JOURNAL OF COMPUTATIONAL PHYSICS 16, 76–92 (1974)

Numerical Experiments on Expanding Gravitational Systems

G. JANIN AND M. J. HAGGERTY

Department of Aerospace Engineering and Engineering Mechanics, and Center for Statistical Mechanics and Thermodynamics, University of Texas, Austin, Texas 78712

Received March 4, 1974

An experimental study of expanding gravitational systems of N bodies is performed by means of computer experiments. A description of the numerical techniques, integration scheme, special handling of close encounters, is given. The effect of the rest of the universe on the system is simulated by adding a smooth time dependent gravitational field. The results are compared with the evolution of similar systems with more discrete particles placed outside. During the computer experiments, a reduction of the number of bodies is sometimes made by reducing small subclusters to single particles at their centers of mass. For $25 \leqslant N \leqslant 200$, the results are shown to be sensitive to nearby external physical sources. Some very accurate, reversible and reproducible runs have been made in order to show that the computations represent purely gravitational interactions, without uncontrolled and unphysical perturbations.

1. INTRODUCTION

The formation of galaxies, clusters of galaxies, and superclusters in an expanding cloud of small lumps of material may be due to relatively close gravitational binary interactions between the lumps [5, 10, and references therein]. The rates have been shown to be insensitive to the internal dynamics of previously separated small clusters, but could depend strongly on the presence or absence of large scale distant aggregations. In the present paper we describe an experimental method, using computer models, for studying the influence of such aggregations. Moreover, results are presented that will provide a justification for procedures used in studies of cosmological clustering [6].

Our models are based on the exact integration of the motion of N point masses interacting gravitationally. The equations of motion are:

$$\frac{d^2x_{i\mu}}{dt^2} = \sum_{\substack{j=1 \\ j\neq i}}^{N} m_j \frac{x_{j\mu} - x_{i\mu}}{(R_{ij})^3} \tag{1}$$

where $(x_{i1}, x_{i2}, x_{i3}) = (x_i, y_i, z_i)$ are the cartesian components of the position $\mathbf{R}_i$ of particle number i with mass m_i, and R_{ij} is the distance between particles i and j. When converting (1) to a first-order system, one writes $x_{i\mu} \equiv dx_{i,\mu-3}/dt$, $\mu = 4, 5, 6$. The universal gravitational constant has been set equal to unity. Initial conditions are to be chosen at some initial time t_0.

This problem, the gravitational N-Body problem, has already formed the subject of numerous studies. All of them show that there is a fundamental instability in the numerical procedure, an instability due to the singularity of the equations of motion when the distance R_{ij} of two particles approaches zero (during an "encounter"). If the particles are not point masses and have a dimension l, the Newtonian force law should be modified for encounters with $R_{ij} < 2l$. In this paper, in order to test the effects of purely gravitational forces between centers of mass of the lumps and small clusters we take l to be small, i.e., $l = 0$.

In order to remove the singularity of the equations of motion for two-body encounters, a mathematical transformation of the equations of motion called regularization is used.

The integration of the equations of motion is performed using a high-order Runge–Kutta integrator with an automatic step-size control. Very high accuracy is obtained by adopting the same step size for integrating the motion of all the particles.

An improved one-step method with variable order is used for systems with a large number of particles ($N > 100$).

When one wants a complete reproducible and reversible evolution, one cannot practically take more than a few hundred bodies into consideration. This means that we will be able to integrate exactly only a small part of a large cloud. One purpose of this study is to check in what manner the neglected or crudely treated parts of the cloud influence the evolution of a given subsystem.

This can be done by comparing the numerical evolution of a system resulting from the adjunction of two or more continuous subsystems with the numerical evolution of each of these subsystems taken in isolation. Such contiguous subsystems have to fit together, so it is convenient to take their shapes as cubical. In order to take into account at least the effect of a smoothed-out mass distribution representing the rest of the cloud, it is reasonable to add an external force acting on the particles, specifically, an asymmetric force field due to a uniform mass density outside the cube but within an enclosing sphere. If such a force were not added, one would expect the cubes to become distorted not only by diffusion due to discreteness effects, but also because of the unphysical pinching of the corners, etc., due to the *mean* field generated by such a truncated system.

In fact we did not find that any such pinching effect became dominant when the external force was turned off. Instead, we found that the external force gives rise to a surprisingly large systematic evolution of the total energy of the system, which

would otherwise be conserved. That in turn greatly affected the systematic evolution of the system. We can therefore think of the external field as representing a large effect due to interactions between the bodies and massive external aggregations. Since the equilibrium size of a new cluster is very sensitive to its total energy (when that is close to zero), such energy channels destabilize the evolution well in excess of naive estimates based on the small magnitude of the additional potential energy associated with the external forces. By retaining accuracy in the N-Body integration, we are able to isolate such a physical instability from the previously mentioned numerical difficulties due to close encounters. Similar physical effects in non-expanding systems have previously been studied by Miller [9] (see also a review of Saslaw [12]).

2. Treatment of Close Encounters

(a) *General Remarks*

The equations of motion (1) for the gravitational N-Body problem have a singularity when R_{ij} approaches zero. This singularity gives birth to unpleasant numerical difficulties when two bodies are very close together.

One simple way this problem can be approached is to introduce a cut-off l of the Newtonian force F_{ij} between the two bodies i and j when their distance R_{ij} becomes small. For example one could specify that

$$| F_{ij} | = G(m_i m_j/(R_{ij}^2 + l^2)).$$

This procedure is plausible when l can be identified with the spatial extension of bodies that have sizes comparable with the distances between neighbors, like star clusters and clusters of galaxies. It has been applied to galaxies and clusters of galaxies by Aarseth [1], Peebles [10] and recently by Press and Schechter [11].

