Scientific Computing on Special-Purpose Computers

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February 19, 2009

Structure of my lecture

- Introduction
  - Who am I?
  - Kepler's problem and the stability of the Solar system
- Stellar Dynamics
  - Example of stellar systems
  - Galactic dynamics
- Gravitational many-body systems
- Building computers for Gravitational many-body systems

Who am I?

- My name is Jun Makino (Junichiro Makino ...).
- Professor at National Astronomical Observatory of Japan.
- That means I am an "astronomer".
- That does not imply I have ever used any telescope to observe anything.

Then what do I study?

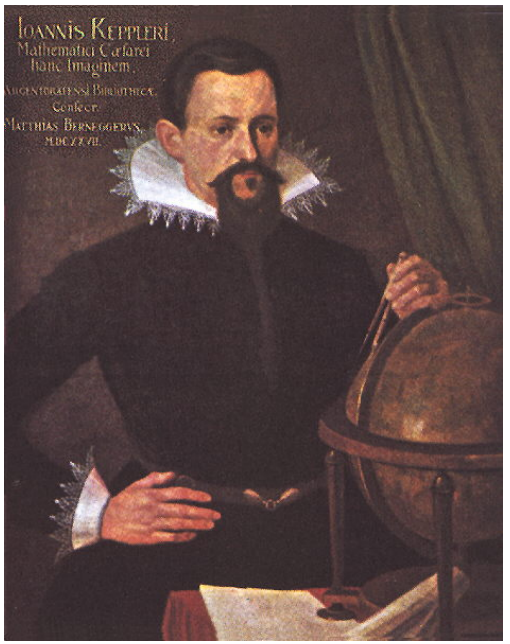
"Theoretical Astronomy"

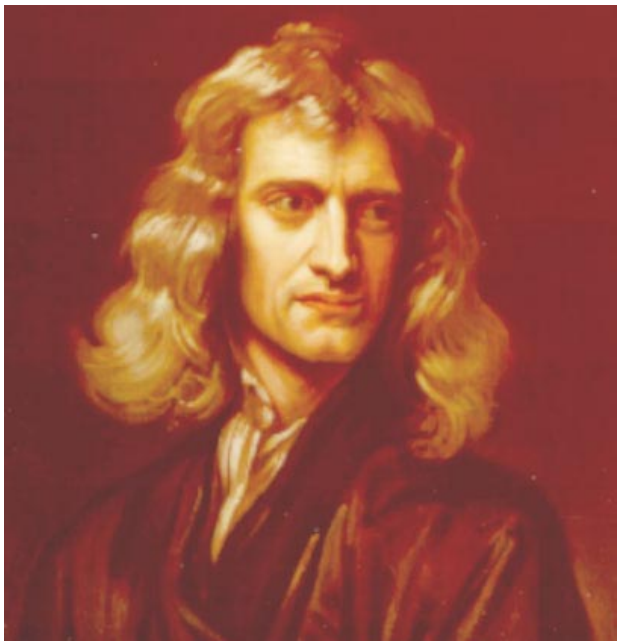
In a simplified sense, its goals are:

- **to understand the observed behavior of astronomical objects in terms of knows laws of physics**
- **to extend the laws if that is really necessary**

First example of Theoretical Astronomy

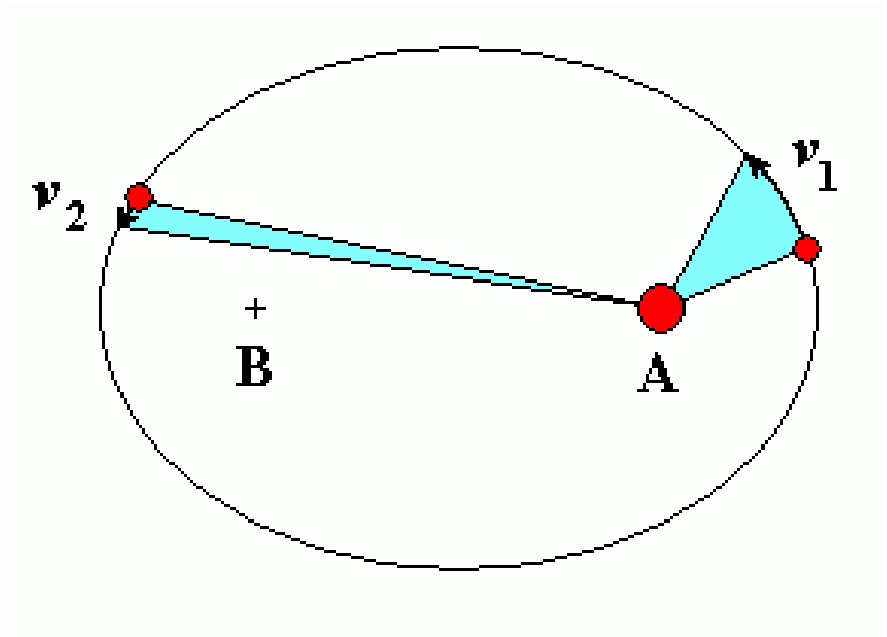
- **Kepler formulated, from Tycho's observations, Kepler's three laws.**
- **Newton showed that Kepler's laws are derived from Newtonian mechanics and Newtonian gravity.**





Kepler's laws

- The orbits of planets are ellipse with one focus at Sun.
- $dS/dt = \text{const.}$
- $T \propto a^{3/2}$



Newtonian equation of motion for planets: Two-body problem

$$\frac{d^2\mathrm{r}}{dt^2} = -GM\frac{\mathrm{r}}{|\mathrm{r}|^3},$$

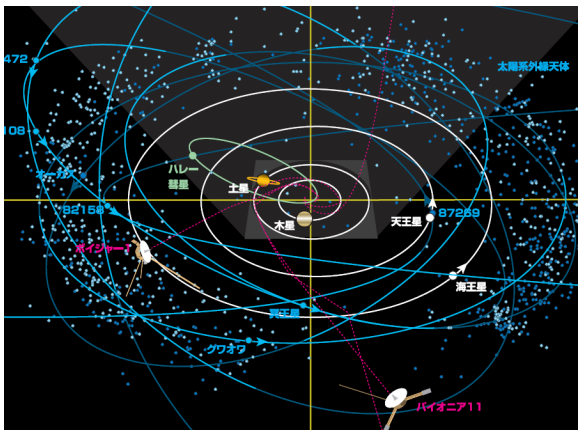
- Gravity from other planets were neglected.
- Simple closed elliptic orbits.

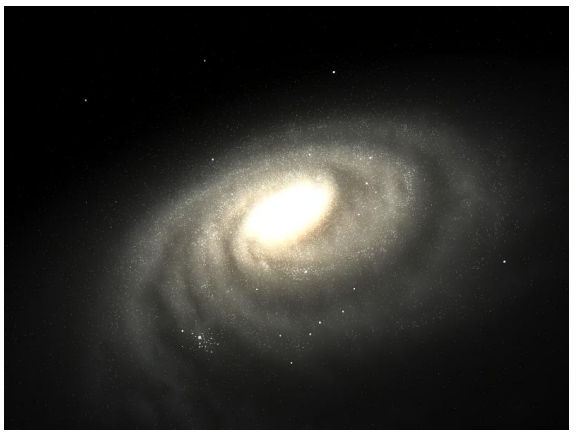
$N > 2$

- Celestial mechanics: What happens if we include planet-planet interaction?
- Stellar Dynamics: How stars themselves move?

Both are very natural "next steps" from the two-body problem.

In both fields, there are significant recent advances.





Two planets

- **Simple example: Mars under the effect of Jupiter**
  - **Gravity from Mars to Jupiter is small**
- **More general case: Saturn and Jupiter**
  - **Saturn is not small**

Perturbation technique

Basic idea:

- **Start from unperturbed Kepler orbits**
- **Derive the equation for the change of orbital elements due to the gravity of Jupiter**
- **Expands it by the mass of the Jupiter**
- **Evaluate the first term (or first few terms...)**
- **(Usually assume that orbits are close to circular and close to coplanar)**

Can be extended to general cases

Success of the perturbation technique

- **Explained high-precision observations of the orbits of planets**
- **Unexplained motions led to**
  - **findings of new planets (Neptune)**
  - **Confirmation of general relativity (Mercury)**

So, is everything OK?

— not quite.

One problem:
Long-term “stability” of the solar system.

Last 20 years of stability study

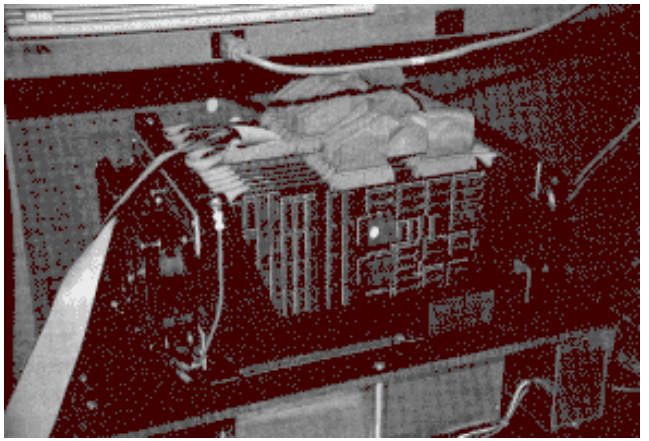
1987: Sussman and Wisdom
850Myrs numerical integration of outer five "planets"

Lyapunov timescale: 20Myrs

Lyapunov timescale: (Roughly speaking) the distance between two (infinitesimally different) systems grows in this timescale

The Digital Orrery

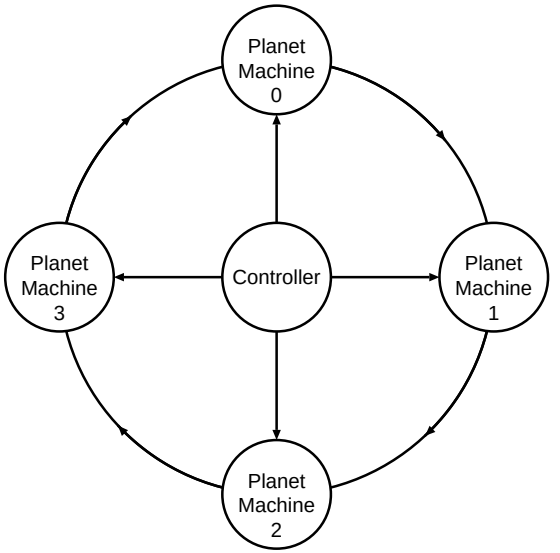
Computer used by Sussman and Wisdom



- A custom-built parallel computer for long-term integration of the Solar system
- Consists of 9 "planet computers" connected in a ring network
- 10 Mflops
- MIT AI lab + Planetary Science

Digital Orrery (2)

- SIMD (Single-Instruction Multiple-Data) parallel computer
- Programmable: Integration scheme etc can be changed
- Effective Quadruple-precision integration



One of (very few) examples of the successful development of special-purpose computer for numerical simulation

Naive question:

Lyapunov timescale $\ll$ Age of the solar system

Is solar system unstable? Why is it there?

