Solving Many Point Particle Interactions Using the Kepler Route

Riadh H. Al Rabeh
College of Engineering, University of Basra, Iraq
Present address: Lydgate Close, Manningtree, Essex, UK. E-mail: alrabeh_rh@yahoo.com

Events in nature can be described using fields and their associated partial differential equations, or equivalently, the mechanics of interaction of point particles described by ordinary differential equations. The field approach can be looked at as the statistical average of the particle approach and in this sense is more economical for computing. The particle approach, on the other hand, is more fundamental but requires enormous computing power as the model has to follow the movements of every individual particle in the interaction. The present work aims at reducing such computing task by solving the problem of many particle interactions (under a central force environment) in an analytical form for one pair of particles using a Kepler type formula- giving the position of the particle as a function of time only. The resulting (analytical) formula is then used to write the result of the many-particle interaction using simple vector superposition. This approach takes less computing time and can give greater numerical stability when the distances between the particles become small and the force grows as the inverse square of the separation distance.

1 Introduction

The problems of physics can be equally described using interacting particles or fields. The flow of fluids, for example, is the result of basic interactions of an enormous number of small particles moving under an inverse square force system. Such processes can be described correctly using force fields that lead to PDE's like those for fluid mechanics and electrodynamics of material media. It is also possible to achieve a description of the same phenomena using interacting particles following what truly happens in the real world. In the present approach, all particles are assumed identical point masses that may carry charges too. The particles interact under a central force environment in which only the separation distance is of any significance. The coupling constants of such interactions can correspond to any of the known forces of nature — gravitation, electrostatic, or any other similarly behaving force. The resultant coupling constant is simply the arithmetic sum of such constants for all the component forces, with a negative sign to distinguish attractive forces from repulsive forces. The numerical values of the individual constants determine the relative strength of each force. In the most basic interaction involving say a doublet of two oppositely charged point masses, the Coulomb force is the most dominant. When very large groups of particles are considered, magnetic, and gravitational forces start becoming more significant.

By using the particle approach, it is possible to do away with the need for closure models (constitutive equations) that describe the properties of matter - such as the elasticity constants in dynamics and the permittivity and permeability of electrodynamics. In fact, one can use the particle interaction model to derive or check the validity of such closure models. The real difficulty with the particle approach is the computing burden which involves solving one ODE corresponding to every single particle in the interaction. We try to address this problem here by performing an initial integration of the ODE, then using vector superposition find the answer of the original many particle interaction problems. In addition to the obvious gain in computing time, the stability of the solution can be enhanced as the singularity is shifted from Inverse Square to simple Inverse of the separation distance. The accumulation error also reduces as a result in long time predictions.

Predicting the behavior of a single particle is well known- as in calculating the position of the landing of a projectile before it is fired for example. The same can be said, at least in principle, for predicting the behavior of multi-point interactions. The equation of motion tells us that once we fix the initial states of position and velocity of every participating point particle, the outcome is determined. The normal way to solve such problems is to find the velocity of each particle from the acceleration by integration (after superposition of all forces) then do a second integration to find the new position and this is to be performed over a large set of simultaneous Ode's since every particle effects every other. In the present work we instead calculate (analytically) the velocity and position in terms of time only for every particle then use vector superposition to find the final picture.

As we are dealing with point particles only, moments of forces and angular momentum and spin are not considered. The gain is an enhanced stability and reduced computing time coming from the fact that we integrate analytically first then use superposition (simple algebraic operation) for displacement as opposed to affecting the superposition of forces first then integrating for the displacement for every point particle. The method can be described as a multi-particle generalization of the Kepler method originally put (and still in use) for the motion of planets.

2 Theory

In an inverse square interaction (electrostatic/gravitational) of point masses, the expression for the force (acceleration since mass is unity) of a pair of such point masses is given by

$$a = \frac{d^2r}{dt^2} = \frac{k}{r^2}\,, \tag{1}$$

where $a = a(t)$, $r = r(t)$ are the acceleration and separation distances between an isolated pair of particles as a function of time t, and k is the coupling constant (negative for attractive and positive for repulsive forces). The magnitude of k is dependent on the type of interaction and equals the sum of the k's of all the forces at play. For example, in the case of repulsive Coulomb forces $k = \frac{1}{4}\pi\epsilon_0$ and for gravitational forces $k = -G$, where ϵ_0 is the permittivity of empty space and G is the universal gravitational constant. For a small number of interacting particles, the Coulomb forces by far dominate all other forces. All charges and masses of all particles are assumed unity as given above. The actual values can be incorporated in the coupling constant. As the interacting masses are points, there is no need to consider angular velocity, spin, angular momentum or any form of moments of forces on the particle. Mass can simply be taken as the number of particles in any setup.