In this project we have introduced no such cut-off: $l = 0$. Although we have in mind the study of the further clustering of loose, extended clusters of galaxies, we should like to be able to study properly the effects of close encounters in systems of particles with concentrated masses, such as stars. But more importantly, it is essential to verify the intuitive idea that long-range gravitational clustering processes are not affected by the precise manner of treatment of close encounters. Thus at least a few tests where no cut-off is introduced ($l = 0$) are appropriate, and it is our purpose to design and conduct such tests.

Therefore we will instead use a mathematical transformation of the equations of the two-body motion for removing the singularity. Such transformations exist and are called "regularizations." The most famous transformations in the tridimensional space is the Kustaanheimo–Stiefel (KS) transformation [13].

(b) *The KS Transformation*

In this regularization procedure, a new independent variable s called fictitious time is introduced by

$$dt = R_{ij}\, ds, \tag{2}$$

where R_{ij} is the mutual distance of the two bodies i and j which motion is to be regularized, and a set of four new dependent variables $\{u_1, u_2, u_3, u_4\}$ defined by a matrix transformation $L(\mathbf{u})$ such that

$$\mathbf{x} = L(\mathbf{u})\mathbf{u}.$$

The equations of motion corresponding to system (1) are in the new variables:

$$\mathbf{u}'' + (h/2)\mathbf{u} = (|\, u\,|^2/2)\, L^T\mathbf{P} \tag{3}$$

where primes denote derivatives relative to s and L^T, the transposed matrix of L, operates on the perturbation force $\mathbf{P}$ which represents the gravitational influence of the $N - 2$ other bodies. In (3), h is the energy of the two-body system and satisfies the differential equation

$$h' = -2(\mathbf{u}', L^T\mathbf{P}).$$

A more detailed collection of related formulas can be found in Stiefel and Scheifele [13, p. 33].

The equations of motion (3) are regular and are equivalent to the equations of an harmonic oscillator for vanishing perturbations. But their numerical integration involves more computations than the integration of system (1); therefore they should be used only for close encounters between two particles and should be switched off when the encounter is over. Several independent encounters can be simultaneously treated in this way.

(c) *Uniform Regular Canonical Elements*

An improvement of the KS procedure is possible. It consists of building a set of elements, which are new dependent variables varying only linearly in the absence of perturbations. In the case of weak perturbations, which is the usual case, the integration of elements will give rise to less truncation errors than the integration of the u variables.

Such a set of elements is easy to establish for pure elliptical or hyperbolic motion. But in the N-Body problem a two-body subsystem can experience a continuous transition between an elliptical and a hyperbolic motion through the influence of a third close body. Stiefel and Scheifele [13] suggest a set of uniform canonical

regular elements which can handle such situations. Their implementation has met with some success. The mean computing time saving for 25-body runs, through this procedure for treating close encounters, was 10% better than with the u formulation (3). However, we do not think that this improvement is large enough for justifying the implementation of this procedure, so we merely refer the reader who wants more details to Stiefel and Scheifele [13, p. 251].

3. The Integration Schemes

The straightforward integration of the $3N$ second-order differential equations of motion (1) from some initial values, with a classical integration scheme, will quickly lead to erroneous trajectories. The rapidly varying functions during close encounters between particles need a variable step size with a good step-size estimation.

Such a method is described in the pioneer work of von Hörner [14]. But a limitation of this method comes from the unavoidable formation of binaries during the evolution of the system. Integration of the motion of these binaries requires a very small step size for too many of the steps.

A major improvement consists of introducing the regularization procedure, outlined at the preceding section, for each of the close encounters and binaries. A test on the mutual force F_{ij} of all the pairs of the system decides at each integration step which pair is interacting strongly enough ($F_{kl} > F_{\lim}$) for applying the procedure. The parameter can be chosen to be of order 10 times the mean force between two neighboring particles of the system. To keep the same independent variable for the whole system of differential equations, the fictitious time of the pair with the smallest mutual distance R_{kl} is chosen as independent variable, and the right-hand side of all equations not belonging to this pair are corrected by the factor R_{kl}, according to Eq. (2). The center of mass of the regularized pairs has to be integrated too. Each regularized pair increases the equations to be integrated by four. Transformation between $\mathbf{x}$ and $\mathbf{u}$ space has to be done at each function evaluation in order to compute the force $\mathbf{P}$ of the $N - 2$ other bodies on the regularized pair.

The frequent switching in and out of regularized variables recommends the use of a one-step integration method. High-order methods have been found to be highly efficient. Attention has been focussed on an eighth-order Runge–Kutta scheme due to Fehlberg (1968) because of its convenient step-size control. In the so-called 7(8) method, at each step a seventh-order and an eighth-order estimation of the solution are simultaneously computed for each equation, and the difference of these two estimations gives an approximation of the truncation error at this step. The largest truncation error is used to predict the size of the next step. Even with

regularization, the step size cannot be taken constant because of eventual multiple collisions.

An N-body program based on the Fehlberg method and regularization of one pair is described in Bettis and Szebehely [3]. Such a program is very efficient for systems of less than 100 bodies (typically 25 bodies), and was used to obtain preliminary results [5]. Even if several pairs are simultaneously regularized, the fact that the same step size (collective step size) is used for the motion of all particles of the system makes this method too slow for $N > 100$.