Even longer numerical integration

- **Kinoshita and Nakai 1996 (4.5Gyrs)**
- **Ito and Tanikawa 2002 (45 Gyrs, 10 times the age of the solar system)**

Solar system seems to be "stable"

What do we mean by "stable"?

- **Planets do not collide, exchange positions, escape from system, etc.**
- **not "linear stability"**

Much simpler setup

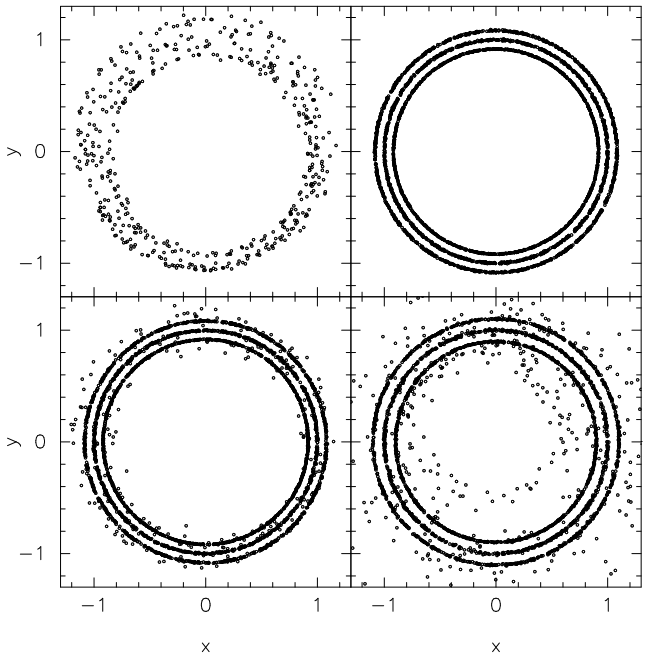
What is known:

- **Sun + two planets: STABLE (if two planets are well separated)**

What happens to the system of *three planets*?

Simple experiment

- **planet mass: 10^{-5} (Sun=1)**
- **planet separation: 0.06, 0.08, 0.1**



Left top: 0.06, T=5000

Right top: 0.08, T=50000

Left bottom: 0.08, T=60000

Right bottom: 0.1, T=90000

“Suddenly” become unstable

Numerical experiments suggest:

- "Instability timescale" $\propto$ exp(separation)
- Weak dependence on the number of planets
- separation normalization: Hill radius $r_H = R(m/M)^{1/3}$
- Initial eccentricity reduces the timescale

Might imply:

- Planetary system (with more than three planets) is unstable, if you wait long enough
- In the case of our solar system, instability timescale is longer than 10$\times$ its age.

Can't we do something better than numerical integration?

Can't we do something better than numerical integration?

- Do not ask me!

Can't we do something better than numerical integration?

- Do not ask me!
- Ask: mathematical physicist

Is the stability of our solar system such an important problem?

- Extrasolar planetary systems
- Trans-Neptunian Objects
- Formation theory for normal planets
- Earth's long-term climate change

Summary for planetary systems

N: number of planets

- **$N = 1$ solved by Newton**
- **$N = 2$: stable if large separation**
- **$N \geq 3$: Everything becomes unstable?**
  - **Why does our solar system exist?**
  - **Wide variety of extrasolar planets**

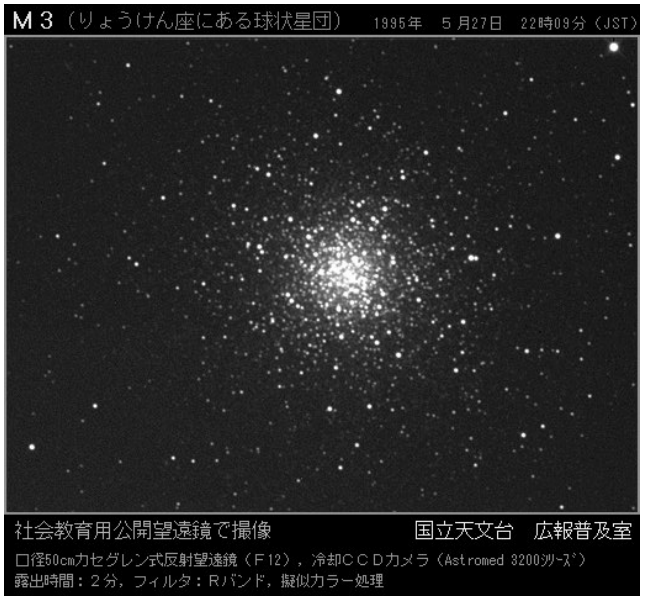
Stellar Systems

Planetary systems: Sun + "small" planets. Kepler orbit+perturbation.

Stellar systems: Consists of many stars

Examples of stellar systems

Globular clusters



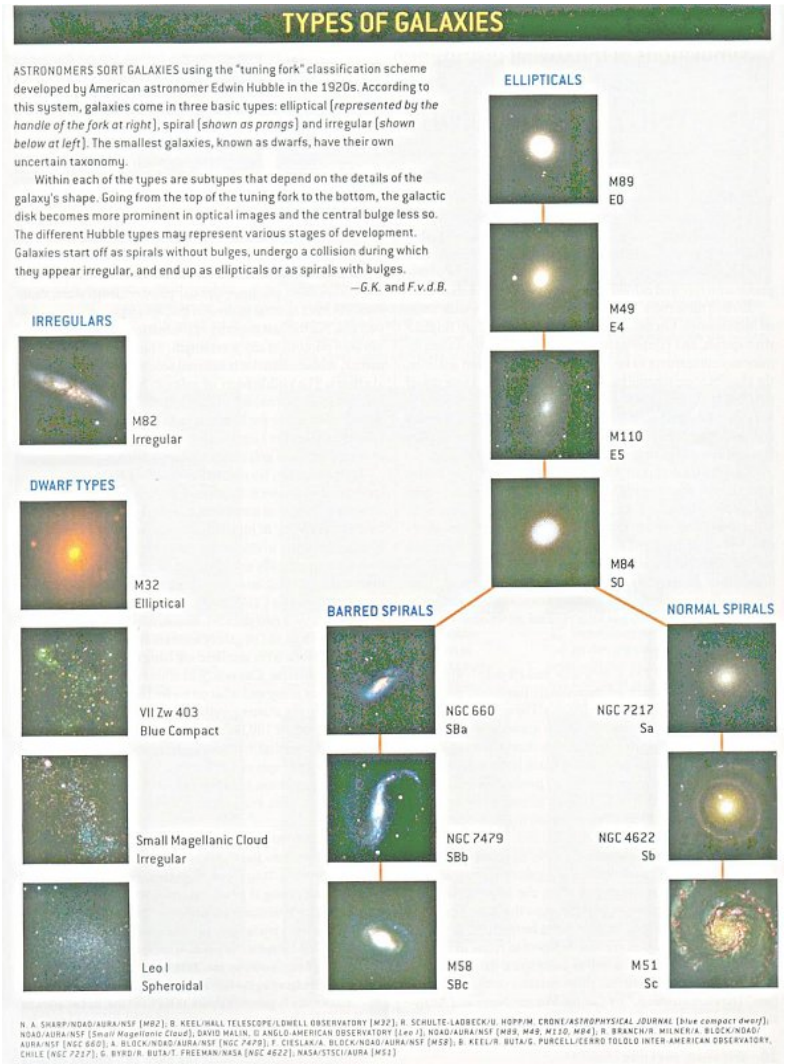
Galaxies

Globular clusters

- 10^5-10^7 stars
- Old stars ,$>$ 10Gyrs (age of the Universe: 13.7Gyrs)
- Mostly spherical (some are a bit elliptical, rotating)
- Globular clusters all look alike
- "Clean" systems, no gas, star formation etc

