A MULTI-PARTICLE REGULARISATION TECHNIQUE*

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Abstract. Certain features of a practical regularisation method, in which the potential or kinetic energy is used as a time-regularising function, are described. For two-body encounters the method is less powerful than Kustaanheimo-Stiefel regularisation, but it has wider applicability.

1. Early experience of N-body computations by many workers made clear the need for an efficient (i.e. rapid and accurate) method of treating close two-body encounters and, in particular, stable binaries. Two methods, both based on a description of such events as perturbed two-body motion, have been proposed and used: the 'binary method' of Aarseth (1970), and Kustaanheimo-Stiefel regularisation, described by Peters (1968). In practice, the binary method is unsatisfactory for moderate or heavy perturbations, and regularisation is inefficient at dealing with relatively stable three-body configurations, where the choice of the pair of particles whose relative motion is to be regularised requires repeated alteration. It is therefore desirable to devise an efficient means of treating such cases, and one possible method is the subject of this paper. Although it is not suggested that the method be used for straightforward two-body encounters, for which powerful techniques already exist, this is nevertheless the simplest situation in which to examine its properties.

In the K.-S. regularisation method, in which both time and position are transformed, the unperturbed relative motion of two point masses is described by the equations

$$u_k'' = \frac{h}{2\mu} u_k \qquad (k = 1, 2, 3, 4) \tag{1}$$

where $\mathbf{u}$ is the 4-vector of transformed coordinates, h is the total energy, μ is the reduced mass, and a prime denotes differentiation with respect to regularised time. Suppose, however, that only the time transformation is performed, that is, we define the regularised time, s, by the differential equation

$$ds = g(\mathbf{x}, \dot{\mathbf{x}})\, dt$$

where g is some well-behaved function of $\mathbf{x}$, the relative position vector, and of $\dot{\mathbf{x}}$, its derivative with respect to physical time t. Then if m_i $(i = 1, 2)$ are the masses of the two particles, and we write $r \equiv |\mathbf{x}|$, the normal Newtonian equations

$$\ddot{x}_k = -(m_1 + m_2)\, x_k r^{-3} \qquad (k = 1, 2, 3) \tag{2}$$

become

$$g^2 x_k'' + g^{-1} \dot{g} \dot{x}_k = F_{ck} \qquad (k = 1, 2, 3)$$

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where F_{ck} is the right hand side of (2). Choosing $g(\mathbf{x}, \dot{\mathbf{x}}) = r^{-1}$, this equation may be written as

$$x_k'' = r^2 F_{ck} + r\dot{r}\dot{x}_k \qquad (k = 1, 2, 3). \tag{3}$$

It is this equation which will be generalised to the N-body problem ($N \geqslant 3$), but in order to study its properties, it is convenient to write it in the form

$$x_k'' = -(m_1 + m_2)\, x_k r^{-1} + r\dot{r}\dot{x}_k - \dot{\mathbf{x}}^2 x_k + \\ + 2x_k \left(\frac{h}{\mu} + \frac{m_1 + m_2}{r} \right) \qquad (k = 1, 2, 3)$$

where, as before,

$$h \equiv \tfrac{1}{2}\mu \dot{\mathbf{x}}^2 - \frac{m_1 m_2}{r}.$$

Hence

$$x_k'' = \frac{2h}{\mu} x_k + C_k \qquad (k = 1, 2, 3) \tag{4}$$

where

$$\mathbf{C} \equiv (m_1 + m_2)\, \mathbf{x} r^{-1} + \dot{\mathbf{x}} \times (\dot{\mathbf{x}} \times \mathbf{x}).$$