A successful improvement is the individual step-size scheme, where each star has its own step size. In the method of Aarseth [2], a polynomial interpolation along the current successive mesh points of the integration of each particle allows the computation of the position and therefore the force on any particle at any time. Regularization is included.

We prefer to orientate ourselves towards another direction. The collective step-size method has the advantage of simplicity. This is important for us as we intend to complicate our system for example by introducing an external field and by changing the integration problem at various times (Section 6 below). In order to define a kind of variable precision in the collective step-size scheme, we propose to have a variable order for the integration method. A high-order scheme is applied for stars involved in a strong interaction while a low-order scheme is sufficient for describing the motion of isolated stars.

A Runge–Kutta method cannot be practically used for this purpose and a new method was developed. This method described in Janin [7] is outlined here.

If one has, for solving system (1) converted to a first-order system, a polynomial approximation $P_{i\mu}^{(L)}(t)$ of order L for the solution $x_{i\mu}(t)$ ($\mu = 1, 2, \ldots, 6$) in the time interval (t_m, t_{m+1}) at the mth integration step, one can build, using the right-hand side of (1), a polynomial approximation $Q_{i\mu}^{(L)}(t)$ of $(d/dt)\, x_{i\mu}$ in (t_m, t_{m+1}). Integration of $Q_{i\mu}^{(L)}(t)$ between (t_m, t_{m+1}) gives an approximation $P_i^{(L+1)}$ of order $L + 1$ of $x_{i\mu}(t)$, using the given initial values $x_{i\mu}(t_m)$. This iterative procedure, called Picard iteration, can be pursued up to any desired order.

In practice, Chebyshev polynomials are used and, at each integration step, successive polynomials of order 0, 1, 2,... are built for each component of each star until a precision test is satisfied. For smoothly behaving stars the test is satisfied already with low-order polynomials, while for stars involved in close encounters, high-order polynomials are required. The collective step size is also variable.

The efficiency of this new method, defined by the number of evaluations of the right-hand sides of the differential equations for a certain accuracy, is much less than for the Runge–Kutta method; however, for a large number of particles ($N > 100$), the reduction of computing time due to the variable-order scheme is predominant and makes the method useful. Therefore we applied it for $N \geqslant 100$

(typically our 200-body system) while we usually employed the Runge–Kutta 7(8) method for $N < 100$ (typically our 25-body systems). The results were equivalent.

The choice of our integration methods and the complication of introducing regularization are made in order to have highly accurate computations of the trajectories. Is such accuracy needed? Previous results [5] suggest that it probably is not, for a global study of the evolution of an expanding system, but it is the only way to be sure the computation is not meaningless. It is well known that the gravitational N-body problem is unstable, and we want to be sure that all statistical fluctuations are associated with the physical approximations and initial conditions, rather than numerical instabilities.

4. A Corrective Force for Cubic Systems

Our aim is to study clustering of gravitational particles in a large initially homogeneous expanding system. The systems we can numerically study are of finite dimension and boundary conditions have to be defined. It is a delicate problem, and no matter how the boundaries are defined, one will have to check experimentally if they are realistic. One way to do it is to consider a system containing a subsystem and to compare the behavior of the particles of the subsystem in isolation (but with the specified boundary conditions) with the behavior under the influence of the other particles of the system. Such a study would not encompass all possible long-range interactions, but would test only the influence of relatively short-range forces, due to particles just outside the subsystem. It is not necessary to completely enclose the subsystem; it is already interesting to extend only one face of a cubical system by adjoining a cube of the same size.

In an effort to reduce spurious effects due to the absence of spherical symmetry, we introduced an auxiliary field to represent the smeared-out material outside the regions containing particles. Equivalently, we may think of the field as being due to a fictitious uniform negative mass density in the regions containing particles, together with a central attractive field that is linear in the displacement from the center.

The gravitational field and potential of a homogeneous cube can be expressed in closed form by a formula containing only elementary functions [8]. This formula has been reestablished in a more elegant way by Waldvogel [15]. The field is computed exactly and added to the interparticle forces. The system is expanding, so that the additional field is time dependent. The appropriate time dependence cannot be precisely determined. A suitable model is specified by considering uniform fluid models with the same initial mass density and mean velocity, without allowing for inward diffusion of the fluid.

5. Initial Condition for Expanding Systems

For the 25-body systems, the particles, each of mass 1 (rather than the somewhat more standard $1/N$) with the gravitational constant $G = 1$, are initially placed at random inside a cube whose sides have length $2(\pi/6)^{1/3}$ (corresponding to a sphere of equal volume and radius 1). Figure 1 shows an (X, Y) projection of such positions.

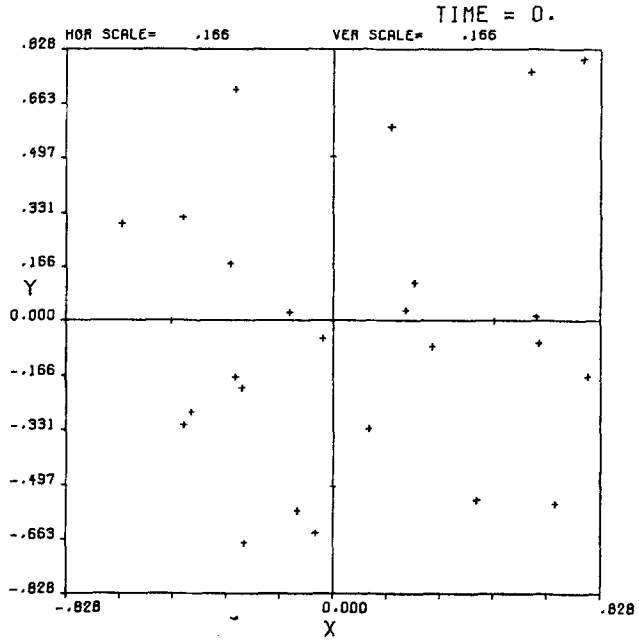

FIG. 1. The initial positions of the 25 lumps in one of eight small cubical systems. A "lump" is a particle of mass 1.

