Astrophysics on the GRAPE Family of Special Purpose Computers

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Abstract

The GRAPE-4, the world's fastest computer in 1995-1997, has produced some major scientific results, through a wide diversity of large-scale simulations in astrophysics. Applications have ranged from planetary formation, through the evolution of star clusters and galactic nuclei, to the formation of galaxies and clusters of galaxies.

Computational physics has emerged as a third branch of physics, grafted onto the traditional pair of theoretical and experimental physics. At first, computer use seemed to be a straightforward off-shoot of theoretical physics, providing solutions to sets of differential equations too complicated to solve by hand. But soon the quantitative improvement in speed yielded a qualitative shift in the nature of these computations. Rather than asking particular questions about a model system, we now use computers more often to model the whole system directly. Answers to relevant questions are then extracted only after a full simulation has been completed. The data analysis following such a virtual lab experiment is carried out by the computational physicist in much the same way as it would be done by an experimenter or observer analyzing data from a real experiment or observation.

Recent increase in computer speed is already significantly more modest than what could be expected purely from the ongoing miniaturization of computer chips. Since the number of transistors on a single chips doubles every 1.5 years, a chip now contains a hundred times more transistors than it did ten years ago. With a clock speed increase of more than a factor ten, one might have expected a speed increase of more than a factor thousand, over the last decade. However, the actual speed increase of a typical computer chip has been at most a factor hundred, lagging far behind theoretical expectations. The reason for this relatively poor performance lies in the significant overhead caused by the growing complexity of a general-purpose chip. Hence, designing a chip for only one specific purpose yields a rapidly growing pay-off. Therefore, the time seems ripe to explore which types of calculations can be realized directly in hardware, in the form of special-purpose computers, rather than run in software on general-purpose computers.

One of these projects has resulted in the GRAPE (short for GRAvity PipE) family of special-purpose hardware, designed and built by a small group of astrophysicists at the University of Tokyo [1]. Like a graphics accelerator speeding up graphics calculations on a workstation, without changing the software running on that workstation, the GRAPE acts as a Newtonian force accelerator, in the form of an attached piece of hardware. In a large-scale gravitational N-body calculation, where N is the number of particles, almost all instructions of the corresponding computer program are thus performed on a standard workstation, while only the gravitational force calculations, in innermost loop, are replaced by a function call to the special-purpose hardware.

Specifically, the force integration and particle pushing are all done on the host computer, and only the inter-particle force calculations are done on the GRAPE (fig. 1). This may seem problematic, given the fact that the intrinsic speed of the GRAPE is a factor of 10,000 times larger than that of the host computer, an ordinary workstation. However, the inter-particle calculations require a computer processing power that scales with N^2, while all other actions on the host scale only in proportion to N. Therefore, each doubling of the number of particles doubles the work load on the GRAPE, relative to that of the workstation. In this way, no matter how slow the workstation is, it will be able to keep up with the GRAPE for large enough values of N.

For some applications, more efficient algorithms have been deviced, that require the computation of a number of inter-particle force calculations that scales with $N \log N$, rather than N^2. It turns out that even these methods can still be efficiently run on the GRAPE [2];

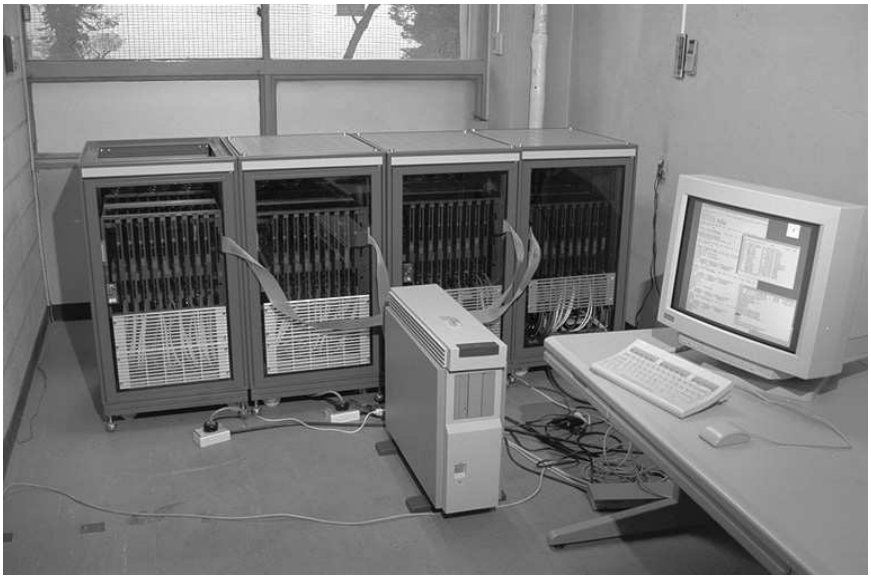

Figure 1: The GRAPE-4 hardware.

