulomb interaction, as described by the potential function (13). Fig. 4 displays the relative deviation of the numerically obtained invariant I from an exact invariant for our simulation. We observe that the main deviations from $I = \mathrm{const.}$ take place at the edges of the focusing lenses. The horizontal sections of the function $\Delta I(t)/I(0)$ — occurring along the drift spaces — indicate that the field-free regions do not significantly contribute to the overall error of our simulation.

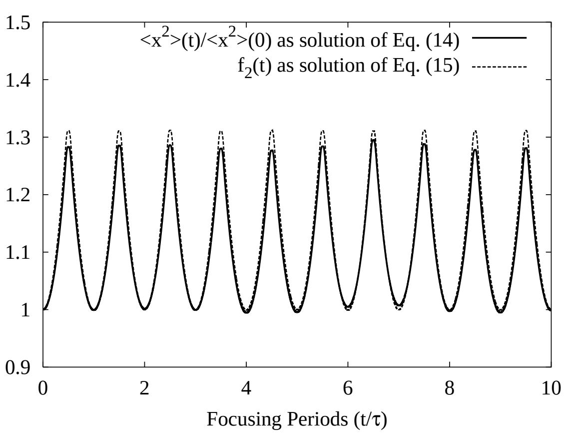

Figure 3: Second beam moment $\langle x^2\rangle$ and f_2 versus time as obtained for 2500 simulation particles in a 3D simulation of an isotropic periodic focusing lattice with strong Coulomb interaction. τ denotes the focusing period common to all three directions.

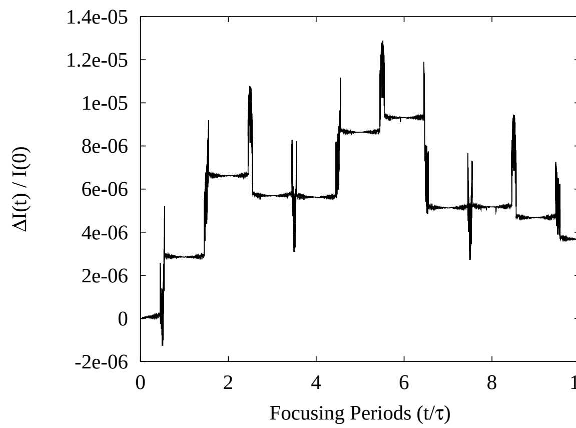

Figure 4: Relative deviation of the numerically calculated invariant (4) from the exact invariant $I(0)$ for the simulation of Fig. 3.

5 CONCLUSIONS

For the special case of a potential $V(\vec x, \vec y, \vec z)$ that is independent of time explicitly, the Hamiltonian (1) yields the system's total energy E. The invariant I then reduces to $I \propto H \equiv E$. For these systems, the time evolution of E is commonly used as accuracy test, which means to check inasmuch the energy is actually conserved in the simulation. On the basis of the general form of Eqs. (5) and (4), this accuracy test may be performed as well for explicitly time-dependent Hamiltonian systems.

REFERENCES

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[2] H. R. Lewis, Phys. Rev. Lett. **18**, 510 (1967); J. Math. Phys. **9**, 1976–1986 (1968).