For 50-body systems we adjoin two such cubes side-by-side and for 200-body systems, eight such cubes to form a large cube with side $4(\pi/6)^{1/3}$.

The velocities are taken as the sum of two terms

$$\mathbf{V}_i = \mathbf{V}_i^{\text{exp}} + \mathbf{V}_i^{\text{pec}}$$

where

$$\mathbf{V}_i^{\text{exp}} \sim \mathbf{R}_i ,$$

a pure expansion term, and $\mathbf{V}_i^{\text{pec}}$, the "peculiar" component, is chosen according to a Maxwellian distribution.

The crossing time

$$t_c = 2\sqrt{2}\,[N\langle R_{ij}^{-1}\rangle^3]^{-1/2}$$

has initially a value of 0.43, but is strongly increasing when the cluster expands.

For the runs described below, the scale of the initial velocities was such that 25-body *spherical* systems are expected to have zero total energy. Therefore the 25-body cubical systems have total energies that are small but positive, the kinetic energy of expansion being affected more than the potential energy by the distortion of the shape. The potential energy of a sphere of mass 1 and vol 1 is $(3/5)(4\pi/3)^{1/3} = 0.967$; the potential energy of a cube of mass 1 and vol 1 is [15]

$$\text{Arsh}(1) + \text{Arch}(2) - (\pi/3) + (1/5)[1 + 2^{1/2} - 2(3)^{1/2}] = 0.941.$$

The ratio of the two, 0.973, deviates from unity by less than the corresponding ratio of expansion kinetic energies, $(5/3)(\pi/6)^{2/3} = 1.083$ (for fixed density and Hubble constant). For the runs shown in Fig. 2, we took the initial motion to be that of

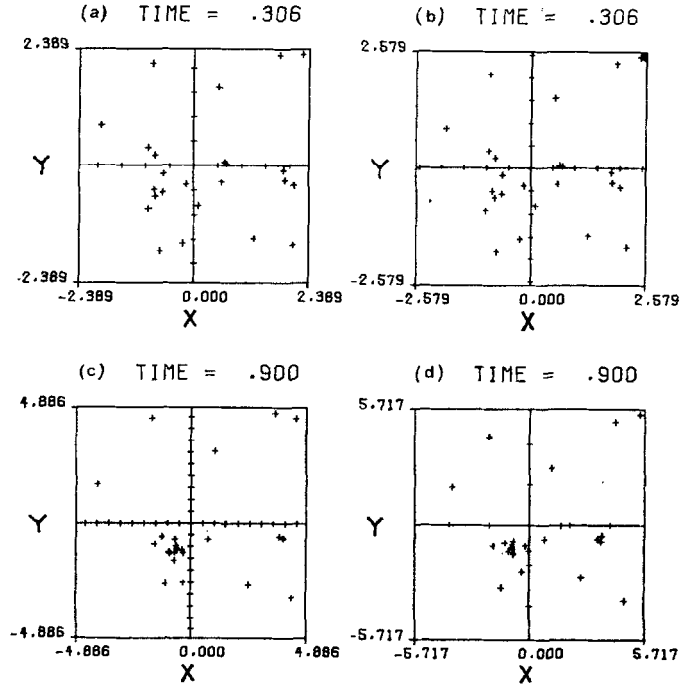

FIG. 2. The evolved positions of the lumps of Fig. 1. (a), (c): external force on. (b), (d): external force off. There were no initial peculiar velocities: $\gamma = 1$.

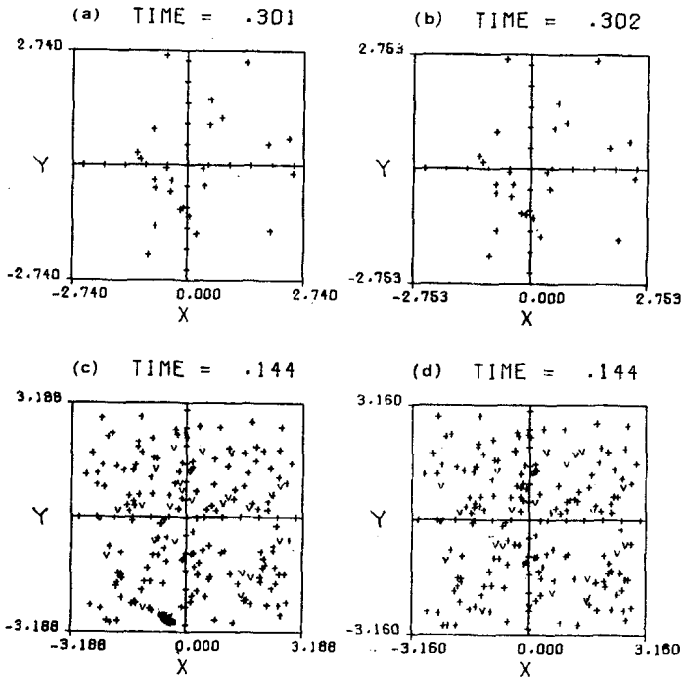

FIG. 3. The evolved positions of a 200-lump system containing the subsystem of Fig. 1, but with $\gamma = 0.75$. (a): subsystem, external force on. (b): subsystem, external force off. (c): system, external force on. (d) system, external force off. The symbol v indicates a combined binary.