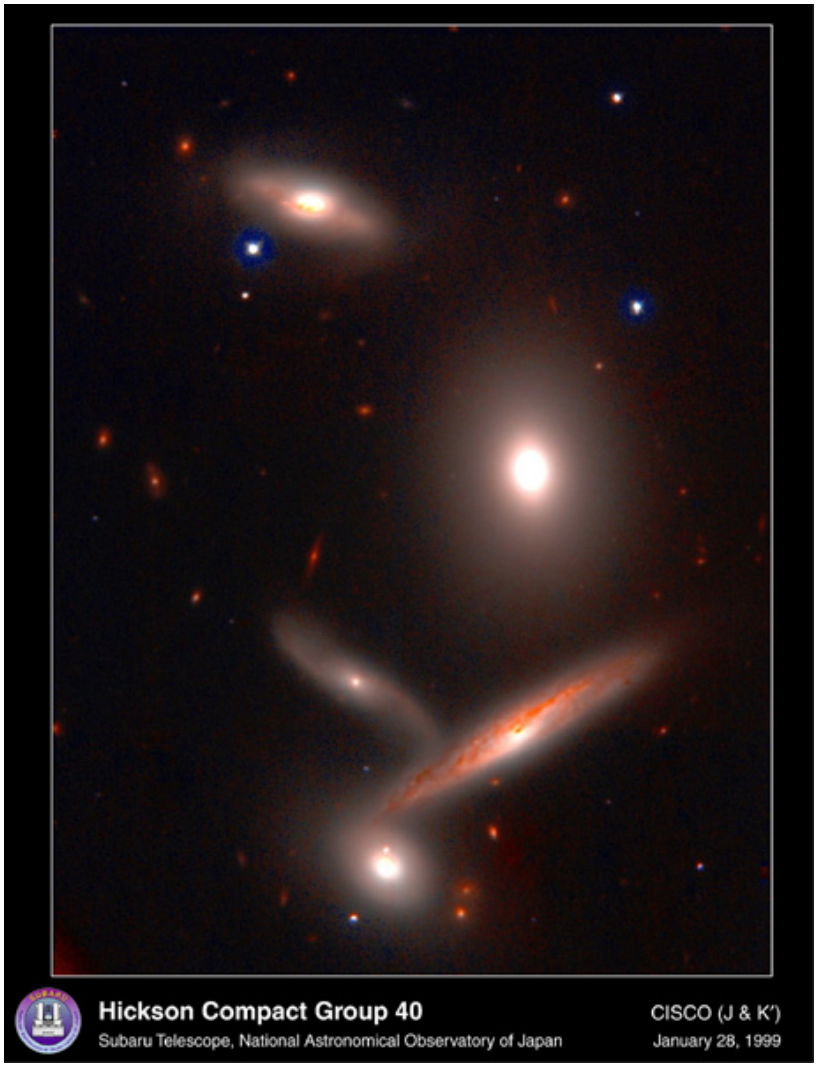
Natural lab for stellar dynamics

Galaxies

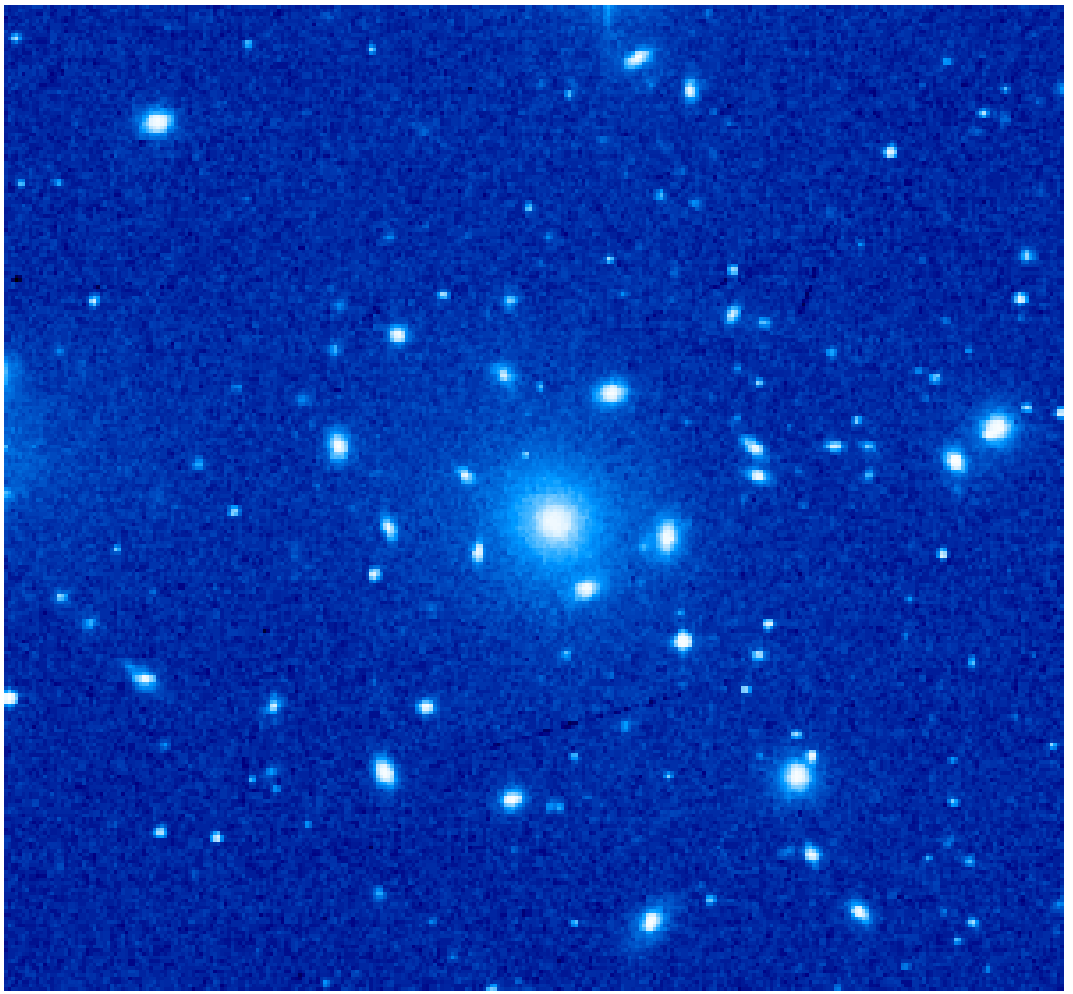


- $\sim 10^{11}$ stars (wide variety)
- Complex systems, gas, stars are forming
- Wide variety in morphology