although the asymptotic scaling advantage is not very large in that case, the overall coefficient in the scaling relation turns out to favor the use of the GRAPE. Some versions of the GRAPE (Table 1) allow arbitrary force implementations, for applications such as molecular dynamics. For example, the MDGRAPE has been used to study the structure of protein molecules [3]. However, most GRAPEs have been used to study astrophysical problems. Below we will review a few representative cases.

Star Cluster Evolution

A globular star cluster [fig. 2; [4]] typically contains about a million stars, packed together much closer than the stars in the solar neighborhood. Such a cluster describes a wide orbit around the parent galaxy, well separated from the stars in that galaxy. If we would live in the core a dense globular cluster, the brightest stars would appear as bright as the full moon, which would make them too bright too look at directly, given their point-like nature. Optical astronomy of anything but the nearby stars in the same globular cluster would be rather difficult, in such a situation.

In the simplest approximation, we can study a globular cluster as a collection of point masses, reducing the problem to the gravitational N-body problem, which was solved by Newton for $N = 2$, but was only studied in detail for $N > 2$ when computers became available. Any localized distribution of particles will tend to become spherical, as a result of forgetting the initial conditions, on a two-body relaxation time scale:

$$t_{rel} \sim 0.1 \frac{N}{\ln N} t_{cr},$$

Table 1: Summary of GRAPE Hardware ([1])

Machine	Year	Peak Speed	Notes
Limited-Precision Data Path			
GRAPE-1	1989	240 Mflops	Concept system
GRAPE-3	1991	15 Gflops	48 Custom chips, 10 MHz clock
GRAPE-5	(1999)	$\sim$ 1 Tflops	under development
Full-Precision Data Path			
GRAPE-2	1990	40 Mflops	IEEE precision, commercial chips
HARP-1	1993	180 Mflops	force and its time derivative
GRAPE-4	1995	1.1 Tflops	1692 Custom chips, 32 MHz clock
GRAPE-6	(2000)	$\sim$ 200 Tflops	under development
Arbitrary Force Law			
GRAPE-2A	1992	180 Mflops	Force look-up table
MDGRAPE	1995	4 Gflops	Custom chip with force look-up table
MDGRAPE-2	(2000)	$\sim$ 100 Tflops	under development

where the crossing time t_{cr} is a measure for the time it takes for a typical star to move across the cluster.

Heat is transported through the cluster, as a consequence of many two-body encounters, on the time scale t_{rel}. On longer time scales, any self-gravitating star system is unstable. Since the system tends to relax towards a Maxwellian velocity distribution, there are always some stars that acquire a velocity that exceeds the escape velocity, after which they are lost from the system. Other stars tend to congregate in the central regions which grow denser at an ever-increasing rate, because higher density implies more frequent encounters and hence a faster two-body relaxation.

This run-away redistribution of energy and mass leads to a phenomenon called gravothermal collapse, often called core collapse, which takes place on a time scale $t_{cc} \sim 10 t_{rel}$. Core collapse was hinted at in numerical simulations [5] in the 1960s, and verified through direct N-body simulations [6] and modeled by semianalytic methods [7] in the 1970s. Core collapse is a fundamental feature of long-term stellar-dynamical evolution, showing the instability that results from the negative specific heat inherent in self-gravitating systems. During core collapse, at first the system can be modeled as passing through a series of self-gravitating equilibrium models exhibiting a maximum entropy for a finite central concentration. Once this maximum is passed, subsequent evolution will increase the entropy, and the structure