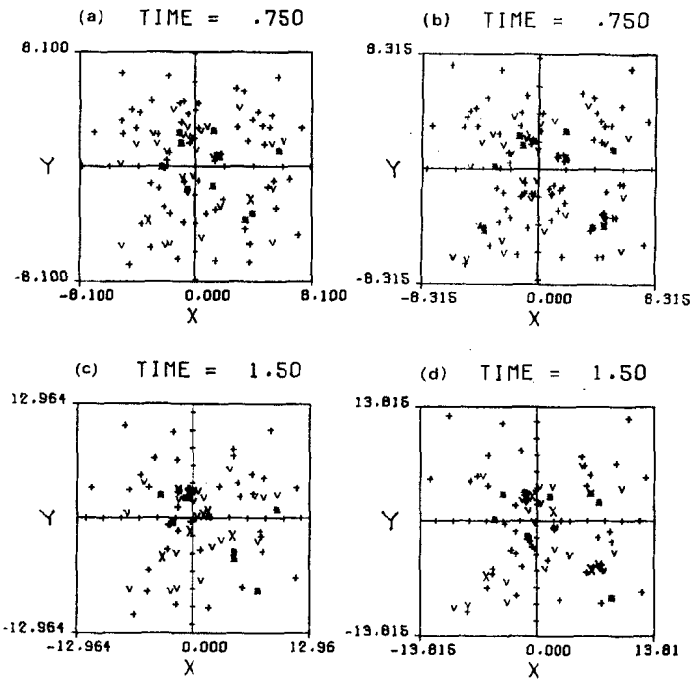

FIG. 4. The evolved positions of the mass-200 systems in Fig. 3(c), 3(d): comparison of positions with and without the external force. The symbol v represents combined clusters of mass 2 or 3. Composite particles of masses 4–7 are indicated by the symbol *; masses 8–15 by $\times$, 16–31 by \$, and 32 and higher by M.

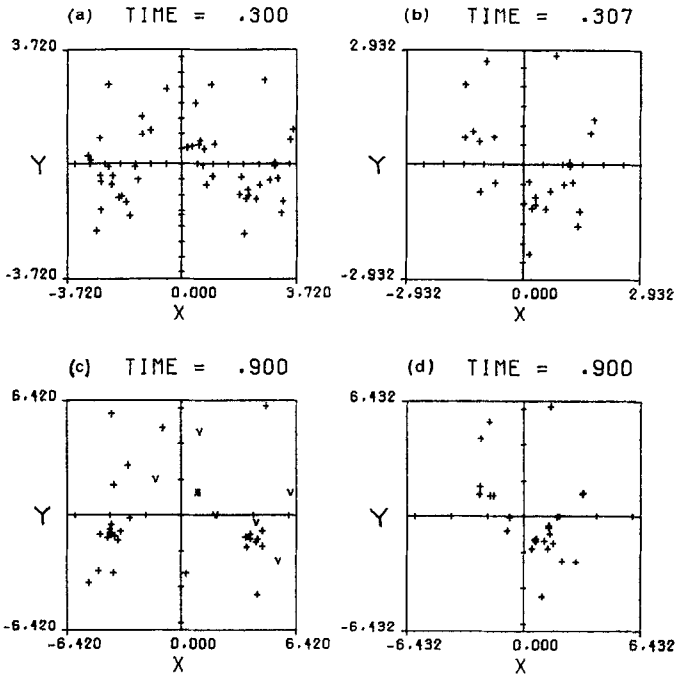

FIG. 5. Comparison of the evolution of mass-25 systems with and without a similar adjoined system. The times are indicated above the graphs. In Figs. 3–6, $\gamma = 0.75$. In Figs. 5 and 6, the external force is on.

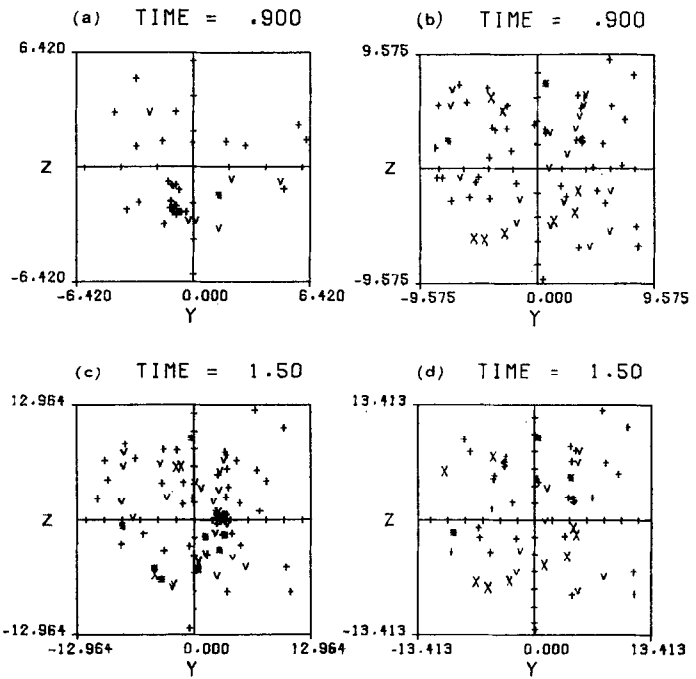

FIG. 6. (a) The Y-Z projection of the mass-50 systems of Fig. 5(c); (b) A mass-200 system composed of mass-50 systems adjoined at different times; (c) The Y-Z projection of the mass-200 system shown in Fig. 4(*c*); (*d*) The evolved positions of the system of Fig. 6(*b*).