Galaxy groups

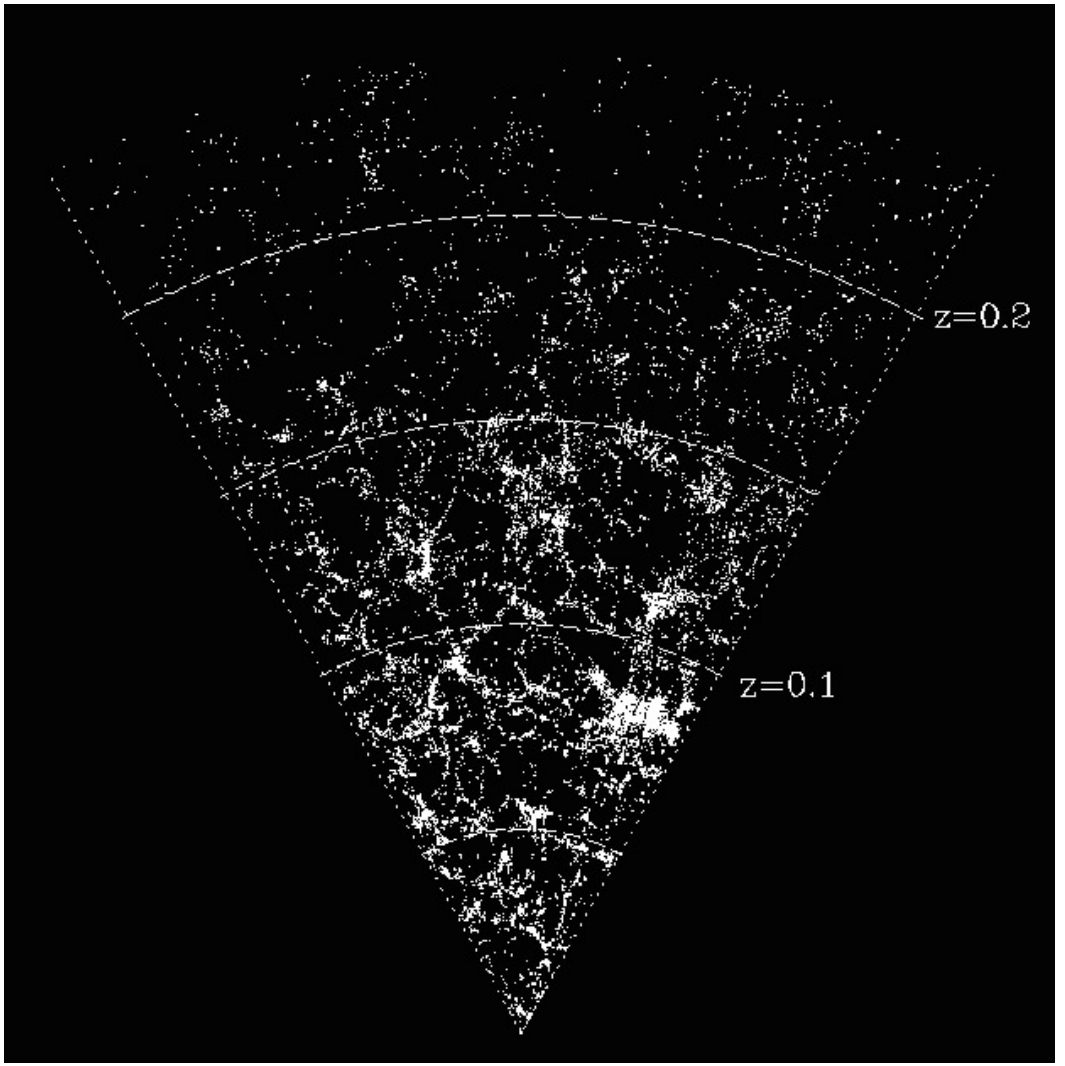


Clusters of Galaxies

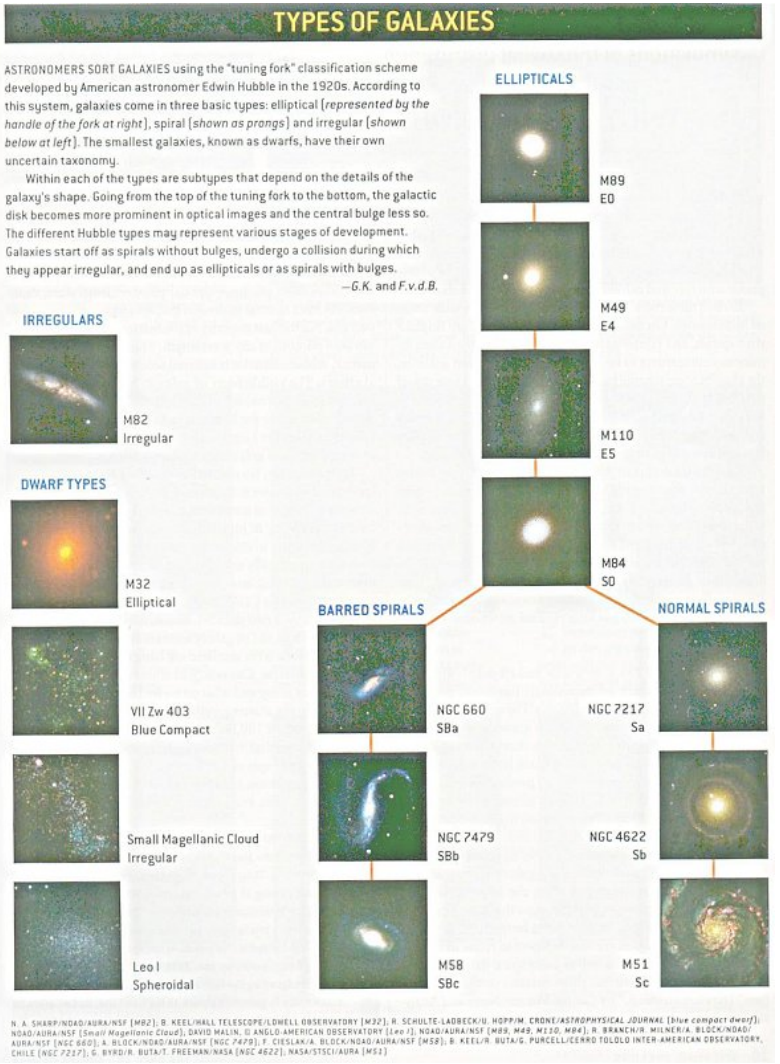


http://antwrp.gsfc.nasa.gov/apod/ap950917.html

Large-Scale Structure



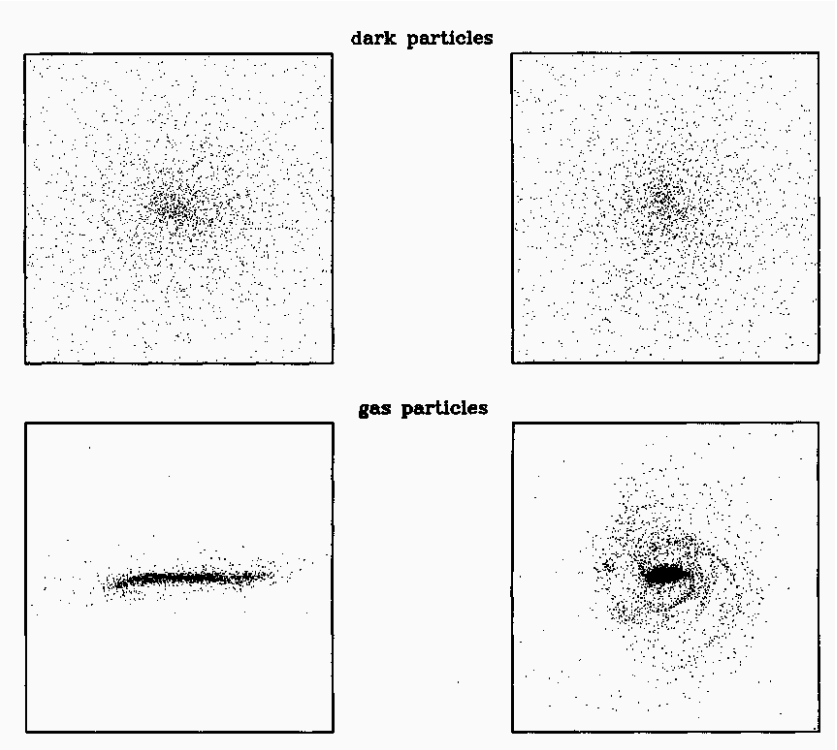
Simulation of galaxy formation



Basic Idea:

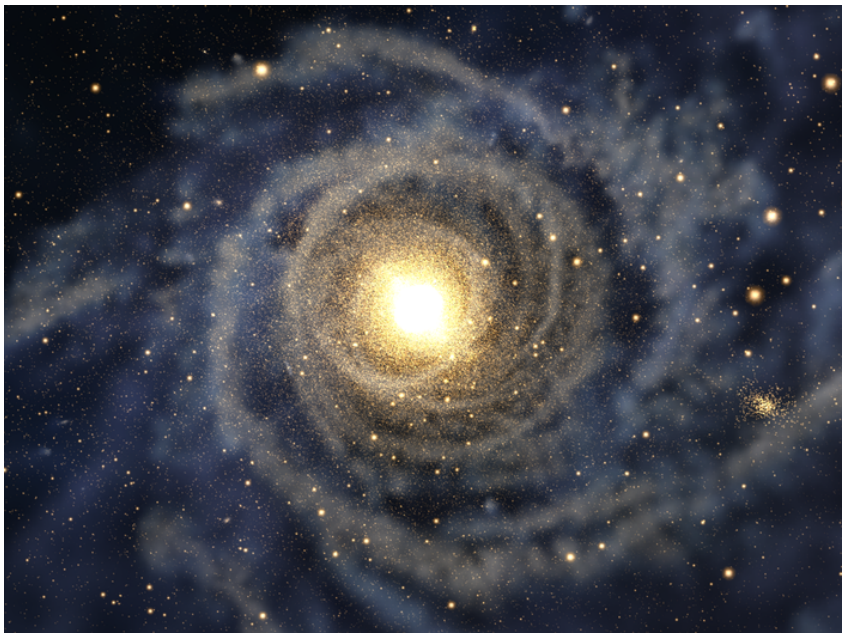
- "Holistic" simulation of galaxy, from initial density fluctuation
- To understand the origin of the variety of galaxies

Katz and Gunn 1992



- Dark Matter + gas + stars
- DM, star: particles gas :SPH particles
- 10^4 particles, Cray YMP 500-1000 hours
- mass resolution : 10^7 solar mass

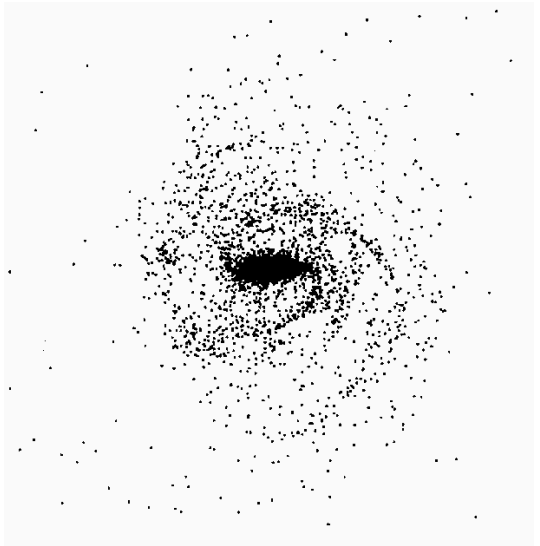
Saitoh et al. 2005



animation

- Dark Matter + gas + stars
- DM, stars: particles gas:SPH particles
- 2×10^6 particles, GRAPE-5 $\sim$ 1 year
- mass resolution : 10^4 solar mass

What learn from improved resolution?



- Not much?
- In this calculation, really not much...
- Impotant things: improved paramtrization of "micro-physics", such as star formation mechanism, energy input from supernovae.

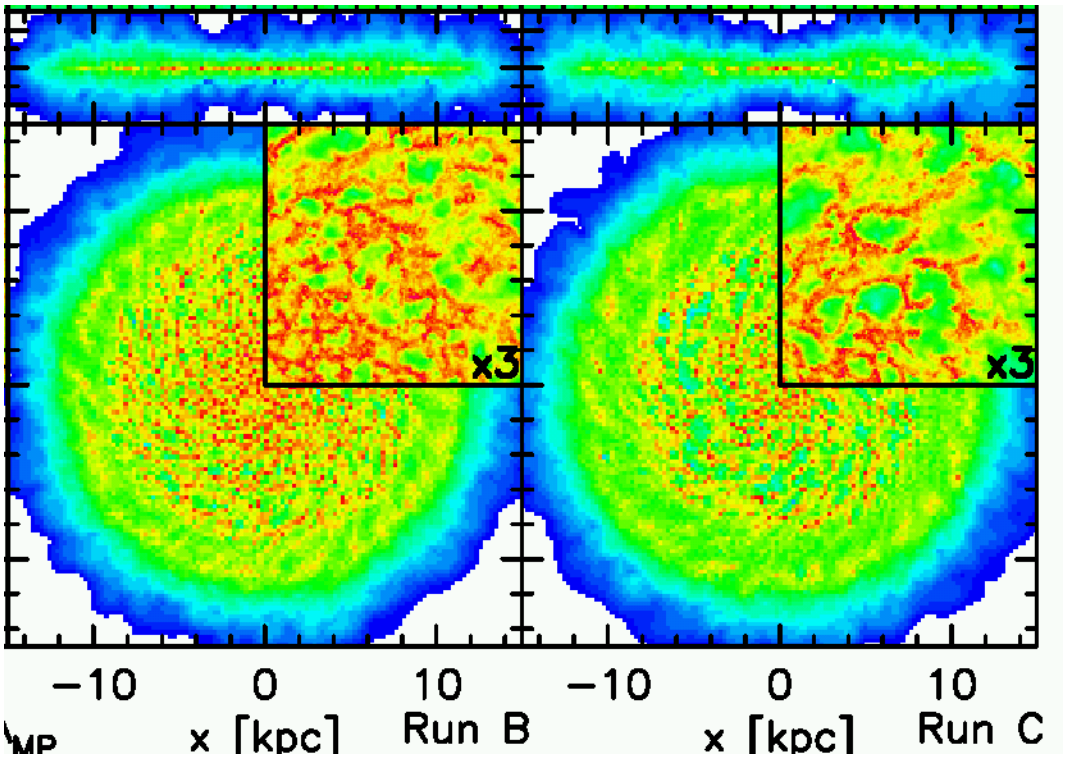
Modelling star formation

- Minimum need for star formation modelling: : 10^{-4} solar mass
- What we can do now: : 10^{3} solar mass (10^{7} times too large)
- Need some way to form stars
  - Usual model: if interstellar gas is dence and cold enough, part of it will become stars in appropriate timescale.
  - three free parameters
  - The structure of the galaxy depends on these parameters
- Similar problem on suprenovae.

