

LA GRANJA: A BEOWULF TYPE COMPUTER FOR NUMERICAL SIMULATIONS IN STELLAR AND GALACTIC DYNAMICS

H. Velázquez and L. A. Aguilar

Instituto de Astronomía
Universidad Nacional Autónoma de México, Ensenada, B. C., México

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RESUMEN

Presentamos una computadora tipo “Beowulf” construida usando componentes comerciales y programas libres. Se compara su rendimiento en capacidad de cálculo y eficiencia en computaciones paralelas con el obtenido para una computadora Origin-2000 de la compañía SGI, usando dos códigos de N -cuerpos diferentes. Se discute el impacto de esta tecnología, que abre la posibilidad de efectuar de manera rutinaria simulaciones con alrededor de un millón de partículas con una computadora “hecha en casa”. Se muestra el efecto de mayor resolución numérica con simulaciones de un colapso sin disipación frío, y del calentamiento de la componente vertical del disco de una galaxia espiral que evoluciona aisladamente.

ABSTRACT

We present a Beowulf type computer built using off-the-shelf hardware and freely available software. Its performance in raw computational power and parallel efficiency is compared with an SGI Origin-2000 computer using two different N -body codes. The impact of this technology in opening up the possibility of making routine $N \sim 10^6$ particle simulations with a “home made” computer is discussed. The effect of higher numerical resolution is shown with simulations of a cold dissipationless collapse and of the vertical heating of the disk component of a spiral galaxy evolving in isolation.

Key Words: MISCELLANEOUS — METHODS: N -BODY SIMULATIONS — METHODS: MISCELLANEOUS

1. INTRODUCTION

The historical development of the field of classical gravitational dynamics has been the opposite to that in most other fields of physics: while usually a macroscopic and empirical description of phenomena precedes the discovery of the basic interaction rules, in classical gravitational dynamics Newton wrote down the basic rule of interaction from the beginning. The interaction rule, unfortunately, does not allow an analytical solution for more than two interacting particles and a numerical solution is mandated for almost any problem.

The N -body problem has had an long and illustrious history in celestial mechanics. The development of many powerful concepts and analytical tools have been derived from it (e.g., the concept of chaos, Poincaré 1890). The first numerical simulation of the N -body problem in galactic dynamics is due to Holmberg (1941) who built an ingenious device to

follow the interaction of two galaxies substituting gravity by light. Subsequent progress in the field of numerical simulations of the N -body problem has sprung from advances in computer technology, either hardware, like the introduction of powerful new generations of computers and novel dedicated machines (e.g., the “digital orrery” of Applegate et al. 1985 and the GRAPE processors of Sugimoto et al. 1990), or in software, like the introduction of novel algorithms to compute forces (e.g., the tree paradigm, Appel 1981, Jernigan & Porter 1989, Barnes & Hut 1986).

The most recent paradigm in computer architecture is the appearance of the “home-made supercomputer” embodied in the concept of the “Beowulf Computer”: a cluster of PC-boards relying on off-the-shelf hardware to run and communicate among themselves, operating with freely available software (Sterling et al. 1999). The first Beowulf-type computer was built in 1994 at the NASA Goddard Space Flight Center. It had 16 Intel 80486 processors run-

ning at 66 MHz and achieved sustained computing rates of 74 Mflops. Two years later, a third generation of Beowulf computers had broken the Gflop barrier and was awarded the 1997 Gordon Bell Prize for best performance to price ratio (Sterling 1994; Sterling et al. 1999).

Today, four Beowulf type machines built in academic institutions appear in the list of the 500 most powerful computers of the world. The Presto III machine built in 2001 at the GSIC Center of the Tokyo Institute of Technology with 256 Athlon processors, running at 1.2 GHz, achieving a maximum LINPACK performance of 331.7 GFlops, and ranked 86th. The CLIC PIII computer built in 2000 at the Technische Universitaet Chemnitz in Germany, with 530 Pentium-III processors running at 800 MHz and with a peak LINPACK performance of 221.6 GFlops, ranked 137th. The Netfinity Cluster PIII built by POSDATA in Korea consists of 320 processors PIII of 1 GHz and ranked 184th reaching a peak performance of 184.4 GFlops. Finally, Kepler, built at the University of Tübingen in Germany in 2000 using 196 Pentium-III processors running at 650 MHz and achieving a peak LINPACK performance of 96.2 GFlops, ranked 495th (see list at <http://www.top500.org>).