pure expansion. For the runs shown in Figs. 3–6, peculiar velocities were added to (reduced) expansion velocities, so that for the 25-body cubes, the ratio

$$\gamma = \left(\frac{\sum | \mathbf{V}_i^{\exp} |^2}{\sum | \mathbf{V}_i |^2}\right)_{\text{initial}}$$

was about 0.75.

Since the peculiar kinetic energy scales as the first power rather than the five-thirds power of the total mass, the adjoined 200-body systems therefore had a slightly negative initial total energy.

6. Experiments with Expanding Systems

(a) *Effect of the External Force*

Figure 2 shows the evolution of the initial positions of Fig. 1 for $\gamma = 1$. The X–Y projections of the positions at times $t \approx 0.3$ (Fig. 2(a,b)) and $t = 0.900$ (Figs. 2(c,d)) are given for a run where the external force was added (Fig. 2(a,c)) and for another where it was turned off (Figs. 2(b,d)). The external force is seen to affect the details of the positions, but not the general distribution of clusters.

Figures 3(a) and 3(b) similarly show the corresponding positions for $\gamma = 0.75$ and $t \approx 0.3$.

Figures 3(c) and 3(d) show the X–Y projection at time $t = 0.144$ of the positions of a mass-200 system for $\gamma = 0.75$. The region $X < 0$, $Y < 0$, $Z < 0$ originally contained the displaced bodies shown in Figs. 3(a,b); the other seven subcubes contain bodies whose positions were determined by mutually distinct sets of random numbers. Figure 3(d) is the result of an accurate, reversible integration, with the external force turned off, followed by the combination of 25 bound binaries into the center-of-mass points indicated by the symbol v (cf. [5]). Figure 3(c) is the results of two accurate integrations, with the external force turned on. The first was to time $t = 0.073$. Then 25 binaries were combined (16 of which were the same as the others). The second was an accurate integration of the resulting 175-body problem, from $t = 0.073$ to $t = 0.144$. We may think of the first integration as providing a set of initial conditions for the second integration. In this sense the combinations do not destroy the accuracy.

Once again, the clusters, though not the exact positions of all the bodies, are independent of the presence of the external force.

Several parameters were examined to determine the most significant deviations. By far the most interesting deviation we encountered was that of the total energy of the N-body system, which showed a surprisingly large systematic evolution when the external force was on. One can understand how the force field would tend to

absorb energy from the outer particles, especially from the escapers, since there is a retardation owing to the positive mass background outside the face centers. The surprise was the magnitude of the effect. It was such as to drive the virial ratio (twice the kinetic energy divided by the interparticle potential energy) from about 2 to about 1 by the time the system expanded by a factor 4 in diameter (see Table I). The energy exchange then slowed abruptly.

TABLE I

Evolution of the Total Energy of the System (Mass 200) Shown in Figs. 3(c), 3(d), 4 and 6(c), and of some central subsystems

	Number of Bodies		Orbital[a] Kinetic Energy		Total Internal[b] Energy		Energy/Mass of Central Sphere[c]		Energy/Mass of Central Cube[d]	
External Force: Time	On	Off	On	Off	On	Off	On	Off	On	Off
0.1441	—	200	—	5744	—	−1188	—	−299/50	—	−276/50
0.1441	175	175	5143	5672	−1711	−1188	−300/50	−300/50	−283/50	−286/51
0.3000	135	175	3268	4031	−1936	−1188	−409/50	−360/50	−332/50	−309/50
0.4500	120	143	2402	3248	−2051	−1188	−413/50	−394/50	−388/51	−378/50
0.7500	97	115	1584	2522	−2234	−1191	−499/54	−387/50	−455/51	−431/50
0.9000	80	90	1208	2191	−2266	−1194	−454/50	−566/58	−448/50	−435/50
1.5000	80	90	1534	1781	−2286	−1194	−458/50	−491/52	−453/51	−457/50

[a] Does not include internal kinetic energy of combined particles. The evolution of the virial ratio may be determined by comparing this column with the next.

[b] Includes a correction ($\lesssim 20\,\%$) due to the binding energy of composite particles, but does not include any potential energy due to the external field. This energy is accurately conserved by the integration method when the external force is off. The change from −1188 to −1194 occurs because of combinations of particles into center-of-mass points.

[c] The particles nearest the center of the system, consisting of approximately 1/4 of the total mass. The energy includes binding energies but not external field potentials.

[d] Let $(j(\nu),\ \nu = 1, 2, 3,\ldots)$ be a sequence of particle labels such that $\max_\mu |X_{j(\nu)\mu}| \leqslant \max_\mu |X_{j(\nu+1)\mu}|$. Then the "central cube" consists of particles $j(1), j(2),\ldots, j(l)$, where l satisfies $\sum_{\nu=1}^{l-1} m_{j(\nu)} < (1/4)M$ and $\sum_{\nu=1}^{l} m_{j(\nu)} \geqslant (1/4)M$. These are different at different times.