What resolution do we need?

- We will know when we reach there....
- Theoretically, if we have sufficient resolution, we can just change all mass to stars (that is what the nature does).
- We are approaching there.
- One or two orders of magnitude more?

Saitoh et al. 2007



Changed the star formation timescale by a factor of 15

little difference in the result

(In low-resolution calculation, the galaxy would have exploded.)

Some more animations

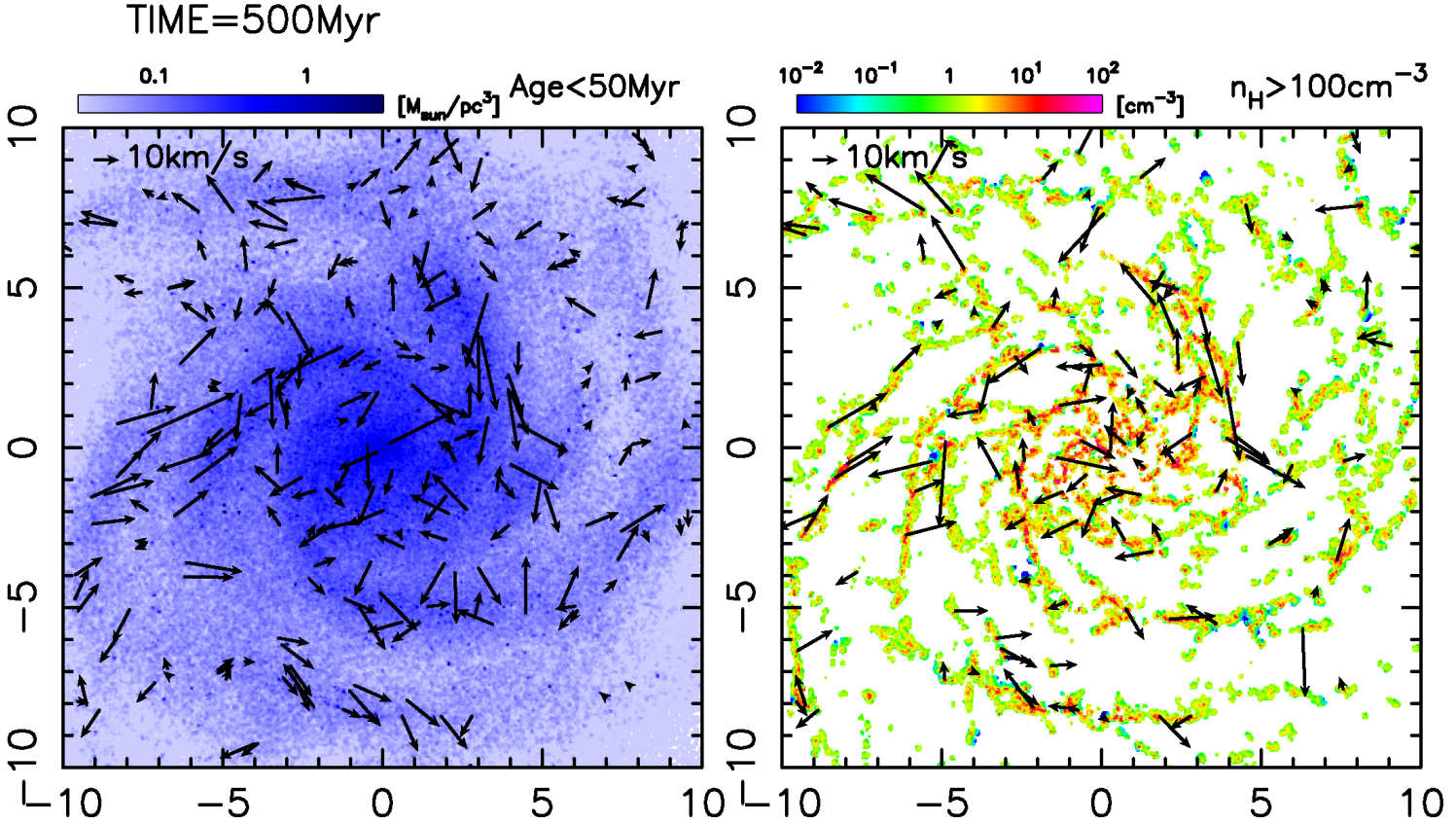
Star formation with SPH

Large scale structure formation with AMR

Galactic disk

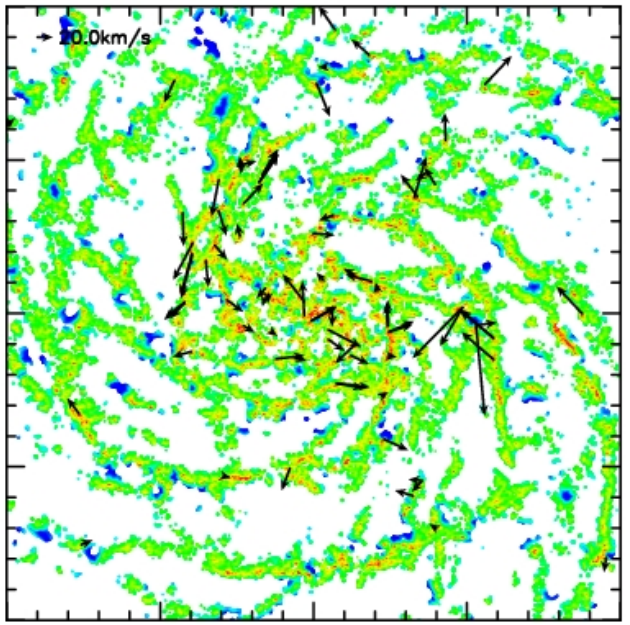
animation 1 2)

Spiral structure and deviation from the circular motion

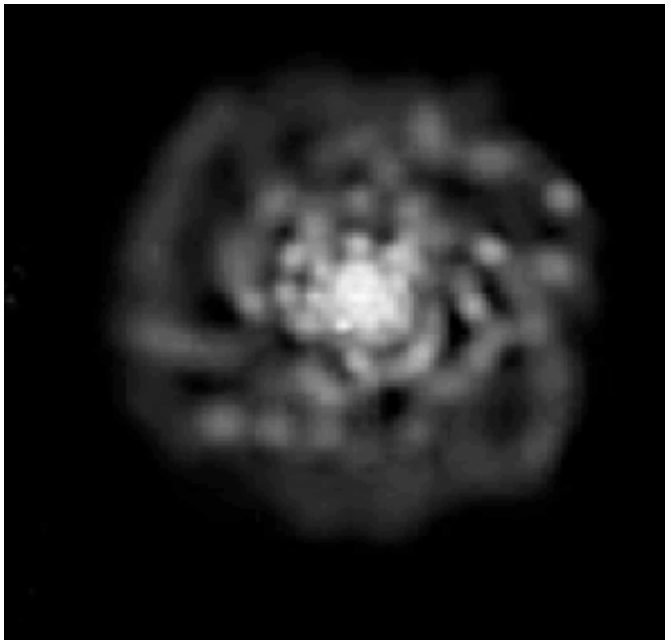


Left: distribution of stars **Right: cold gas**

High-resolution model and observation



Low-resolution model and observation



Gravitational Many-Body problem

Equation of Motion:

$$m_i \frac{d^2 x_i}{dt^2} = \sum_{j \neq i} f_{ij} \tag{1}$$

x_i, m_i: position and mass of particle i

f_{ij}: gravitational force from particle j to particle i

$$f_{ij} = G m_i m_j \frac{x_j - x_i}{|x_j - x_i|^3}, \tag{2}$$

G: gravitational constant.

This equation, however, does not tells much about the behavior of the system.

Why not?

- the equation does not have analytic solution
- there are special cases....
  - $N = 2$
  - $N = 3$ from special initial condition
  - Solar-like systems (well....)
  - $N \to \infty$, dynamical equilibrium

On the other hand, we can numerically integrate the equation of motion using computer. Isn't that enough?

Numerical integration

In principle, numerical calculation should be enough.

In practice, it is not.

Reason:

- **Computers are not fast enough**
- **Additional physics**
  - **gas dynamics**
  - **stellar evolution**
  - **...**

Computer power and calculation cost

A naive estimate:

If we have N stars, calculation cost per timestep is N^2.

A 10^8-body system would need a computer 10^8 times faster than a 10^4-body system needs.

Three ways to reduce calculation time

- Improve numerical methods to reduce operation count
- Buy faster computers
- Build faster computers

Improve numerical methods to reduce operation count

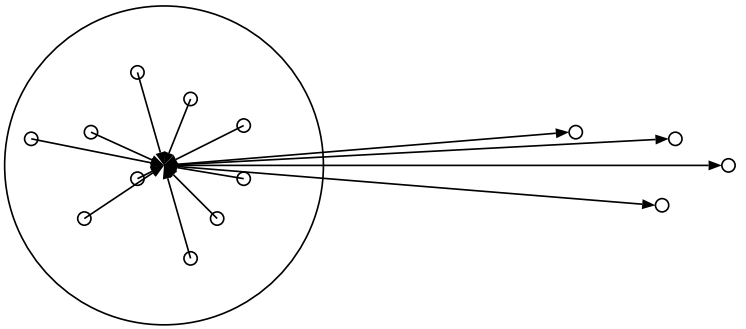
- Better methods for orbit integration
  - high-order integrator
  - symplectic/symmetric methods
  - hybrid
  - ...
- Fast and approximate methods for interaction calculation
  - Tree and FMM

Basic idea for tree method and FMM

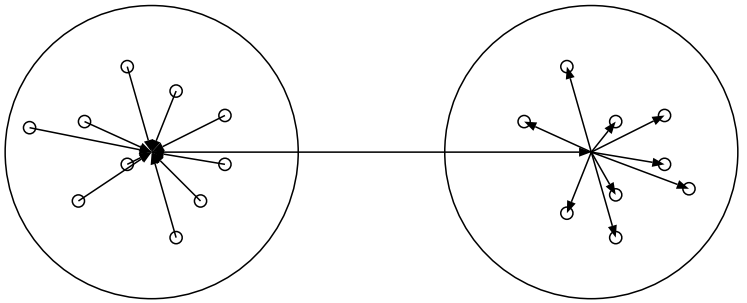
Force from distant particle: Weak

↓

Can't we evaluate many forces at once?