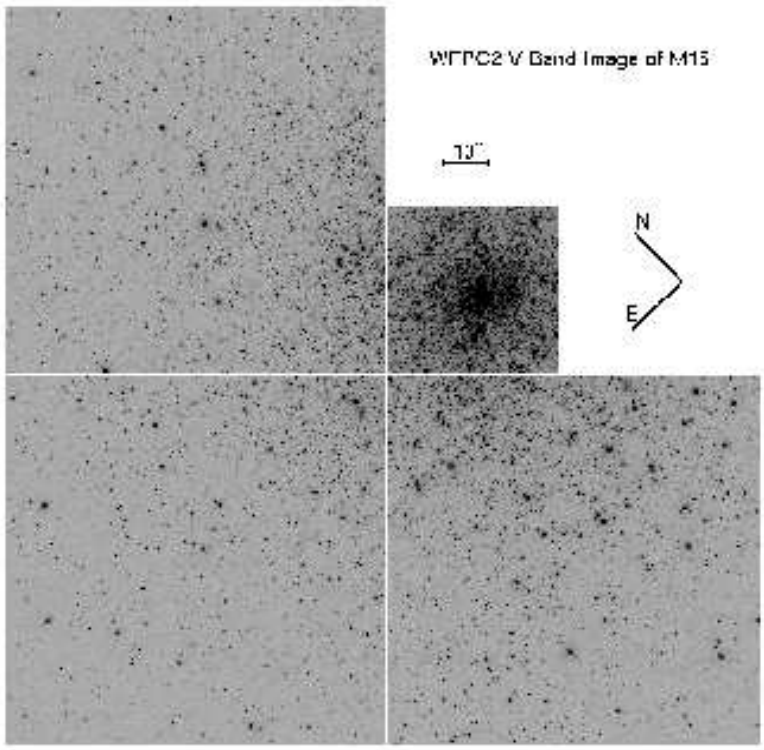

Figure 2: A globular cluster, M15, as seen by the Hubble Space Telescope[4]

of the star cluster is forced to deviate from that of an equilibrium model.

Even in an idealized system of self-gravitating point particles, core collapse will be halted before an infinite central density is reached. When the central density is high enough, occasional close encounters between three unrelated particles will form bound pairs (binary stars in the case of star clusters), with the third particle carrying off the excess kinetic energy required to leave the other two particles bound. Subsequent encounters between such pairs and other single particles tend to increase the binding energy of these pairs, which leads to a heating of the surrounding system of single particles.

When enough pairs have been formed in this way, the resulting energy production will reverse the process of core collapse. After reaching a minimum radius and a maximum density, the core region will expand again. Core collapse, when threatened to occur by the collective effects of two-body relaxation, can thus be narrowly averted by a handful of crucial three-body or four-body reactions in the dense core of a nearly collapsed cluster. What will happen next depends on the total number N of particles in the system. If this number is sufficiently small, $N \lesssim 10,000$, the whole system will slowly and steadily expand. In this case a steady-state equilibrium can be found between the steady energy production in three-body encounters in the center, and the continuous loss of energy through the outskirts of the system.

If the total number of particles exceeds 10^4, however, a different behavior emerges. The more particles there are in the system, the higher the central density has to become to halt core collapse. As a result, the post-collapse phase features a short relaxation time in the center of the cluster, shorter than the relaxation time in the outer regions, where most of the particles can be found. From the point of view of the inner core dynamics, the bulk of the mass further out seems almost frozen. It is this discrepancy in time scales that can cause the inner core to become 'impatient', and to revert to a local collapse, triggered by the slightest fluctuation in the direction of the energy flow produced by stochastic three- and four-body interactions.

What happens then is that about 1% of the inner particles will go into a coherent collapse, locally reminiscent of the original core collapse. As before, bound pairs of particles spring into action, generate energy, and manage to reverse the collapse in the nick of time, preventing an infinite central density from building up. This process repeats itself, leading to irregular oscillations of the core of the cluster.

The existence of these oscillations was unknown until 1983, when they were first found in approximate simulations [8]. Dubbed 'gravothermal oscillations', they were subsequently analyzed in detail with semi-analytic methods [9]. Their occurrence was confirmed in a variety of approximate numerical simulations [10], and shown to correspond to low-dimensional chaos for large N values [11]. Direct verification of the existence of these oscillations was attempted, using the fastest supercomputers available, but these attempts were unsuccessful [12, 13].

The reason that they were so hard to confirm through direct N-body simulations lies in the fact that it has not been possible to model star cluster evolution with more than 10,000 particles until the advent of the GRAPE-4. This may seem surprising, given the fact that cosmological simulations now routinely handle up to a billion particles. The main difference between the two type of calculations lies in the higher accuracy required for star cluster simulations, together with the much larger number of time steps required, in comparison with cosmological simulations.