It would be tempting to interpret this evolution as a relaxation towards a state satisfying the virial theorem (cf. [9]), made possible by the breaking of the symmetry of energy conservation by the opening of a channel of interaction between the bodies and the massive effective sources of the external field. Subsequent extended runs did *not* verify that such an interpretation is generally valid; indeed, sometimes the evolution reversed itself, and the virial ratio became once again greater than 2.

Thus one must be very cautious about drawing firm conclusions on the basis of a few runs with many of the parameters fixed.

Table I also shows that in both cases the magnitude of the energy of the central regions of the system also increases, and that the rate of increase was rather independent of whether the extermal force was on or off. That suggests that material in neighboring regions of comparable size, rather than material at a great distance, contributes most to such energy exchanges.

Figure 4 shows the same pair of runs at times 0.75 and 1.5 (with similar reductions from $N = 175$ to $N = 80$ and 90). The deviation of the parameters of Table I is not reflected by any large deviation in the overall appearance of the system.

(b) *Effect of Distant Discrete Particles*

In Fig. 5 we study (at $t = 0.3$, 0.9) the effect of a single plane boundary by comparing the evolution of a 50-body system with shape $2 \times 1 \times 1$ with one of its halves, the right half. The displaced positions (at $t = 0.0$, 0.3) of the left half were shown in Fig. 1 and 3(a). Some combinations were made at $t = 0.3$, so that a 36-body problem was integrated from 0.3–0.9.

Our general impression is that the motion of the particles *near* the boundary is *severely* affected by the presence or absence of particles on the other side of the boundary. For instance, in one case but not the other a large cluster may form, may interact strongly with another large cluster in the interior, and may be transported inward. An attempt to fit together the single cubes at an advanced time by comparing positions of the corresponding particles was a failure (even if the original cubes were allowed to overlap and to contain common particles). More progress could be made by forgetting the initial labeling of particles, considering only the instantaneous distributions of positions and velocities, and fitting various averages of these with the corresponding parameters of fluid models.

However, at a distance from the boundary under study, the particles can easily be identified by their common positions, and the clustering is unaffected.

In Fig. 6 we change perspective from the X–Y to the Y–Z projection. Figure 6(a) shows the same positions as Fig. 5(c), except viewed from the end of the double-cube. Figure 6(b) gives the same view at the same time $t = 0.9$ of a mass-200 system obtained by joining side-by-side the positions from two mass-100 runs. One set (displaced to the region $Y \lesssim 0$) was the result of taking the mass-50 system of Fig. 5(c) but at time 0.61, displacing it to the region $Z \lesssim 0$ and adjoining a similar set of positions with $Z \gtrsim 0$. This similar set was obtained with different random numbers determining the coordinates of the original 50 lumps. After a reduction of the mass-100 set to $N = 47$, an integration to $t = 0.9$, and a further reduction to $N = 35$ by making combinations of small bound clusters into center-

of-mass points (cf. Section (a) above), the system was adjoined to a second set of 34 bodies obtained similarly but displaced to $Y > 0$.

Figure 6(b), then, is a 69-body cubical system of mass 200, consisting of four double-cubical regions bounded approximately by the $Y = 0$ and $Z = 0$ planes. The positions were obtained by integrating the system without allowing any communication between the $Y > 0$ and $Y < 0$ parts, and allowing interparticles interactions between the $Z < 0$ and $Z > 0$ parts only for $0.6 < t < 0.9$. All interactions across the $X = 0$ plane were taken into account from the beginning. The comparison is with Fig. 6(a), representing the region $Z < 0$, $Y < 0$ integrated in isolation. In this case the similarity of the two is not striking, partly because of different combinations in the two cases.

Figure 6(d) shows the result of integrating the coordinates of the system of Fig. 6(b), reduced to a 50-body problem, and integrated from $t = 0.9$ to $t = 1.5$. That is to be compared to Fig. 6(c), which is the same as Fig. 4(c) but viewed from the Y–Z plane. It represents the integration of the same 200 lumps to the same time, but with full communication. Again the general distribution of clusters is comparable.

(c) *Adjunction of Subsystems*

The rules for displacing the center-of-mass positions and velocities of the subsystems out of communication (in the Z direction at $t = 0.6$ and the Y direction at $t = 0.9$) were difficult to specify. The rates of expansion of the various systems was due not only to the initial expansion bias in the velocities, but also to the pressure associated with the peculiar kinetic energy. Diffusion owing to cluster interactions caused penetrations of subsystems into each other and fluctuations in the magnitude of all these effects.

We avoided the difficulties by simply using the evolution of the mean velocity field in a perfect fluid model with *zero* total energy. The amount of displacement was taken as

$$R_d = (1 + 3(25/2)^{1/2}\, t)^{2/3}(\pi/6)^{1/3},$$

which was a slight overestimate for $\gamma = 0.75$ (see Table II), but resulted in relative positions such as those in Fig. 6(b), where the density is fairly continuous near $Y = 0$. In specifying the displacement in velocity, we compensated by retaining a factor $\gamma^{1/2}$; to get

$$V_d = [50\, \gamma/R_d]^{1/2}(\pi/6)^{1/3}.$$

Table II and Fig. 6(c,d) show that this is the right order of magnitude.