In México, the first Beowulf computer built in an academic institution was “Hormiga”, assembled by Alberto Vela of CINVESTAV in 1997–1998 (A. Vela 2002, private communication). It had 10 Pentium II processors running at 233 MHz, linked using twisted pair Ethernet running at 100 Mbps. It is interesting to note that this computer was built using computers stored in a warehouse pending construction of a terminal room at CINVESTAV. The second Beowulf machine built in México at an academic institution is the machine we describe here: “La Granja”, built at the Ensenada branch of the Instituto de Astronomía of the National Autonomous University of México (IAUNAM). As far as we know, there is only a third Beowulf computer built in México in an academic institution. This is a 20 Pentium III processor built at the México City branch of the IAUNAM (D. Page 2002, private communication).

La Granja is currently the largest such machine in México. It has been devoted to run N -body simulations for research in stellar and galactic dynamics and several codes have been ported to it. There is an SGI Origin-2000 mini-supercomputer at IAUNAM/Ensenada with 6 MIPS R10000 processors. We use this machine as a point of comparison to gauge the performance of our home-made computer. In § 2 we describe the hardware of the machine and

the software used. Section § 3 briefly describes the numerical experiments used to carry out our study. In § 4 we compare “La Granja” with an SGI Origin-2000 mini-supercomputer; the performance in computational power and efficiency of parallelization are contrasted using the same code and problem. Also, the cost of running the computer is assessed. In § 5 we use simulations of a cold dissipationless collapse and a disk galaxy to illustrate the importance of numerical resolution in N -body experiments. Finally, in § 6 we discuss the impact that the availability of this type of computer can have in our field of research and we present possible upgrades.

2. THE COMPUTER

La Granja is a Beowulf-class parallel computer built from cost-effective and mass-market components. This has the advantage of reducing the price of technical massive computing and providing a facility to run numerical simulations with a great price/performance ratio as compared with conventional supercomputers (e.g., Origin-2000).

2.1. Hardware

In its present configuration, it consists of 16 nodes each one with the following hardware components:

- 2 Pentium III processors of 450 MHz each one with a cache size of 512 KB.
- 512 MB of SDRAM at 66 MHz.
- A 12 GB hard drive.
- A Fast Ethernet card (10/100 Mbps).

No graphics and sound cards, floppy, keyboard, mouse or cdrom are needed. La Granja is interconnected by its own private LAN through a Fast Ethernet Switch (100 Mbps). We have chosen a Bay Stack 450 Fast Ethernet Switch (100 Mbps) since it provides an ample backplane of 2.56 Gbps which guarantees a fast communication among nodes with a latency as low as $9\mu\text{s}$ for short messages of 64 bytes. A schematic representation of La Granja is shown in Figure 1 where a server works as the user front-end.

A steady power supply for La Granja is provided with a Mitsubishi UPS unit with a capacity of 6 KVA. A key problem that had to be addressed is cooling. La Granja consumes 1.6 KW of power and this requires an active cooling system. Our computer is located in a closed air-conditioned room on

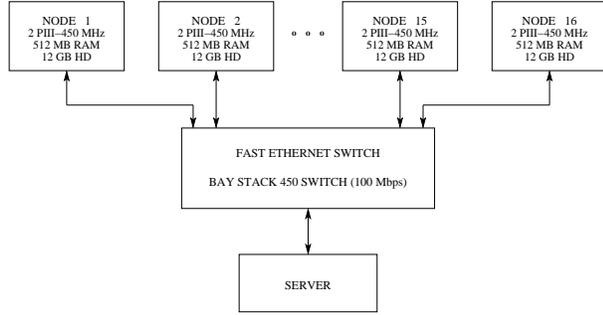


Fig. 1. La Granja: a schematic representation. It consists of 16 nodes and a server as front-end. Everything is connected through a 100 Mbps Fast Ethernet switch.

a stack of four shelves. This is a compact space-saving configuration, but the sides of the node cases are required to be kept open in order to allow air circulation. An air conditioning unit with a capacity of 3 tons of cooling (i.e., 36,000 Btu per hour) can adequately maintain an operating temperature of 20–21 degrees Celsius. It is not possible to operate La Granja without the use of the air conditioning unit, as the temperature of the room reaches 50 degrees Celsius within several minutes of turning off the air conditioner. A steady supply of clean electricity and active cooling are essential for the proper working of La Granja.

2.2. Software

La Granja uses the RedHat distribution release of LINUX (version 6.2) as the Operating System (OS). We have recompiled the kernel in order to include patches for improving the TCP (Transmission Control Protocol) communication between nodes for short messages. Both the OS and TCP patches are freely available at the following web sites: <http://www.redhat.com> and <http://www.icase.edu/CoralProject.html>.

TCP communication between nodes is achieved through the PVM (Parallel Virtual Machine) and MPI (Message-Passing-Interface) libraries. MPI is implemented into MPICH (MPI-Chameleon) and LAM (Local-Area-Multicomputer). We have also used the GNU compilers: gcc and g77.