As for the first point, following the gravothermal collapse requires a very accurate integration of the equations of motion. The required accuracy is difficult to achieve using approximate schemes like tree codes [14]. Therefore, traditional direct summation schemes have to be used. Even on supercomputers the maximum particle number is thus limited to about ten thousand.

The second point is related to the fact that N-body simulations play a very different role in the modeling of star clusters, and of cosmological large-scale structure formation. In the case of star clusters, each particle stands for an individual star, and thus has a direct physical meaning. In the case of a cosmological simulation, each galaxy is represented by a relatively small number of particles, that sample the distribution of stars in phase space. Each particle thus represents the average behavior of many millions of stars. The time steps used can therefore be much larger than would be the case if we were to follow the close encounters of individual stars.

Finally, the existence of gravo-thermal oscillations was proven when they were seen in a

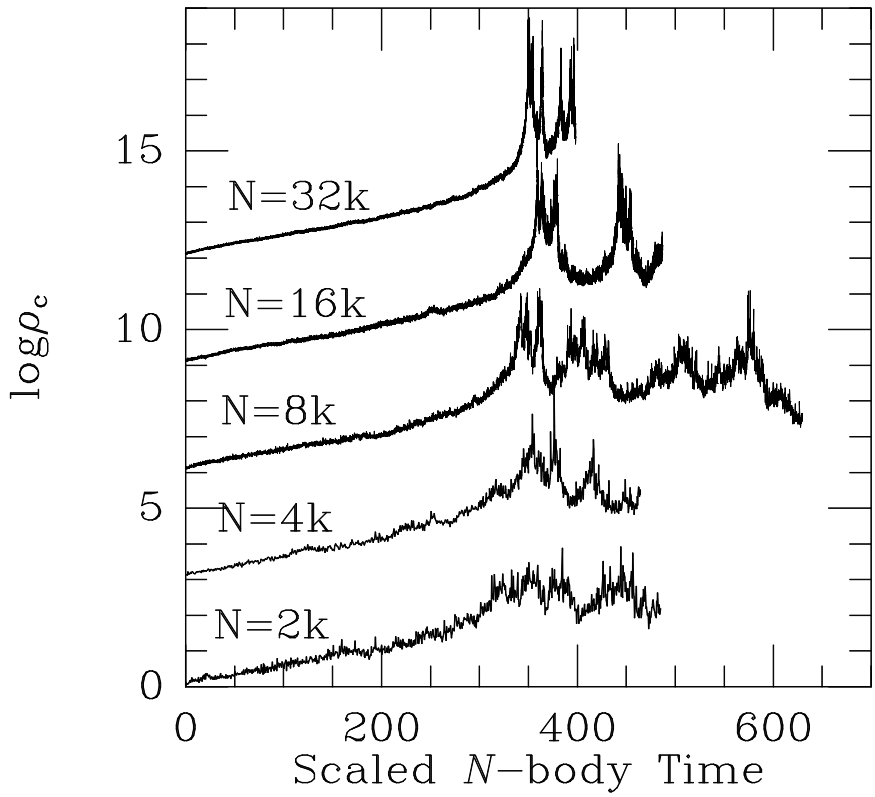

Figure 3: The evolution of the central density ρ_c. Thirty time units correspond roughly to one initial half-mass relaxation time. Curves for different values of N are vertically shifted by 3 units.

direct N-body simulation on the GRAPE-4 that was able to incorporate N values beyond $N = 10,000$ [15], as illustrated in figures 3 and 4.

After core collapse, the fluctuations in central density grow with increasing N values, as is clear from figure 3. For the largest N values displayed, the typical behavior of core oscillations emerges, with its deep and long-lasting throughs punctuated with brief interludes of high core density. For smaller N values, some oscillatory behavior seems to be present, but less pronounced. The results of the central density evolution, while suggestive, do not answer the question of the existence of gravothermal oscillations.

Figure 4, however, provides the proof of the gravothermal nature of these oscillations [16]. The thermodynamic cycle exhibited by the central density and 'temperature' (as measured by the velocity dispersion), is traversed in the opposite direction from that of a Carnot engine: the decompression stage takes place at a lower temperature than the compression stage. This is a reflection of the negative heat capacity of self-gravitating systems: compression leads to a temperature increase resulting in more heat loss and hence more compression, with the opposite effects holding during decompression. The period of decompression finishes when the core expands beyond the central isothermal area.