With the aid of (2) it is easy to show that $\mathbf{C}$ is a constant vector, which, incidentally, is directed along the line of apsides. It is of interest to note that, since (4) may be readily generalised to the case of perturbed two-body motion and the first derivatives of $\mathbf{C}$ and h are regular at $r = 0$, these equations could be used in a two-body regularisation method; however, that is not the subject of this paper. Comparison of (4) with (1) shows that, when the coordinate transformation is performed, the period of the motion (in case $h < 0$) is doubled. Therefore, we may expect that, to achieve a certain accuracy in a numerical integration, twice as many steps per physical orbit are needed to integrate (3) as to integrate (1). That (3) is nevertheless generally more efficient than the ordinary equations (2), can be appreciated in the following way. Suppose one uses a time-step criterion based on the rate of convergence of the Taylor series for the velocity, such as

$$(\Delta t)^2 = \eta^2 \frac{\eta |\dot{\mathbf{x}}| + \Delta t |\ddot{\mathbf{x}}|}{\eta |\mathbf{x}| + \Delta t |\mathbf{x}^{\mathrm{IV}}|}$$

and the analogue for Δs, the regularised time-step for integrating (3). In this expression, which is a modification of that used by Aarseth (1968), η is an adjustable constant. Then at pericentre one finds the approximate result

$$\left(\frac{\Delta t_3}{\Delta t_2} \right)^2 = \frac{2a}{r} \tag{5}$$

where a is the semi-major axis, and subscripts refer to the above numbering of the equations; one sees that, for close encounters, a much larger timestep can be taken for system (3) than for system (2). In practice the advantage gained is not as great as this, for reasons that will appear later.

2. In general, a close 2-body encounter in an N-body problem ($N \geqslant 3$) can be treated similarly if the total potential energy, V, is used as the regularising function, for V is dominated by any two-body encounter. The regularised force per unit mass on any particle is

$$F_k = V^{-1}(V^{-1}F_{ck} - V'x_k') \qquad (k = 1, 2, 3) \tag{6}$$

where F_{ck} is the corresponding Newtonian force. This system of equations is unsatisfactory for two reasons:

(i) A close encounter between two bodies reduces the time step for all bodies, because of the second term in the expression for the force. This is very inefficient for large N.

(ii) The calculation of V, involving about $\frac{1}{2}N^2$ full precision distance calculations per step, is very time-consuming. It could be calculated from the regularised kinetic energy, T, and the total energy, H, by the relation

$$V^2T - V - H = 0.$$

However this procedure is very inaccurate, because (Figure 1) $(\mathrm{d}T/\mathrm{d}V) = 0$ at $V = -2H$, i.e. when the virial ratio is unity. In most practical cases, V soon tends to fluctuate about this value, and then it is ill-determined by T.

The second objection can be met by using as regularising function the kinetic energy

$$\mathscr{T} \equiv \tfrac{1}{2}\sum_{i=1}^{N} m_i\dot{\mathbf{x}}_i^2.$$

Because of the presence of the term in $\mathscr{T}'$ in the regularised force, $\mathbf{F}$ must be known for every particle at each time-step. An explicit calculation is too expensive if individual

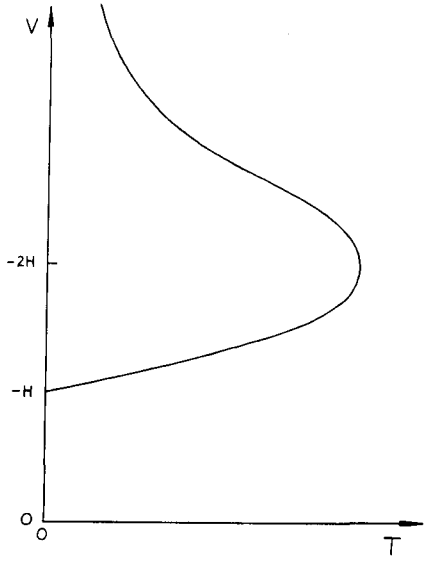

Fig. 1. The relation between V and T for $H < 0$, where T is the V-regularised kinetic energy.

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time-steps are taken by each particle, and one can show that the method is unstable if **F** is extrapolated from previous, explicitly calculated values. It is therefore expedient to use the same time-step for each particle, which reinforces the first objection above.

One may meet the first objection by taking as regularising function the kinetic energy, $\mathscr{T}^*$, of a small number N_{reg} of the particles, where $N_{reg} \ll N$. In practice one selects those involved in binaries or in encounters, so that very often $N_{reg}=0$ or 2; and one's choice is reviewed from time to time. Then one still uses the unregularised equations, and individual time-steps, for all other particles. For the 'regularised' particles, analogues of (6) are used, with a common time-step: this is not inefficient if N_{reg} is small, and indeed the efficiency may be improved, because several parts of a time-step calculation are shared between all such particles. At this stage there is little to choose between $\mathscr{T}^*$ and V^* as regularising functions, and in the remainder of the paper the former is referred to.