3. NUMERICAL EXPERIMENTS

In this section we briefly describe some experiments used to quantify and compare the performance and resolution reached with this home-made computer. For this purpose we use simulations of a cold dissipationless collapse and a spiral galaxy. These examples are typical of those found in studies of the dynamics and evolution of galaxies.

3.1. Cold Dissipationless Collapse

Cold dissipationless collapse has been studied by several authors as a possible mechanism for the formation of elliptical galaxies and triaxial dark haloes (Polyachenko & Shukman 1981; Aguilar 1988; Aguilar & Merritt 1990; Palmer & Papaloizou 1987). In an important work, van Albada (1982) demonstrated that a dissipationless cold collapse produces a final configuration similar to an elliptical galaxy with a surface density profile well described by a de Vaucouleurs law. Previous N -body simulations by Gott (1973) failed to produce this profile because they lacked enough dynamical range. Cold dissipationless collapses produce triaxial configurations which are associated with the so-called “radial orbit instability”, that affects systems dominated by radial orbits. More recently, dissipationless collapse has been put forward as a possible mechanism to form cuspy density profiles, like the ones observed in ellipticals (Hozumi, Burkert, & Fujimara 2000). The fact that this is a problem where a large numerical resolution is paramount, and that has been thoroughly investigated in the past using N -body simulations, makes it ideally suited as a test bed for our computer.

To generate the initial conditions for our dissipationless collapse experiments, we set up the particle positions from the following spherical density profile:

$$\rho(r) = \frac{M}{2\pi R^2} \frac{1}{r}, \quad (1)$$

where M is the total mass and R is its maximum extent.

Velocities are randomly generated from an isotropic Gaussian distribution, such that the initial virial ratio is $\eta = 2K/|W| = 0.01$, where K and W are the kinetic and potential energies of the system, respectively.

For this case, we have chosen a system of units such that $G = 1$, $M = 1$ and $E = -1/4$, E being the total energy of the system. We use a total of 10^5 , 10^6 , and 10^7 particles to carry out these tests. With these units the free-fall time scale is about $t_{\text{ff}} \approx 5$.

3.2. Spiral Galaxy

Simulations involving realistic models of spiral galaxies are by far more complex to carry out than spherical ones, due to the wide spatial and mass range imposed by the cold disk component. First attempts to simulate encounters between disk galaxies were performed in the early 70’s (Toomre &