Tree



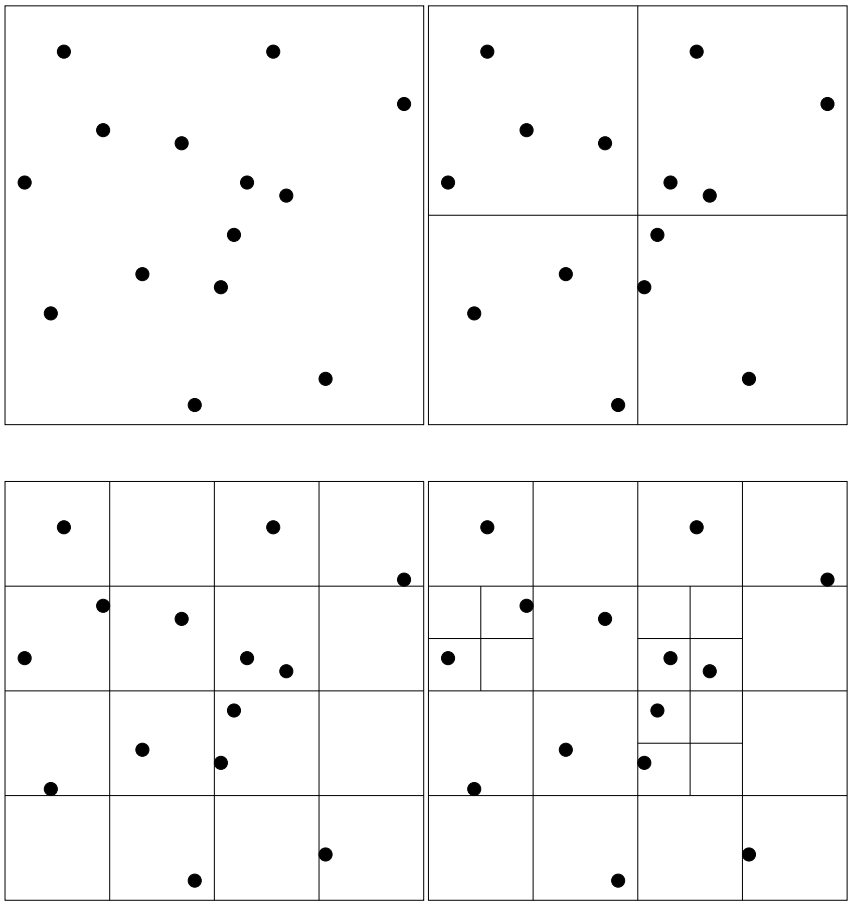
FMM

- Tree: aggregate stars which exert the forces
- FMM: aggregate both side

How do we aggregate — Barnes-Hut tree

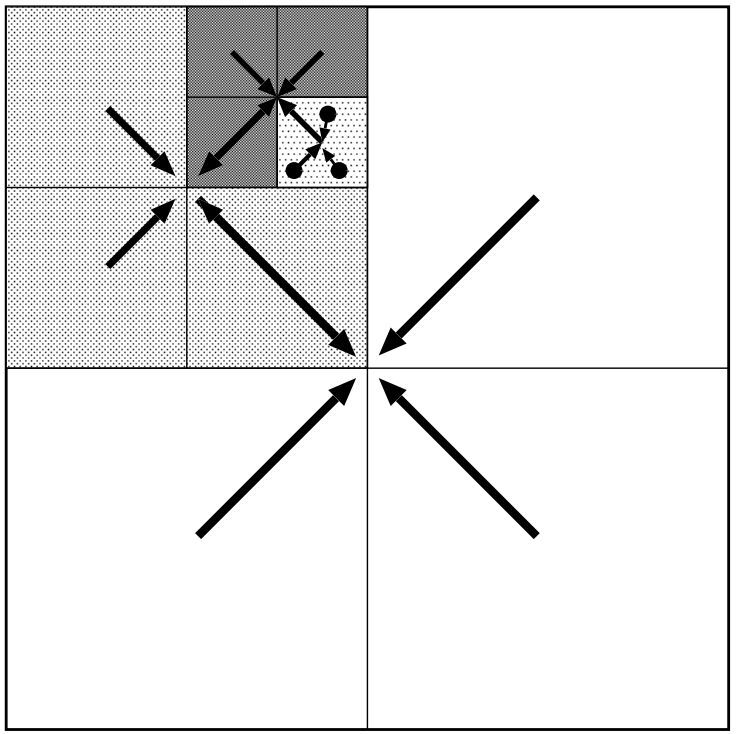
Use tree structure

- First make a cell with all stars in it
- Recursively subdivide the cells to 8 subcells
- Stop if there is small enough stars



Construction of the multipole expansion

Form the expansion for cells.

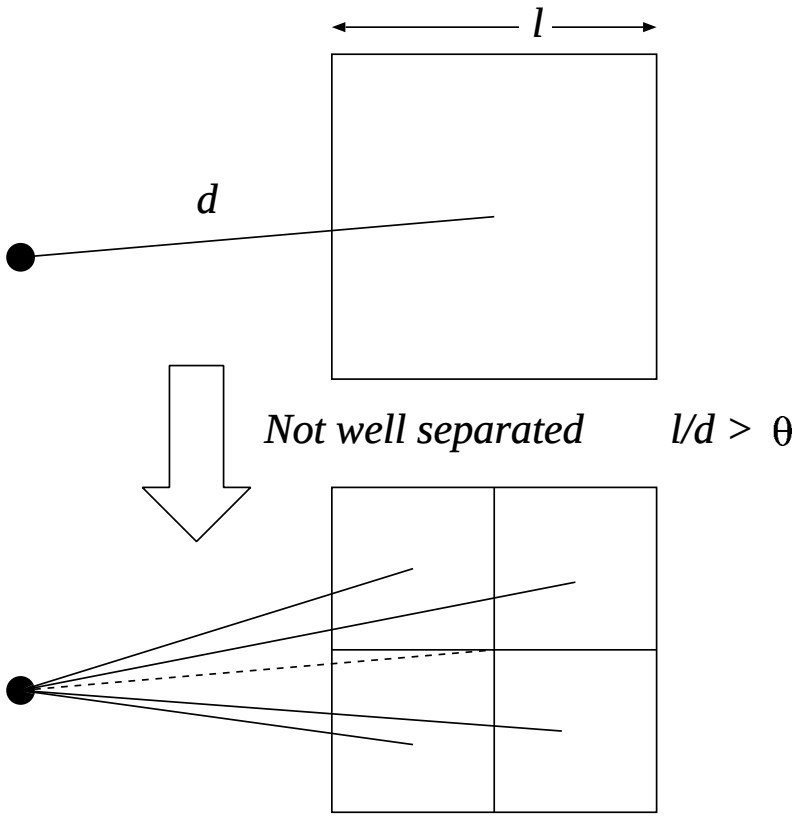


- **lowest-level cells: Directly calculate the expansions for stars in it.**
- **Higher-level cells: Shift and add the expansions for child cells.**

Calculate bottom-up.
Calculation cost: $O(Np^4)$ (p: expansion order)

Force calculation in tree method

Recursive expression:



- **Well separated: apply the multipole expansion**
- **not: take summation of the forces from the child cells**

Total force = force from the root cell

Second approach: Buy fast computer

We can do fast calculation by using fast computer.

... not that simple ...

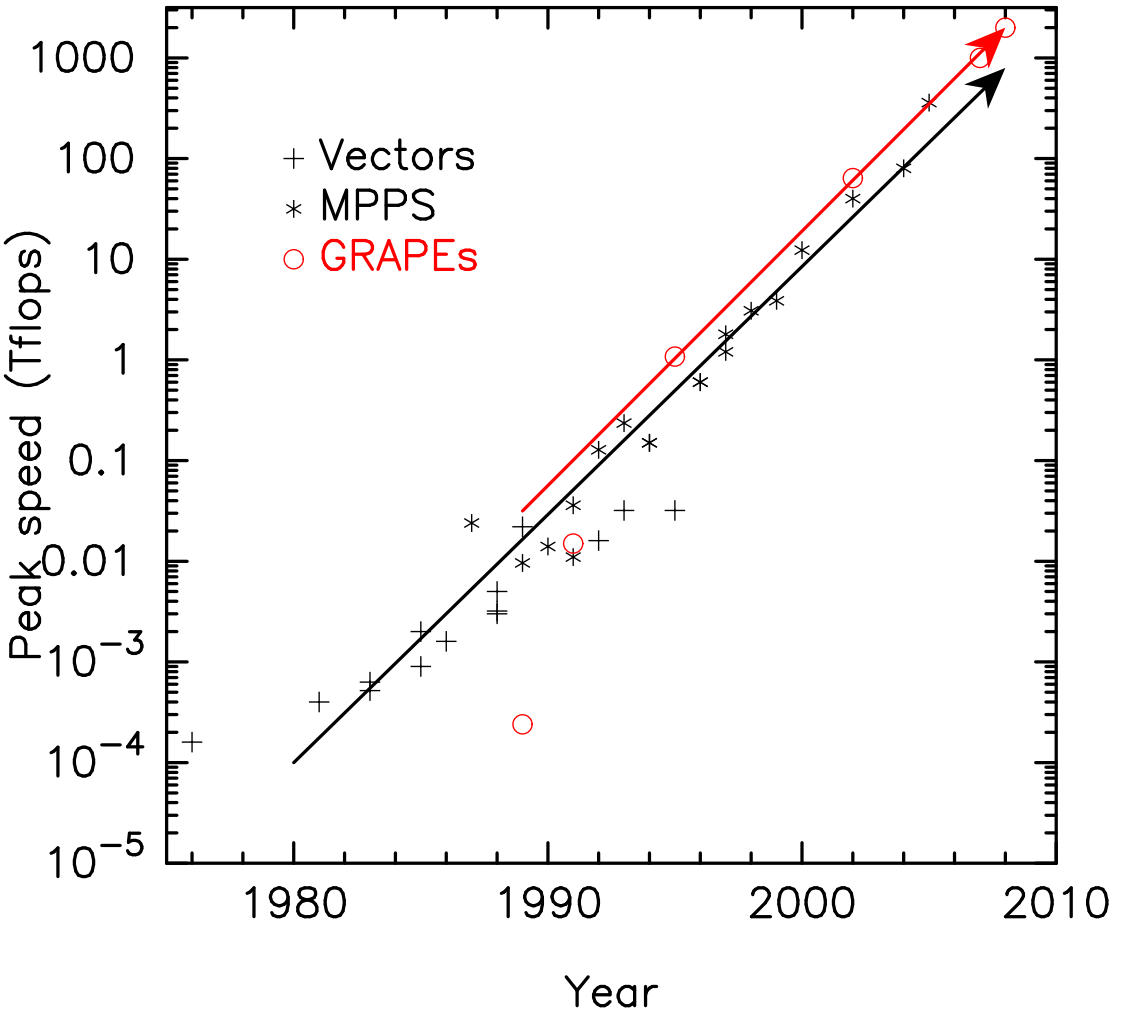
Basic reason:

The development of high-performance computers in the last 30 years made it more and more difficult to use them

Advance in computers

Speed improvement: 10^{10} in 50 years

Roughly exponential in time



How the exponential increase made possible?