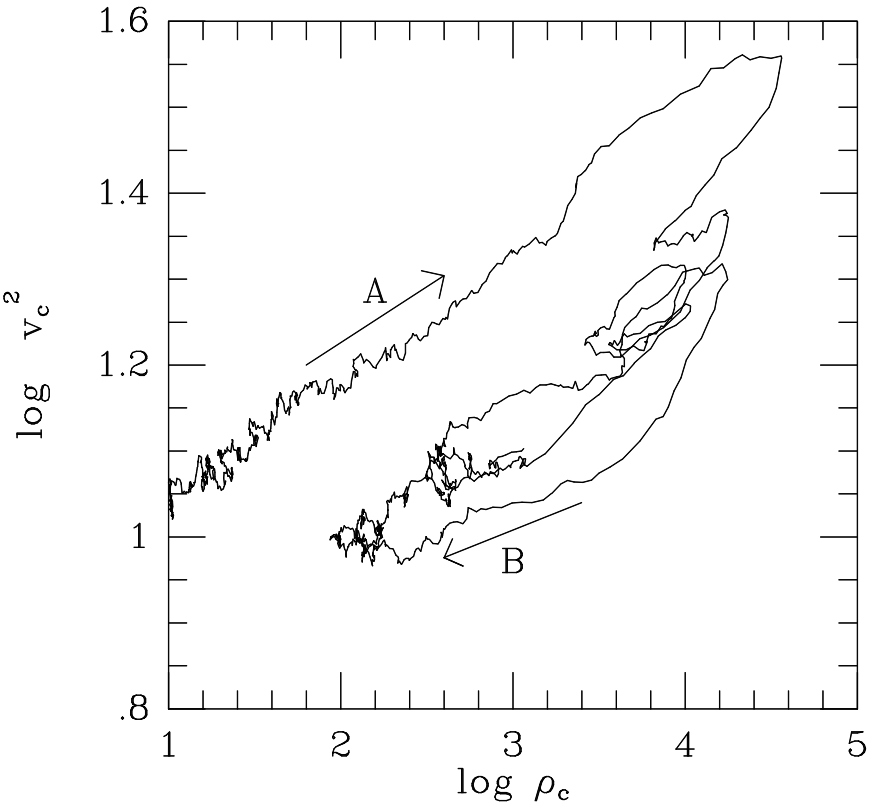

Figure 4: Changes in central density ρ and central velocity dispersion v_c^2, for a simulation with 32k particles. Each data point presents a time average, obtained by averaging ρ and v_c^2 over 80 snapshots. Arrows indicate the direction of evolution.

Having clarified the fundamental behavior of self-gravitating point mass systems, in the limit of very large numbers of particles, we are currently working on more realistic treatments of star clusters, where the evolution of individual stars is modeled [17].

Black Hole Spiral-In

When two galaxies collide, they are likely to stick together, if their relative speed is not too high. Within a few crossing times, the transient ripples and distortions will be smoothed out, and the resulting single galaxy will settle down into a new equilibrium configuration. While all this is going on, the dense cores of both galaxies will spiral in, as a result of dynamical friction, in the central regions of the collision. Finally they, too, merge to form a single core.

Many, if not most, galaxies harbor a massive black hole in their center. Recently, many such black holes have been detected, with masses spanning a range from a million to a billion solar masses, up to 0.1% of the mass of the parent galaxy [18]. When two galaxies collide and stick together to form one large merger remnant, the dense nuclei of the two parent galaxies will spiral in, within the central region of the newly formed galaxy. These nuclei

will merge to form a single dense nucleus, as soon as they come in contact with each other. What will happen, if each nucleus contains a black hole, however is far from clear.

At first, they will keep circling each other, within the single newly formed dense nucleus. Although dynamical friction tends to let them spiral in rapidly at first, this process becomes considerably less efficient by the time the amount of mass in stars between the two holes becomes smaller than the mass of the holes themselves. The stars that initially tend to be most efficient in providing a braking mechanism are scattered into different orbits. As a result, the system may reach a stagnation point, in which little further dynamical friction occurs.

The prediction of this stagnation process was made almost twenty years ago [19], and since then many attempts have been made to check this prediction quantitatively, using large-scale N-body calculations. Until the advent of the first GRAPEs, this problem was completely intractable, even on the largest supercomputers available. One reason that the GRAPE computers are suitable for this type of problem is the intrinsically high dimensionality of the problem. With two black holes in an eccentric orbit around each other, there is no symmetry in either configuration space or velocity space. As a result, the stellar dynamics problem is truly six-dimensional, when seen as a fluid flow in phase space.