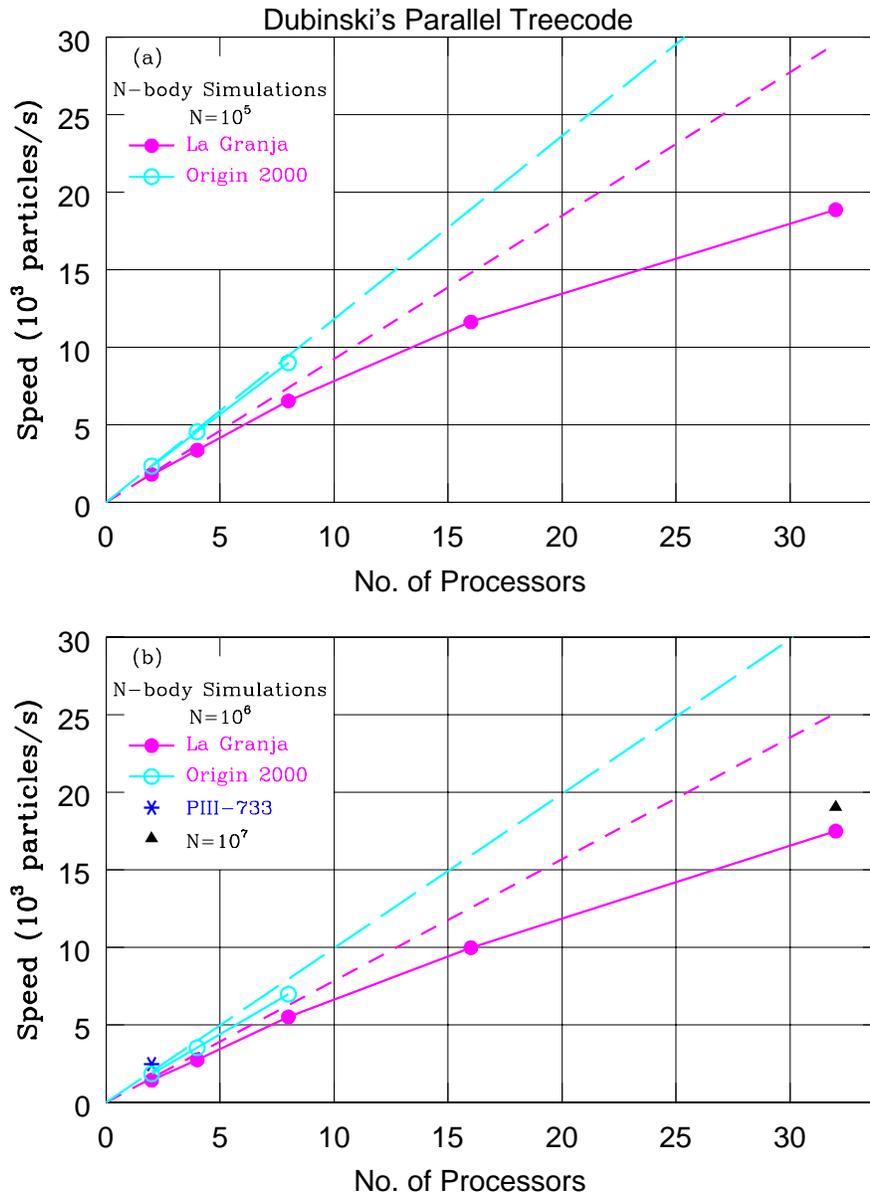


Fig. 2. Dubinski's parallel treecode performance for cold dissipationless collapses. For these simulations we used 10^5 (upper panel), and 10^6 (lower panel) particles, and both our Beowulf computer and the Origin-2000. The straight lines represent an ideal performance for a perfectly load-balanced DPTC code for this simulation: the long-dashed line for an Origin-2000 and the short-dashed for our computer. We have also indicated a 10^6 -particle test done on a system with dual Pentium III at 733 MHz (star symbol), and a simulation consisting of 10^7 particles ran on La Granja (filled triangle).

Toomre 1972); however, they did not successfully explain the observed continuous extension of the spiral arms right into the galaxy center, since they ignored self-gravity in their test particle representation of the disk component (Toomre 1981). Recent improvements in setting up stable self-gravitating disk

galaxy models (Hernquist 1993; Kuijken & Dubinski 1995) have allowed one to address, in detail, mergers and encounters between spiral galaxies (Barnes 1999 and references therein), and even clusters (Moore et al. 1999), although these N -body simulations have required a large number of particles. This is also

the case when studying the heating of galactic disks by accretion of satellites (e.g., Quinn & Goodman 1986; Quinn, Hernquist, & Fullagar 1993, Font et al. 2001), and bar formation and its subsequent evolution (Debattista & Sellwood 1998), providing important clues about the models of galaxy formation by constraining the accretion rate of matter and the inner structure of galaxy haloes, respectively. For these reasons, we have included a simulation of an isolated disk galaxy to test the performance of our computer.

Our numerical spiral galaxy is a composite model of a disk, a spherical bulge and a halo. The particle positions are generated from the following density profiles:

$$\rho_D(R, z) = \frac{M_D}{4\pi R_D^2 z_0} \exp(-R/R_D) \operatorname{sech}^2(z/z_0), \quad (2)$$

$$\rho_B(r) = \frac{M_B}{2\pi} \frac{a}{r(r+a)^3} \quad (3)$$

and,

$$\rho_H = \frac{M_H \alpha}{2\pi^{3/2} r_{\text{cut}}} \frac{\exp(-r^2/r_{\text{cut}}^2)}{R^2 + \gamma^2}, \quad (4)$$

where M_D , M_B , and M_H are the disk, bulge and halo masses. The disk structure is characterized by a radial R_D and a vertical z_0 scale length, while a corresponds to the bulge scale length. r_{cut} and γ are the cut-off and core radii of the halo and α is a normalization constant. A detailed description of the method used to set up a spiral galaxy is beyond the scope of the present paper; we refer the reader to Hernquist (1993). In Table 1 we list the parameters that define our galaxy model. We have adopted $G = 1$, $M_D = 1$, and $R_D = 1$ as our unit system. Assuming a disk mass of $5.6 \times 10^{10} M_\odot$ and $R_D = 3.5$ kpc, the units of time and velocity are 1.3×10^7 yr and 262 km s^{-1} , respectively.

3.3. Numerical Tools

To assess the performance of our computer to carry out N -body simulations we use two versatile algorithms: a Parallel Tree Code kindly provided by Dubinski (Dubinski 1996), hereafter DPTC, and GADGET (Springel, Yoshida, & White 2001). Both codes are easily implemented in La Granja since they rely on the portability of the MPI libraries. Dubinski's parallel tree code uses a fixed timestep, while GADGET has the advantage of assigning individual timesteps to the particles.