1. Moore's law: Size of transistors halves every three years
   - 4 times more transistors
   - 2 times faster
2. Change in computer architecture
   Scalar $\rightarrow$ Vector $\rightarrow$ distributed parallel

We need parallel algorithm which is efficient on parallel machines with relatively slow network

(I'll not discuss it here...)

Third approach — build your own computer

Using fast computers is not easy...

- **In 10 years, computer architecture might completely change, making your program totally useless. (Have changed in every 10 years)**
- **Using modern machines is hard:**
  - **Parallelization on distributed-memory machine**
  - **Cache reuse**
  - **Other complicated techniques**

Isn't there a somewhat better way of life?

One approach: build your own computer

It's difficult to use the computer somebody else mad for some other purpose

Could be simpler to design the machine suited for your goal (special-purpose hardware).

Why consider special-purpose?

(Might be) faster and cheaper than general-purpose computers.

Why?

- Characteristics of the problem itself
- Technical aspects
- Historical, economical aspects

Characteristics of the problem itself

Stellar system :one star interacts with all other stars

- Large calculation cost (compared to memory requirement)
- Calculation is simple loop
- Communication pattern is simple

We do need some additional considerations for individual timestep and tree code.

Classification of the physical systems

Continuous:(Hydro etc): regular, near-neighbor communication, small calculation cost

Particles: regular $N \times N$ comm), high calculation cost

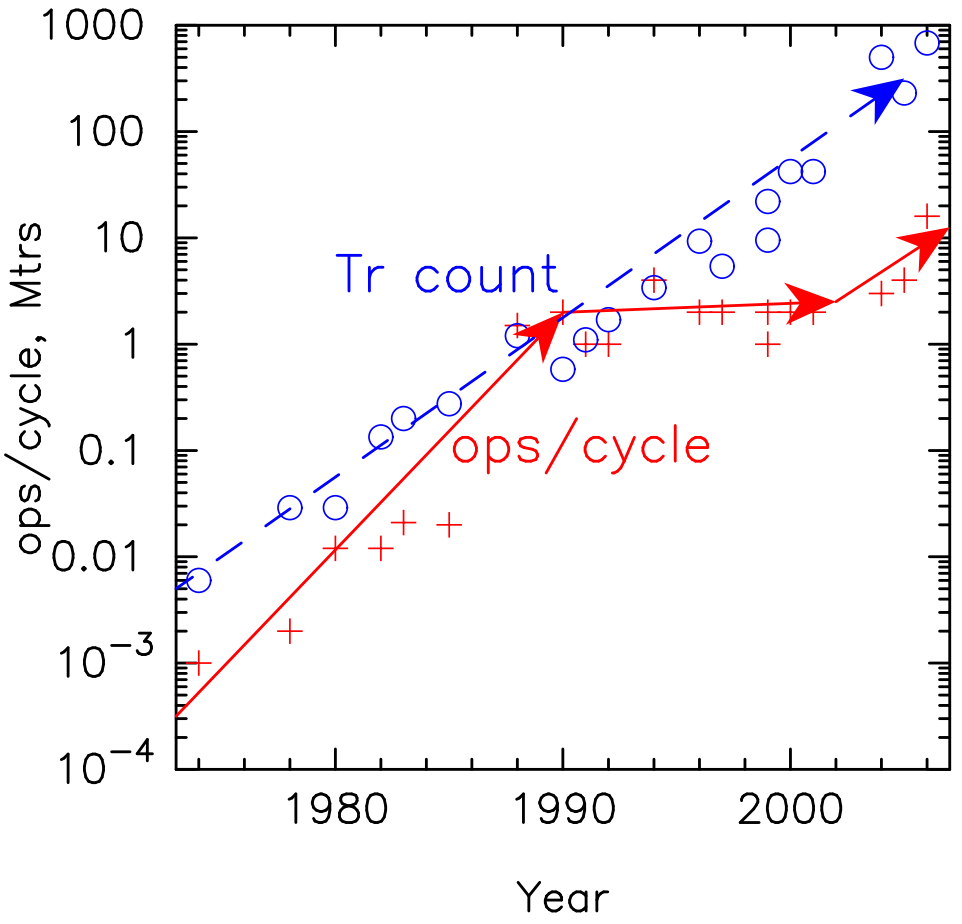
Others(discrete irregular systems)

Regular and costly = suited to special-purpose hardware

Technical aspects

- Advance in semiconductor technology: Large-scale circuits with large number of arithmetic units becomes technologically feasible
- Limit in design method = rapid decrease in transistor efficiency

"Evolution" of microprocessors

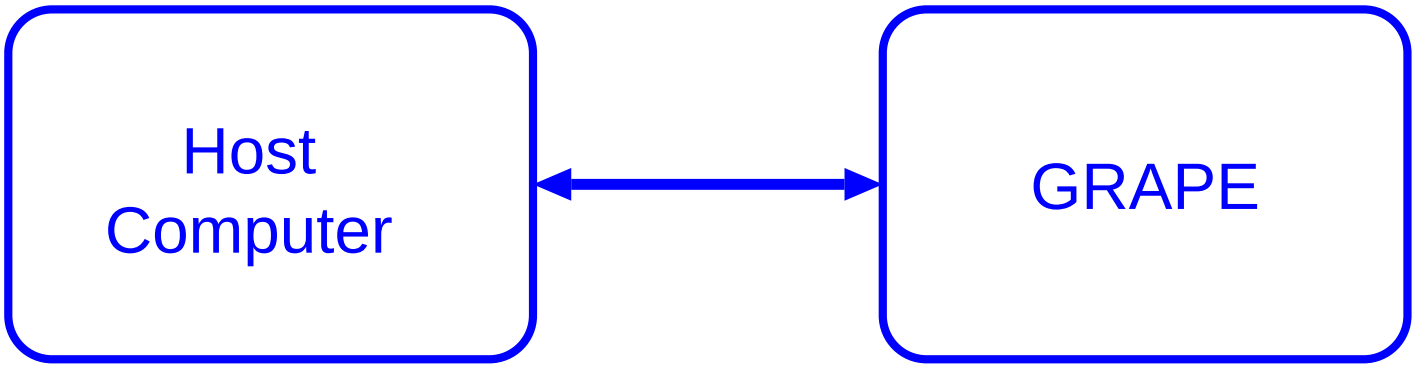


Number of transistors and Number of arithmetic operations per clock cycle

Transistor number increases exponentially Operation count stuck at 1

Could be improved?

Basic idea of GRAPE



Time integration etc.

Interaction calculation

Special hardware: **interaction calculation**

General-purpose host: **everything else**

Special-purpose hardware

- Pipeline processor specialized for interaction calculation
  - Large number of FPUs
  - Small overhead
  - All FPUs always run in parallel

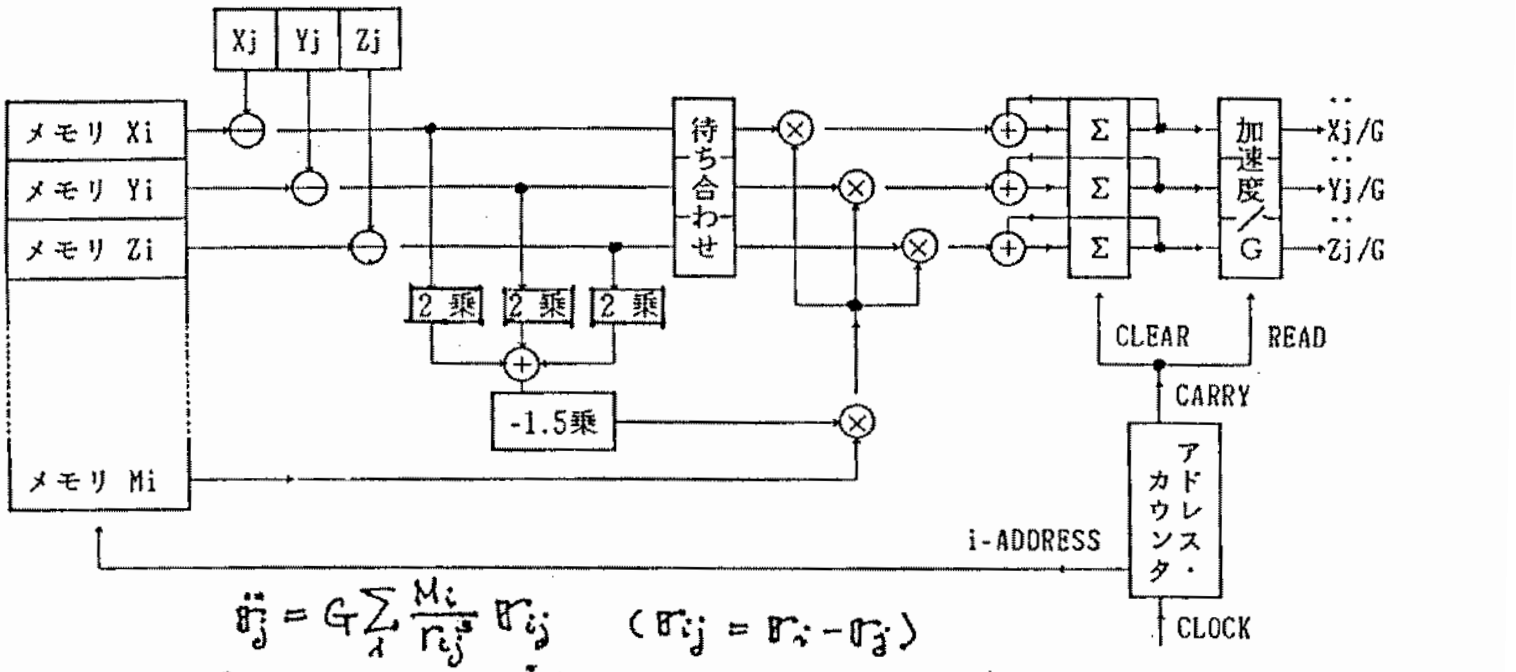
  $\rightarrow$ Very high performance

Important condition: low memory bandwidth requirement

General-purpose host computer

- "High-level" languages (Fortran, C, C++...)
- Existing programs with minimal changes
- Individual timestep, tree method, FMM