In contrast, modeling a globular cluster is often done by assuming spherical symmetry, which leaves only one spatial dimension (radial) and two velocity dimensions (radial and tangential) to worry about. In practice, further simplifications have often been made, in which the distribution function of the stars is assumed to be dependent only on energy, or sometimes on energy and angular momentum. Fokker-Planck methods have therefore been very useful, initially, in modeling globular clusters, especially during the core collapse phase. After core collapse, during the reexpansion phase, the effects of binaries have to be taken into account, an extremely granular process that defies the main Fokker-Planck assumptions of smoothness of the distribution function. However, even so, it has been very useful to compare the full N-body calculations in the post-collapse domain with approximate Fokker-Planck treatments. However, a Fokker-Planck treatment of a six-dimensional system is completely impractical from the outset.

The first attempts to use the GRAPE to tackle this problem, were made in 1990 [20], using the GRAPE-2, followed by more recent attempts [21] on the GRAPE-4. Three important conclusions have emerged from these studies. (i) When two identical galaxies, each harboring a central black hole, merge, they will produce a merger remnant with a ratio of core radius r_c to half-mass radius r_h that is comparable to that of the original galaxies. In contrast, galaxies without black holes tend to produce merger remnants in which r_c/r_h is smaller than in the original galaxies. In the former case, $r_c/r_h \sim M_{BH}/M_{tot}$, where M_{BH} is the mass of the central black hole, and M_{tot} is the mass of the whole galaxy. (ii) This 'core', formed around the black hole binary after the merging of the two galaxies, does not have a completely flat density distribution in the center. In fact, it looks more like the 'weak cusps' observed in many galaxies by the Hubble Space Telescope [22]. The formation mechanism of this cusp is not well understood. (iii) Whether or not a black hole binary, lurking in the core of a merger remnant, has had time to spiral in within the current age of the Universe, and under which circumstances, is still largely an open question. We expect the continuum limit to be

reached for $N \simeq 10^7$. These calculations will only be feasible with the GRAPE-6 (Table 1).

Formation and Evolution Processes, from Planets to Galaxy Clusters

We will briefly discuss how the GRAPE computers have been used to study the origin of structure in the Universe, from very small scales to the largest scales that can be observed. On the small end, the coagulation of grains and boulders to form planets has been modeled, in order to understand the formation process of our own planetary system, as well as that around nearby stars. Increasing the length scale of interest by a factor of a billion, we discuss the formation of galaxies. Multiplying the size by another factor of a thousand, we reach the scale at which rich clusters of galaxies evolve.

Planet Formation

After the Sun was formed, some matter of the proto-solar nebula was left in a disk around the Sun. Grains that condensed out of the original gas coagulated through collisions to form larger and larger particles, the size of pebbles, boulders, and larger proto-planetary bodies. To model this process in detail has turned out to be difficult, because significant evolution takes place on a time scale larger than a crossing time, by a factor of a million or more.

The main stumbling block has been the need to simultaneously model the presence of a wide variety of particle sizes, or equivalently, masses. A little more than ten years ago, it was realized that dynamical friction plays an essential role in planetary formation. [23, 24] This process forces more massive particles to have smaller random velocity, which effectively increases their collision cross section. Thus, massive particles can grow much more rapidly than less massive particles.

Kokubo and Ida [25] used the GRAPE-4 to model this type of growth of planetesimals, under the assumptions that the accretion was perfect (*i.e.* the collisions were totally inelastic) and that there was no gas left in the system to cause non-gravitational drag on the particles. They found the mass distribution to relax quickly to a continuous power-law mass distribution with $dN/dm \propto m^{-2.5}$, where N is the cumulative number of bodies, independent of the initial mass distribution (a result that was subsequently derived analytically [26]). Their most interesting result was that the heaviest body would subsequently detach from the continuous power law distribution, featuring a much more rapid growth in mass, called runaway growth, that could lead to the formation of a planet.

Kokubo and Ida [27] again used the GRAPE-4 to study the later stages of planet formation, on a more global scale. The earlier local run-away studies, leading to the formation of a single protoplanet, give rise to multiple protoplanet formation when a large fraction of the protoplanetary disk is modeled. They found that such protoplanets are formed and keep growing independently provided their orbital separations are wide enough. After a while, the growth rate of these protoplanets slows down, because their gravitational perturbations increase the random motion of the swarm of planetesimals they are embedded in. A continuous mass distribution of relatively light planetesimals can thus coexists with a small number of large protoplanets, for millions of years.