In the case of the cold dissipationless collapse with the DPTC code, we use a tolerance parameter of $\theta = 0.75$ and a timestep of $\Delta t = 0.01$, with

TABLE 1
SPIRAL GALAXY MODEL

Disk		Bulge		Halo	
M_D	1	M_B	0.3	M_H	8.0
R_D	1	a_B	0.2	γ	1.0
z_0	0.2	ϵ_B	0.05	r_{cut}	25.0
Q_\odot	1.5	N_B	20,000	ϵ	0.05
R_\odot	2.43		2500 ^a	N_H	400,000
ϵ	0.05				50,000 ^a
N_D	100,000				
	12,500 ^a				

^aRefers to the galaxy model with the lowest resolution.

the quadrupole terms of the force included. For GADGET tests, the individual timesteps are determined by a criterion based on the particle acceleration, and are defined by $\Delta t = \eta_v/|\mathbf{a}|$ with $\eta_v = 0.02$ (see Springel et al. 2001 for a detailed description of this code). In both cases, the softening parameter was fixed to be $\epsilon = 0.01$. With these parameters the energy conservation was better than 0.5% for about $5t_{\text{ff}}$ in both cases.

To simulate the evolution of the disk galaxy we use the DPTC code with a tolerance parameter of $\theta = 0.75$ and a timestep of $\Delta t = 0.1$ (~ 1.3 Myr). This simulation was evolved for about 250 time units (~ 3.25 Gyr) with a energy conservation better than 0.3%.

4. PERFORMANCE

In this section we compare the performance obtained in La Granja with that for an SGI Origin-2000 using both codes: DPTC and GADGET. The Origin-2000 has 8 processors MIPS R10000 running at 195 MHz and with 2 MB of cache each. We should mention that for the simulations in the Origin-2000 we used the latest proprietary version of MPI (1.2) available from the Silicon Graphics Web page. To compare the performance of both computers we used only the N -body simulation of a cold dissipationless collapse.

4.1. Performance under DPTC

In Figure 2 we have plotted the speed, in particles per elapsed wall-clock time, obtained on La Granja and on Origin-2000, as a function of the number of processors and the number of particles. The straight lines refer to an ideal performance for a perfectly load-balanced DPTC code: long-dashed lines correspond to the Origin-2000 and short-dashed lines

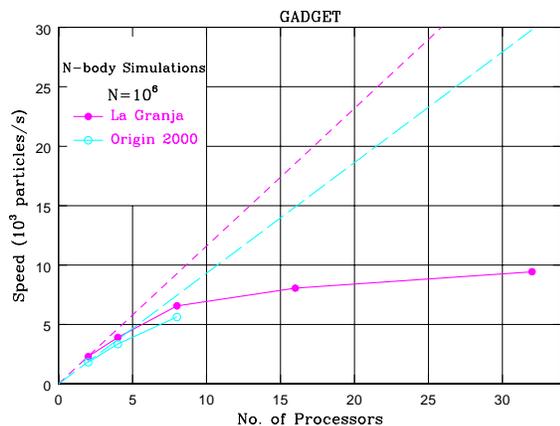


Fig. 3. Overall GADGET speed for a cold dissipationless collapse with 10^6 particles as a function of the number of processors for our Beowulf computer and the Origin-2000. As in Fig. 2, the straight lines show the ideal performance for a perfectly load-balanced GADGET: the long-dashed line corresponds to an Origin-2000 and the short-dashed line to La Granja.

to our computer. We have also included a 10^6 particle experiment done on a dual system of PIII at 733 MHz (star symbol) and a simulation with 10^7 particles ran on La Granja (filled triangle). Some trends are clearly observed. (1) In each instance the Origin-2000 is faster than our computer, but not by much, at most by a factor of 1.3. (2) Comparing both panels of Fig. 2 we see that the speed of an 8-processor Origin-2000 has dropped by about 30% when we increase the number of particles from 10^5 to 10^6 in our N -body simulation, while this reduction is about a factor of two less for our computer with 32 processors. This result suggests that the cache of the processors does not play an important role once it is completely saturated. (3) The DPTC code scales well with the number of processors in both computers, indicating that this code is more CPU-limited than limited by communication, for this number of processors.