For a group of interacting particles, the net acceleration of particle j is given by

$$\left.\begin{aligned} a_j &= \frac{dv_j}{dt} = \sum_i \frac{k_{ij}\, r_{ij}}{r_{ij}^3} \\ r_{ij} &= |r_{ij}|\,, \qquad i, j = 1, 2, \ldots N \end{aligned}\right\}, \tag{2}$$

where a_j is the resultant acceleration, v is velocity, k_{ij} is the total coupling constant between particles i and j, and $r_{ij} = r_j - r_i$ is the vector from i to j positions and N is the total number of particles. Equation (2) is a set of simultaneous Ode's that must be integrated once in order to find $v_j(t)$ and twice to find the position $r_j(t)$. For a large number of particles, the task becomes formidable. One way to reduce this burden is by going back to (1) and performing the integration for a pair of particles first, then use the resulting closed form formula to perform superposition of displacements and find the result of the interaction. Since the function $r(t)$ is not known before hand, we follow the Kepler route [2].

Assume a solution in the form $r = t^n$, where t is time and n is an exponent. Substituting in (1) we find that for the equality to hold for any r, the value of n should be $\frac{2}{3}$, and hence,

$$r = \frac{9}{4}\, k t^{2/3}. \tag{3}$$

This result can be directly checked by differentiating twice and substituting back to recover the original inverse square law. We are using scalar quantities because the force, acceleration and displacement are all along the separation line. The form of (3) is similar to Kepler's third law for orbital motion. In the original Kepler form the distance r refers to the average radius of the orbit and t refers to the mean time of one revolution. Formula (3) however, is more general and refers to motion along the line joining any two interacting particles under an inverse square relation. It is seen that the same formula is suitable for both types of motions. In fact direct substitution in the centrifugal force formula v^2/r using (3), with $v = dr/dt$ gives the same relation between r and t as that derived form (3). A similar result is obtained if we substitute for the Coriolis and the magnetic (Ampere) forces. In fact, such a substitution in the general acceleration definition d^2r/dt^2 reduces it to an inverse square relation. Kepler formula is also shown to be a direct consequence of mechanical similarity [1], and the form $1/r^n$ satisfy similarity for any n, but only $n = (2, -2)$ produces bounded motion, which corresponds to the inverse square force and to the space oscillator type (spring oscillators) interaction forces. The spring type force is also shown to be a special case of the inverse square law for small displacements around an equilibrium point. When (3) is differentiated with respect to time we get

$$v(t) = \frac{dr}{dt} = \frac{2}{3}\, k t^{-1/3} = k r^{-1/2} \tag{4}$$

further differentiation gives

$$a(t) = \frac{d^2r}{dt^2} = \left(-\frac{2}{9}\right) k t^{-4/3} = \left(-\frac{2}{9}\right) k r^{-2} \tag{5}$$

thus we have recovered the inverse square law. Substituting from (4) for the centrifugal force gives

$$\frac{v^2}{r} = \frac{4}{9}\, k^2 t^{-4/3} = k^2 r^{-2} \tag{6}$$

which is, apart from a constant, has the same form of dependency of t on r. The velocity is given by

$$v_j = v_{j_0} - \frac{2}{3}\, t^{1/3} \sum_i \frac{r_j - r_i}{|r_j - r_i|}\,, \quad j, i = 1; n\,, \quad i \neq j \tag{7}$$

and the position r_j is given by the vector relation

$$r_j = r_{j_0} + v_{j_0} t + \frac{9}{4}\, t^{2/3} \sum_i \frac{r_j - r_i}{|r_j - r_i|}\,, \tag{8}$$

where r is the net position vector of all particles and is given, for each, as the vector sum of $n - 1$ vector displacements in addition to the initial position of the particles r_0 and the initial velocity v_0 multiplied by the time t.

The form in (8) is similar to the usual form of the equation of motion for n interacting particles which can be written as

$$r_j = r_{j0} + (dt)\, v_{j0} + (dt)^2 \sum_i \frac{r_j - r_i}{|r_j - r_i|^3} \tag{9}$$

with the obvious difference that (9) involves dt rather than t and therefore must be advanced in very small steps to reach the final solution.

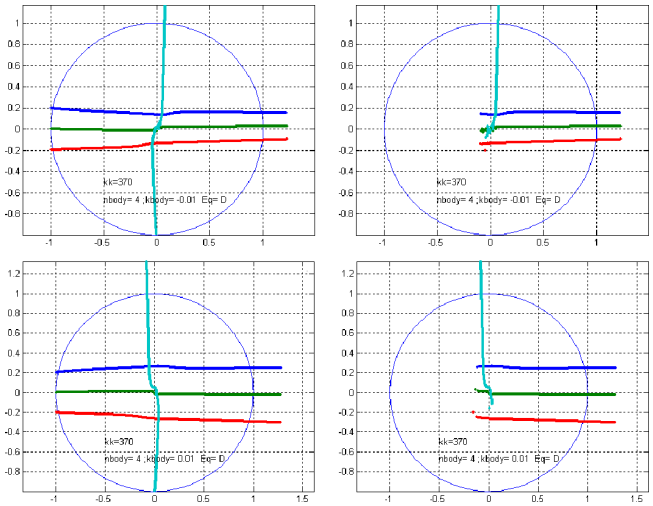

Fig. 1: Four point particles interacting under attractive (top) and repulsive inverse square forces (bottom). Prediction using (8) starts from time step $kk = 1$ (left) and $kk = 150$ (right), showing the capability of writing the correct solution for many particles at any time without going through time evolution.