Galaxy Formation

To study the formation of a single galaxy, it is important to model its environment, out to large distances, given the long-range character of the gravitational force, which through tidal effects influences the angular momentum distribution within the contracting gas clouds destined to form galaxies.

In addition, it is essential to model the gasdynamical effects that influence the early phases of galaxy formation. While the GRAPE has been designed primarily for stellar dynamical computations, it has proved to be flexible in accommodating deviations from an inverse square law. A key property of the GRAPE hardware is that it uses the inter-particle distances, that are computed in order to calculate the pair-wise gravitational forces, to construct for each particle, a list of neighboring particles that reside within a prescribed distance.

Using this neighbor list, hydrodynamical simulations can be run on the front end workstation. The prime example here is smoothed particle hydrodynamics, or SPH [28]. Examples of these types of simulations include the formation of galaxies [29], the physical origin of Ly-α and metal line absorption systems [30], the structure of galaxy clusters [31], and the fragmentation of molecular clouds [32].

Simulations of galaxy formation have demonstrated that structure, kinematics and chemical evolution of model galaxies which form in hierarchical clustering scenarios agree with corresponding properties of observed galaxy populations [33]. The major shortcoming is that simulated galaxies are too concentrated. This is usually referred to as the angular momentum problem [29] and suggests that efficient feedback due to late stages of stellar evolution (for example winds, and supernovae) is needed for a successful galaxy formation model.

Simulations of damped Lyman-α absorption systems demonstrated that non-equilibrium dynamics can easily explain the apparent discrepancy between the observed high velocity of low ionization lines and the relatively small circular velocity predicted by hierarchical models of structure formation. [30] The evidence that damped Lyman-α absorbers at high redshift are related to large rapidly rotating disks, which would disagree with the hierarchical clustering hypothesis, is thus not compelling. [34]

Galaxy Cluster Evolution

Galaxies are formed in a long drawn out process, starting somewhere within the first billion years after the Big Bang, and continue to form today. Most galaxies are formed in isolation or in small groups, but some galaxies are form in much richer groups, called clusters of galaxies, or even superclusters of galaxies. The typical properties of galaxies formed in such clusters are different from galaxies that were formed elsewhere. For example, most galaxies in clusters are elliptical galaxies, whereas most field galaxies are spiral galaxies. [35]

To what extent do these differences reflect the different formation history of the galaxies, as they may have been affected by, for example, the much higher matter density in the sites where rich clusters of galaxies were born? And to what extent do the differences reflect later modifications to the galaxies, as a result of the different dynamical environment of a rich cluster? In attempts to resolve this nature versus nurture debate, the GRAPE has been used

to model the internal evolution of a rich galaxy cluster.

Apart from the calculations by Bartelmann and Steinmetz [31], already mentioned in the previous section, earlier work by Funato *et al.* [36] simulated the evolution of clusters of galaxies containing 32 to 128 galaxies. What they found is that 'passive' evolution of galaxies, caused by mutual encounters as well as by the influence of the tidal field of the parent cluster, alters the mass and size of individual galaxies. In particular, they found that passive evolution leads to a distribution of masses with $M(\sigma) \propto \sigma^4$, where σ is the internal velocity dispersion of the stars within a galaxy.

To understand the detailed mechanism of this passive evolution, Funato and Makino [37] used the GRAPE-4 to study a large number of encounters between two isolated galaxies, in order to determine how the resulting changes of mass and binding energy depend on the models used for the galaxies, and on the parameters describing the type of encounter. They then estimated the cumulative effect of encounters, in the setting of a rich cluster of galaxies. They again found that the mass distribution of galaxies tends to approach $M(\sigma) \propto \sigma^4$, for the mass M of a galaxy as a function of its velocity dispersion σ.

Their results resembles the observational Faber–Jackson relation, the empirical result that the luminosity of a galaxy $L(\sigma) \propto \sigma^4$, for elliptical galaxies. Note that the remnants of collisions between galaxies typically resemble elliptical galaxies, even if the progenitors were spiral galaxies or other types of galaxies. Because it is also reasonable to assume that $M \propto L$, this agreement with observations suggests that the encounters of galaxies play an important role in the evolution of galaxies in a cluster of galaxies.

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