4.2. Performance under GADGET

We have repeated our cold dissipationless collapse experiments with 10^6 particles, but now using GADGET. In Figure 3 we show the performance (the overall code speed in particles per elapsed wall-clock time) obtained in these simulations. We can notice that: (1) In this case our computer outperforms the Origin-2000 regardless of the number of processors. (2) The scaling of GADGET on La Granja is not very good as we go from 8 to 16 or 32 processors; it shows a poor load-balance, which may be due to

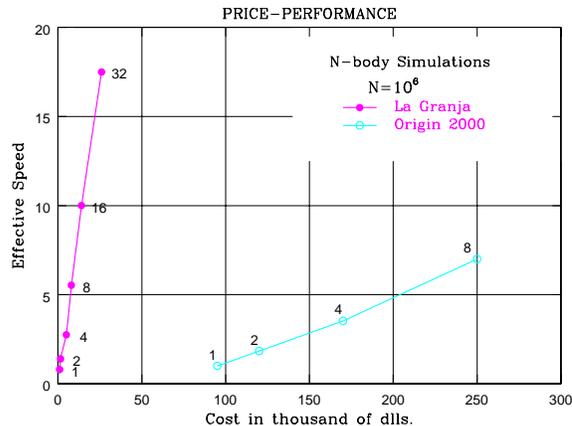


Fig. 4. This figure shows the speed, normalized to that of an Origin-2000 with one processor, of our Beowulf computer and an Origin-2000 as a function of their cost¹. The simulation is that of a 10^6 particles of a cold dissipationless collapse with the DPTC code. The huge gain in performance to cost ratio obtained with our home-made computer is remarkable.

the limited communication bandwidth provided by our Fast Ethernet switch. For a full-load run on La Granja, this factor alone accounts for $\sim 40\%$ of the total elapsed wall-clock time. Unfortunately, we do not have access to a faster communication switch to check its impact on reducing the wall-clock time in the load-balancing step. Obviously, GADGET is more a communication-limited code than a CPU-limited one.

4.3. Operational Costs

One of the greatest advantages of Beowulf clusters is that they provide supercomputer power at a reduced cost, compared with a conventional supercomputer. Furthermore, the maintenance of a Beowulf class computer is minimal.

In Figure 4 we show the “effective” performance (using DPTC) for both computers, relative to a one single processor R10000, as a function of their cost.¹ This figure clearly shows the huge gain in performance for this particular code of our home-made computer, which turns out to be equivalent to an Origin-2000 with 17 *effective* processors at just 10% of the price of an 8-processor Origin-2000.

A final comment on operational costs: the power consumption of our Beowulf cluster, at full operation, is similar to the power required by the Origin-2000 with 8 processors (~ 1.6 KW).

¹Prices for the Origin-2000 are *circa* 1997 scaled from a 6-processor machine. Prices for La Granja are scaled from our 32-processor machine and are *circa* 1999.