In a subsequent paper [6] we will therefore feel free to treat systems of 800 of the original lumps by doing integrations on subsystems with $N \leqslant 200$, and adjoining

TABLE II

A comparison of the center-of-mass position and velocity components normal to the bounding planes of various slices of the mass-200 cubical systems ($t = 0.9$, $\gamma = 0.75$) of Fig. 3(*c*), 3(*d*), 4, 6(*b*), 6(*c*), 6(*d*)

	200-body system						Adjoined 50-body systems		
	External force *off*			External force *on*			External force *on*		
Halves[a]	Mass	Center-of-mass pos.	vel.	Mass	Center-of-mass pos.	vel.	Mass	Center-of-mass pos.	vel.
$X_\mu < 0$	100	−2.63	−1.27	101	−2.22	−0.48	109	−2.20	−0.77
$X_\mu < 0$	92	−3.83	−2.27	92	−3.27	−1.16	94	−4.33	−2.55
$X_\mu < 0$	102	−3.52	−2.11	99	−3.31	−1.61	99	−4.00	−2.05
$X_\mu > 0$	100	3.67	2.27	99	3.34	1.56	91	3.63	1.72
$X_\mu > 0$	108	2.73	1.45	108	2.46	1.01	106	3.24	1.55
$X_\mu > 0$	98	3.86	2.39	101	3.46	1.84	101	4.15	2.26
Central Quarter Slices[b]									
$X_\mu < 0$	50	−1.01	−0.26	50	−0.82	0.07	51	−0.54	0.11
$X_\mu < 0$	59	−2.69	−1.29	51	−1.85	−0.08	60	−3.23	−1.63
$X_\mu < 0$	60	−2.15	−1.00	62	−2.26	−0.98	55	−2.64	−1.03
$X_\mu > 0$	50	1.70	0.82	54	1.70	0.47	54	2.35	0.72
$X_\mu > 0$	52	1.56	1.11	50	1.26	0.74	57	2.11	0.88
$X_\mu > 0$	52	2.22	1.33	50	1.66	0.58	50	2.42	1.12

[a] "Halves": Subsystems ($M \approx 100$) bounded by a plane $X_\mu = 0$ ($\mu = 1, 2$ or 3).
[b] "Central Quarter Slices": Subsystem ($M \approx 50$) bounded by $X_\mu = 0$ and $X_\mu = \text{const.}$

the subsystems after suitable time intervals (with R_d and V_d increased by a factor 2). It turns out that the process cannot be carried on indefinitely to an arbitrarily large number of lumps, because too many of them remain unclustered for too long. However, much computer time can be saved in this manner, and the identification of clustering in such few-body models with clustering in a large expanding universe is made more convincing by these comparisons.

7. Conclusion

In this paper we have described an improvement in the efficiency of accurate 200-body integration routines by the use of a one-step variable-order method with a collective step size and several simultaneous regularizations.

The method was applied to the study of the effect of boundary conditions on clustering in expanding systems. We showed that there can be a surprisingly large systematic exchange of energy across such a boundary and that the formation of

clusters of a particular size and mass depends greatly on the presence or absence of adjacent material of similar size and mass.

The details of the formation of particular small clusters are much more severely affected by changes in distant boundary conditions than by the previously studied combinations of other small clusters into center-of-mass points [5]. However, the generic rate of formation of small clusters in large systems seems approximately independent of the conditions at distant boundaries.

ACKNOWLEDGMENTS

Support from the Janggen–Pöhn Stiftung (St-Gall, Switzerland) and the Fonds National Suisse de la Recherche Scientifique, permitting one of the authors (G. J.) to begin this research at the University of Texas at Austin is acknowledged. The other (M. J. H.) was supported by the Welch Foundation and is indebted to I. Prigogine for his constant interest in the work.

We thank H. W. Harrison, D. G. Bettis, V. Szebehely and particularly O. Graf for many helpful discussions during the course of this project, and R. H. Miller and S. J. Aarseth for useful comments on the manuscripts.

REFERENCES

1. S. AARSETH, *M.N.R.A.S.* **126** (1963), 223.
2. S. AARSETH, *Astrophys. Space Sci.* **14** (1971), 118.
3. D. G. BETTIS AND V. SZEBEHELY, *Astrophys. Space Sci.* **13** (1971), 365; **14** (1971), 133.
4. E. FEHLBERG, NASA TR R-287, 1968.
5. M. J. HAGGERTY, "Formation of Clusters in 25-body Systems with Free Boundaries," unpublished report, 1972. A summary is to be published.
6. M. J. HAGGERTY AND G. JANIN, Numerical experiments on cosmological clustering," *Astron. Astrophys. J.* (1974), to be published.
7. G. JANIN, "Proceedings of the conference on the numerical solution of ordinary differential equations" (October 19–20, 1972, the University of Texas at Austin), *in* "Lecture Notes in Mathematics," Vol. 362, Springer–Verlag, Heidelberg, Germany, 1974.
8. W. D. MCMILLAN, "The Theory of the Potential," New ed., Dover, New York, 1958.
9. R. H. MILLER, *Ap. J.* **180** (1973), 759.
10. P. J. E. PEEBLES, *Comments Ap. Space Phys.* **4** (1972), 53.
11. W. H. PRESS AND P. SCHECHTER, *Ap. J.* **187** (1974), 425.
12. W. C. SASLAW, *P.A.S.P.* **85** (1973), 5.
13. E. STIEFEL AND G. SCHEIFELE, "Linear and Regular Celestial Mechanics, Springer–Verlag, Berlin, 1971.
14. S. VON HÖRNER, *Z. Astrophys.* **50** (1960), 184.
15. J. WALDVOGEL, The Newtonian potential of a homogeneous cube (1972), unpublished.

Printed in Belgium