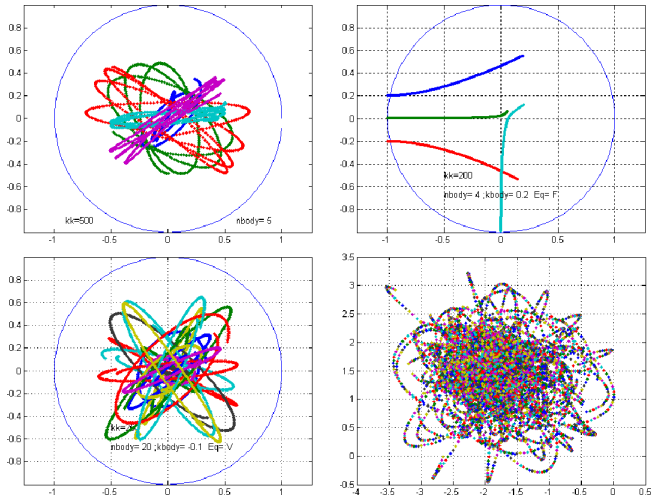

Fig. 3: T: interaction using force (9) for five bodies (confined) and three bodies (not confined). B: interaction using velocity formula (7) for 20 & 200 particles under attractive forces with and without a restraining circular boundary.

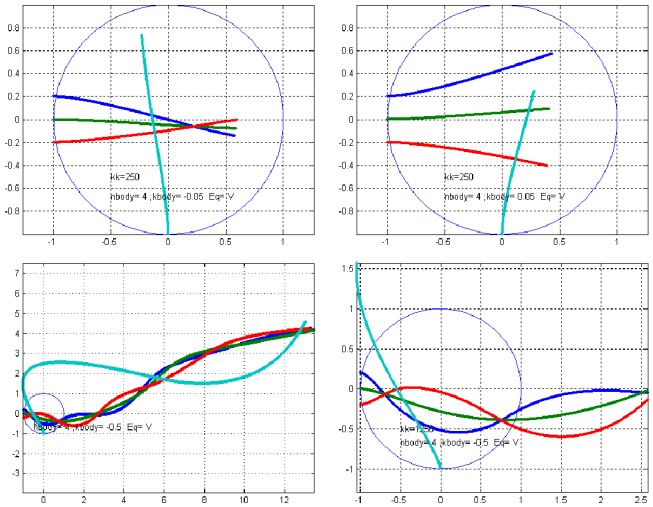

Fig. 2: Predictions using (7) keeping the circular boundary neutral. T: four point particles interacting under attractive and repulsive inverse square forces. B: four point particles interacting under attraction forces for longer time showing the stability of the velocity solution at close encounters. Particle paths interweave as a result of the attraction forces and the (inertia) forces.

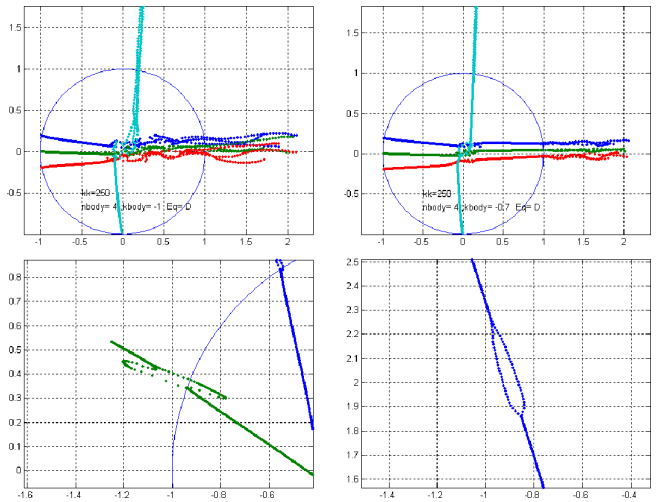

Fig. 4: Instability in the distance formula (8) at small interaction distances. Each particle path branches into three but recovers back to a single path as the particles further separate (top figures). The path disintegrates to only two branches at the encounter of a particle and a wall of particles. The minimum separation distance needed for such behaviour increasing with the increase in the value of the separation constant.