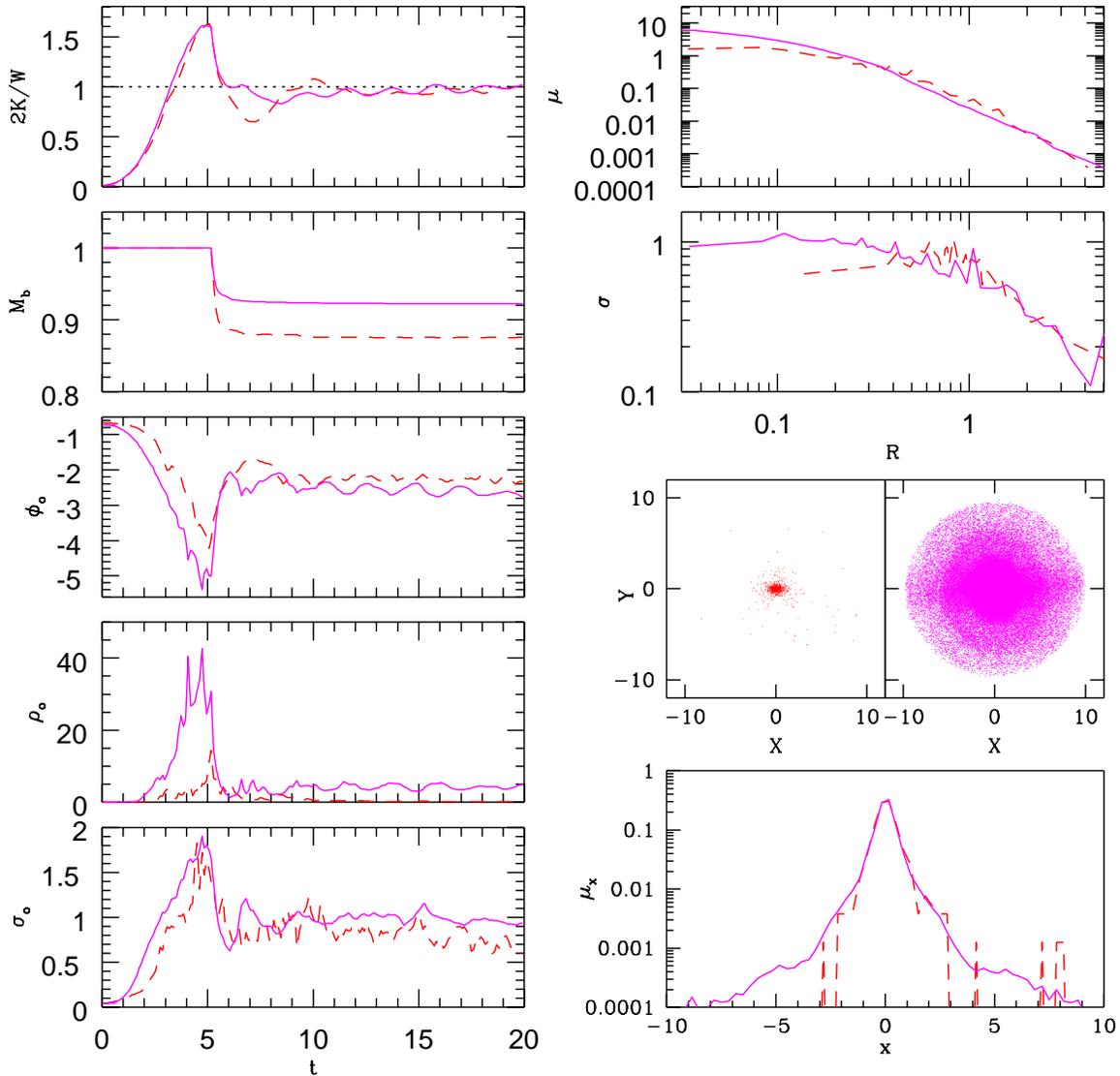


Fig. 5. Cold dissipationless collapse simulations with 10^3 (dashed lines) and 10^6 (solid lines) particles. We plot several global properties such as the virial ratio (upper left panel), total bound mass (next left panel down), final projected surface density profile (upper right panel) and final velocity dispersion profile (next right panel down). We also plot local parameters like the value of the central potential (middle left panel), central density (next left panel) and central velocity dispersion (bottom left panel). The middle right panels compare projected scatter plots of both simulations and the bottom right panel compares projected surface densities sections along the x-axis.

5. NUMERICAL RESOLUTION

Availability of La Granja has allowed us to perform 10^6 -particle class simulations in a routine manner. The increased particle number translates into a higher spatial resolution, which is crucial in the investigation of many stellar and Galactic dynamical problems. In this section, we present a couple of illustrative examples to contrast the quality of the results obtained with simulations of the same initial conditions, performed with different number of particles.

5.1. Cold Dissipationless Collapse

A full study of this issue is beyond the scope of this paper. Here, we just want to illustrate the impact of higher numerical resolution in numerical simulations of this problem. To this end, we carry out two simulations of the same experiment: one with 10^3 particles and the other with 10^6 particles. For each simulation we have computed as a function of time global quantities like the virial ratio and bound mass, and local properties like the depth of the potential and central values of density and velocity dis-

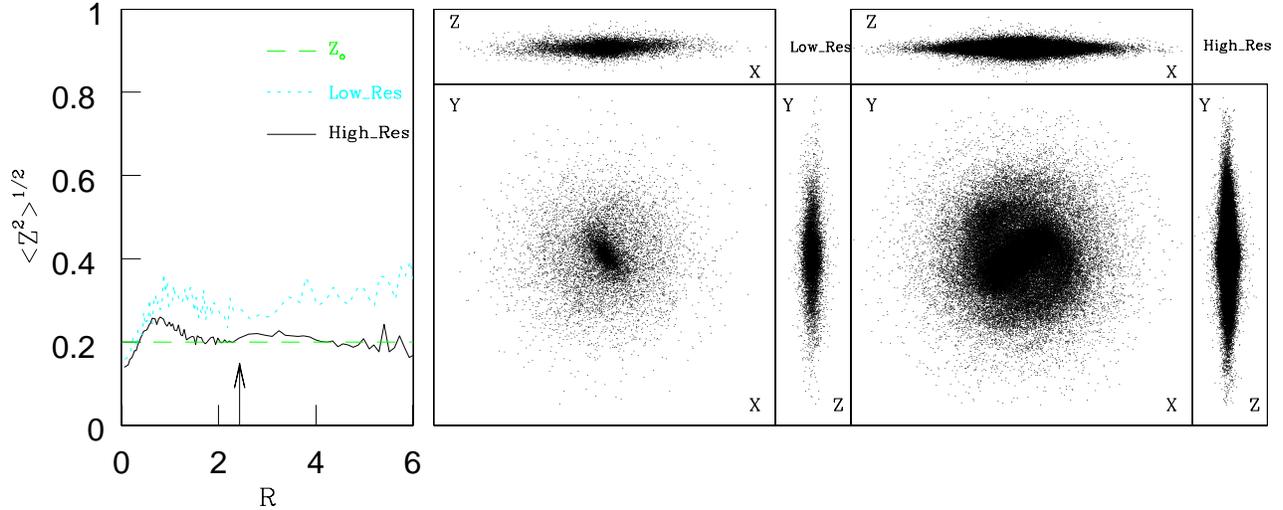


Fig. 6. Simulation of a disk spiral galaxy with a lower (middle panel) and higher (right panel) numerical resolution. The resulting vertical scalelength after 250 time units (3.25 Gyr) of evolution is shown in the left panel. The arrow indicates the Sun’s position (8.5 kpc), and the horizontal straight line corresponds to the initial vertical scalelength (Z_0) of the disk.