3. It remains to point out a number of features of the equations which become apparent in practical application. Here reference is made to computations carried out on the Institute's IBM 360/44, in which variables are normally carried to a standard precision of about six significant decimal digits; for very accurate work, a facility exists whereby the precision may be extended to up to about sixteen digits.

Consider an isolated binary system. Suppressing the asterisks, we have

$$\mathbf{x}_i'' = T\,(T\mathbf{F}_{ci} - \mathscr{T}'\mathbf{x}_i') \qquad (i = 1, 2) \tag{7}$$

where $T\mathscr{T}=1$. Weighting each equation by the corresponding mass and adding, one obtains, for the motion of the centre of mass, the equation

$$\bar{\mathbf{x}}'' = -\,T\mathscr{T}'\bar{\mathbf{x}}'$$

which is unstable if $\mathscr{T}'<0$, i.e. after pericentre. In practice this instability is not serious.

It is usually sufficient to compute and carry the force in standard precision, and so it is subject to considerable rounding error which may sometimes feed back into the force via T, the regularised kinetic energy. This cannot be obviated by reducing the steplength if the rounding error in the force has non-zero expectation, which is the case with those computers in which conversion from extended to normal precision is effected by truncation rather than by rounding. Equations (7) are not easy to discuss, but the one-dimensional analogue of the equation of relative motion of the two bodies reduces, in case $m_1=m_2=2$, to

$$x'' = (x')^4 x^{-2}\,(1 + \varepsilon f(s))$$

which will be adopted as a model of the system (7). Here, $\varepsilon f(s)$ is the rounding error, so that $f(s)=\mathrm{O}(1)$ as $\varepsilon \downarrow 0$; in practice $\varepsilon \approx 10^{-6}$.

Using ε as expansion parameter we find, for $\varepsilon \downarrow 0$, the particular asymptotic solution

$$x \sim x_0 + \varepsilon x_1$$

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where

$$x_0 \equiv \tfrac{1}{8}s^2$$

and

$$x_1 \equiv -\tfrac{1}{12}s\int_{s_0}^{s} f(v)\,dv + \tfrac{1}{12}s^4\int_{s_0}^{s} v^{-3}f(v)\,dv$$

if $x_1(s_0)=x_1'(s_0)=0$; $s_0<s<0$ during the approach to encounter. If a stepwise integration procedure is used, these integrals must be replaced by sums, and one finds that, as $s\uparrow 0$ (i.e. for very close encounters), the first term of x_1 dominates. If the expectation of f vanishes, this term is $O(s\sqrt{\Delta s})$ as $s\uparrow 0$, where Δs is the steplength, and if the expectation of f is non-zero it is $O(s)$; in this case, the relative error is of order $\varepsilon|x|^{-1/2}$. Experience confirms the presence, during particularly close encounters, of an instability that cannot be removed by a reduction in steplength; it can be obviated by reducing ε (e.g. by calculating the force in extended precision), and little inefficiency is introduced as this procedure is required only in rather exceptional cases. It is probable that this instability would be less serious in a computer with a more accurate standard precision. Rounding error can still be introduced in the higher terms of the integration scheme, but may be controlled by a modest reduction of steplength. Because of velocity-dependent terms in the force, significant truncation error in the velocity must be avoided, by the same reduction in the time-step. It is for reasons such as these that Equation (5) overestimates the efficiency of the method.

A computer program, constructed on these principles, has been written in FORTRAN IV and applied to some standard problems. For example, the IAU 25-body problem (Lecar, 1968) has been integrated to $t=10$ in 16 min, the energy decrement being only 8×10^{-7}, although this results from the fortuitous near-cancellation of two decrements of 3×10^{-6}. Even so, the test compares very well with all those discussed by Lecar. In two integrations of comparable accuracy up to $t=5$, respectively with and without regularisation, it was found that regularisation effects a reduction in computing time of about 50%.

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