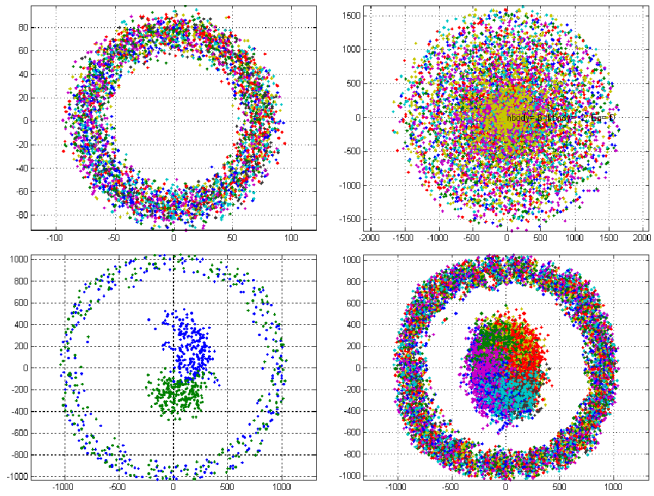

Fig. 5: Rotation, stratification and condensation for large numbers using (8). T: 150 particles under attractive forces only but at different coupling constants. B: one time step and many time steps results of the interaction of 500 particles of equal mix of charges.

3 Results

In this section we concentrate on showing that (7) and (8) give the expected behavior in the case of interacting particles under attraction or repulsion for the case of free particles and for the case of particles trapped inside a constraining circular wall. Comparison is then given with predictions using the usual integration of the inverse square law (9). The distances and coupling constants in these tests are arbitrary- chosen to produce magnified effects of the forces involved. The actual values used are marked on each figure.

Figure 1 shows four particles moving to the right with initial velocities mainly in the horizontal direction. The relative values of initial kinetic energy and the coupling constant determine the behavior of the interacting particles. When the initial velocity is large, as expected, the particles do not change direction appreciably, and when it is small, the repulsion and attraction forces have bigger effect — creating appreciable changes in the particle path. The trajectories are calculated using the displacement expression (8). When using this method it is possible to write the solution at any required time instant as shown in the right hand side frames, wherein the solution is now started at an advanced time location (at the 150th time step kk) and still agreeing with the results of the previous solutions starting at the first time step ($t = 0$) — using the same original set of initial conditions.

Figure 2 shows the results using the velocity expression (7) for the case of attractive and repulsive forces. The stability of the solution is clearly demonstrated by the last frame showing an interweaving paths forced by the equally effective inertial and attractive forces. The velocity formula gives more stable solutions at closer encounters because of the absence of the inverse square term from (7), being replaced by a quantity dependent on t. We should note here also that we still have the direction cosines to consider for the vector superposition. This, however, has a more favorable behavior at very small separation distances since the quantities x_{ij}/r_{ij}, go to unity as r goes to zero.

In Figure 3, the top two frames show the results of using the force formula (9) for the case of four free particles and five particles respectively confined in a circular boundary. The bottom two frames show the result for large number of particles, when using the velocity formula (7), in which 20 particles are confined in a circular boundary and 200 particles under attraction without a restraining boundary.

Problems have been experienced when using the distance formula (8) when the separation distance is small. As shown in Figure 4, the particle path divides into 3 branches but recovers afterwards as the two bodies separate and the separation distance increases depending also on the strength of the coupling constant. Note the effects on the path even before the target is reached. At the interaction with a wall of charges, the path divides instead, into two parts and recovers back again. This phenomenon requires further investigation as it is found to occur only at larger separation distances if the coupling constant is increased. It is numerical in origin, which is somehow different to what one would expect of this formula.

Figure 5 shows the results of using (9) for a large number of particle interactions. Results for 150 and 500 particles under attractive forces are shown. The results show signs of rotation and pulsation behavior as well as coagulation to form separated groups.

4 Conclusion

It has been shown that it is possible to reduce the computation time and enhance the solution stability for multi-point particle interactions. As a result it has been possible to follow the interaction of very large number of particles using modest computer memory and time. In the author opinion the method shown here is worthy of further development and use to numerically investigate the fascinating world of particle interactions. Evidence of grouping appears when the number of interacting particles is large and without the need of retaining external boundaries or forces.

A consistent phenomenon of path splitting into three and two branches has been observed. It is a direct result of evaluating distances using the square root, as it is treatable by adding a very small constant value to the inverse of the rooted quantities. Clearly this phenomenon needs to be corrected first before the present method acquires its full potential.

Submitted on September 12, 2009 / Accepted on October 19, 2009

References

1. Landau L.D., Lifshitz, E.M. Mechanics. Pergamon press, 1960.
2. Murray C.D. and Dermott S.F. Solar system synamics. Cambridge University Press, 2000.