persion. We also plot projected density and velocity dispersion profiles at the end of the simulation. Although similar in their rough behaviour, all quantities plotted as a function of time present differences between both simulations. The virial ratio shows smaller fluctuations and the model loses less mass in the higher resolution experiment. On the other hand, variations in the central values of density and potential are more pronounced at the time of first collapse ($t_{\text{ff}} \sim 5$ time units) for the same higher-resolution experiment. The final density and velocity dispersion profiles, although similar in the external part, go deeper in the higher-resolution run, developing a power-law central cusp in the former and more spikes in the latter. These spikes are due to collapsing shells that have not yet been erased by the process of violent relaxation. Finally, a comparison of the projected scatter plot of both simulations reveals more structure in the higher resolution simulation, like a bar-like structure, whose long-axis was rotated to be oriented with the x -axis, and a shell of material.

5.2. Spiral Galaxy

Another interesting example where the mass and spatial resolution plays an important role is provided by numerical simulations of disk galaxies, since their disk component is quite thin, supported by rotation and prone to instabilities. Controlling numerical diffusion is fundamental in studies of disk heating by accretion of satellites (Quinn et al. 1993; Walker, Mihos, & Hernquist 1996; Huang & Carlberg 1997; Velázquez & White 1999), and bar formation

and secular evolution (Debattista & Sellwood 1998), among others.

The importance of reducing numerical noise is best illustrated by the change in disk thickness due mainly to the discrete representation of the halo component. In Figure 6 we have plotted the final snapshot of the simulations listed in Table 1 at $t = 250$ model units (~ 5 Gyr): the middle and right panels correspond to the three main projections (XY , XZ , and YZ) for our lowest (65,000 particles) and highest (520,000 particles) resolution experiments, respectively. We characterize the change in the vertical structure of the galaxy disk through its vertical scale-length defined as: $z_0(R) \equiv \langle z(R) \rangle^{1/2}$. In the left-panel of this figure we show the resulting vertical scale-length of the disk for our low (dotted-line) and high (solid-line) resolution simulations. The long-dashed line corresponds to the initial value of the vertical scalelength. It is easy to see that the simulation with lower resolution has increased its vertical scalelength by $\sim 40\%$, while the one with higher resolution has suffered an increase of just 5% at the Sun’s position (indicated by the arrow).

6. CONCLUSIONS AND FUTURE WORK

We summarize our main conclusions as follows:

- A Beowulf home-made computer offers super-computing performance to carry out high resolution N -body simulation of stellar systems at a small fraction of the cost of a conventional supercomputer. Therefore, for a country with limited financial resources a Beowulf computer is a viable alternative.

- La Granja allows us to carry out N -body simulations with 10^6 particles in a routinely manner, increasing the mass and spatial resolutions available to us. This is particularly important in order to address problems such as the formation of cuspy density profiles in galaxies, the secular evolution of bars and its relation with the inner structure of halos, among several interesting problems.
- We proved that currently available state-of-the-art codes can be easily ported to our computer. We have found that Dubinski's parallel tree code scales quite well with increasing number of processors, while GADGET scaling is strongly affected by the poor load-balance on La Granja, due to the reduced bandwidth provided by our Fast Ethernet Switch of 100 Mbps.

The continuing advance in technology opens the possibility to build even faster and better Beowulf-class computers. We could incorporate new and faster processors and new communication technologies such as Gigabit, or Myrinet, which provide faster communications by an order of magnitude at low latency, but still keep the costs to a minimum. The impact of faster processors is illustrated in Fig. 2 where we performed a test with a system consisting of a dual Pentium III running at 733 MHz and with 256 KB of cache (star symbol). We observed a gain in performance by about a 70–80% with respect to a single node of La Granja. Of course, incorporating faster processors will require better communication technologies, so it is important to reach a compromise between these factors.

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Luis A. Aguilar y Héctor Velázquez: Instituto de Astronomía, UNAM, Apdo. Postal 877, 22860, Ensenada, B. C., México (aguilar, hmv@astro.unam.mx).