GRAPE Pipeline



$$\ddot{\vec{r}}_j = G\sum_i \frac{M_i}{r_{ij}^3}\vec{r}_{ij} \qquad (\vec{r}_{ij} = \vec{r}_i - \vec{r}_j)$$

+，－，×，２乗は１operation，　-1.5乗は多項式近似でやるとして10operation 位に相当する．
総計24operation．
各operation の後にはレジスタがあって．全体がpipelineになっているものとする．
「待ち合わせ」は２乗してMと掛け算する間の時間ズレを補正するためのFIFO(First-In First-Out memory)．
「Σ」は足し込み用のレジスタ．N回足した後結果を右のレジスタに転送する．

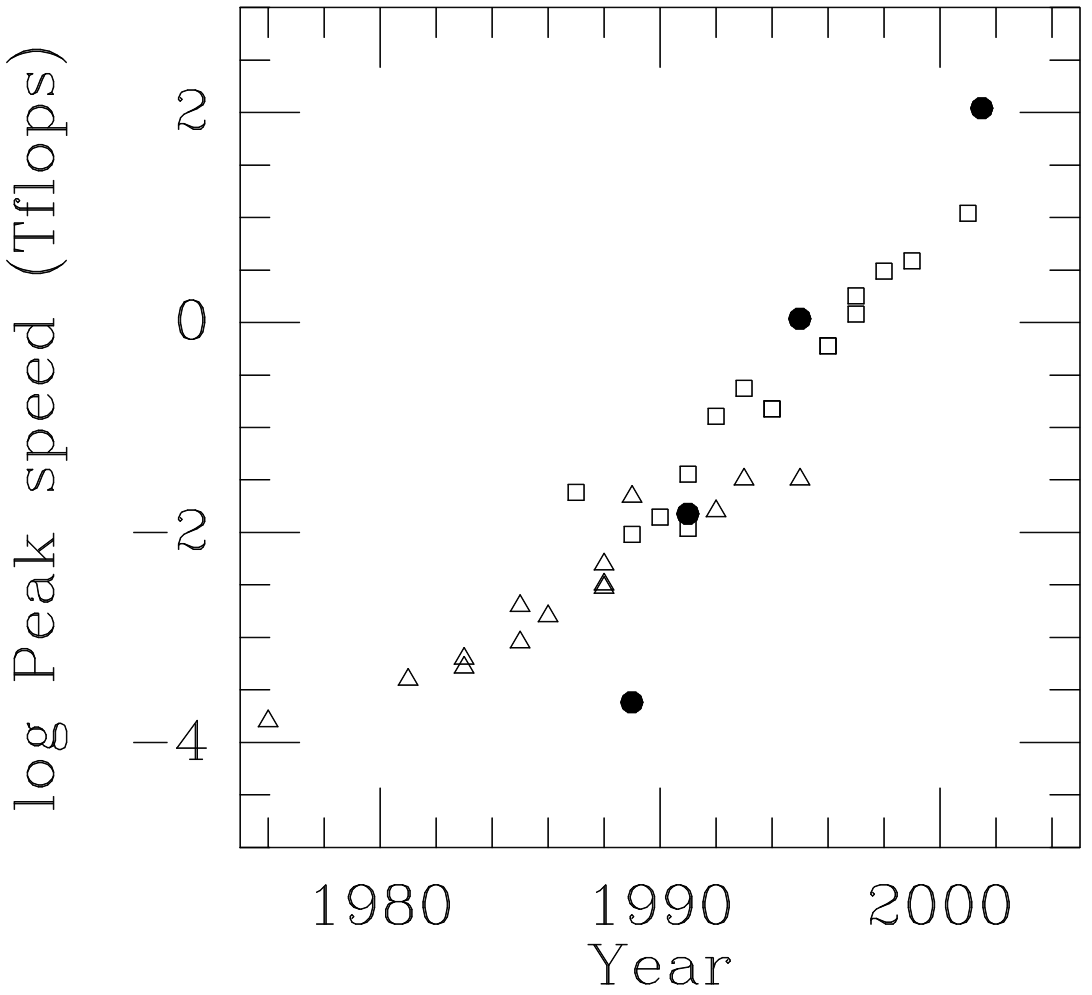
図２．N体問題のj-体に働く重力加速度を計算する回路の概念図．

(Chikada1988)

Evolution of GRAPEs

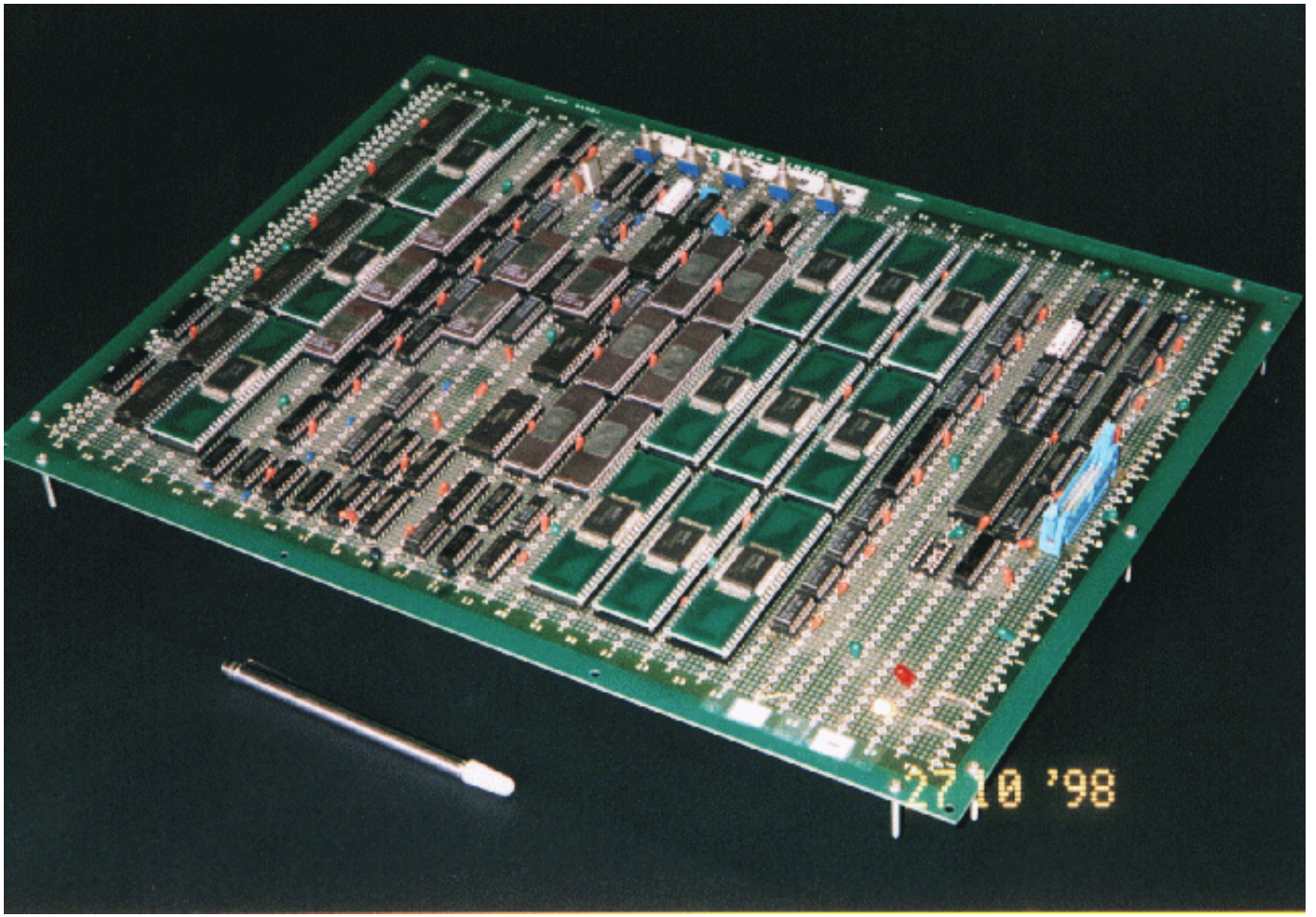
1989	**GRAPE-1**	**low acc, EPROM**
1990	**GRAPE-2**	**high acc, FPU chips**
1991	**GRAPE-3**	**low acc, Custom LSI**
1995	**GRAPE-4**	**high acc, custom LSI, Massively Parallel**
1998	**GRAPE-5**	**low acc, two pipes in a chip**
2001	**GRAPE-6**	**high acc,six pipes in a chip, MP**
2005	**GRAPE-7**	**low acc, 20 pipes in a chip**

Evolution of speed



filled circles: GRAPE

GRAPE-1



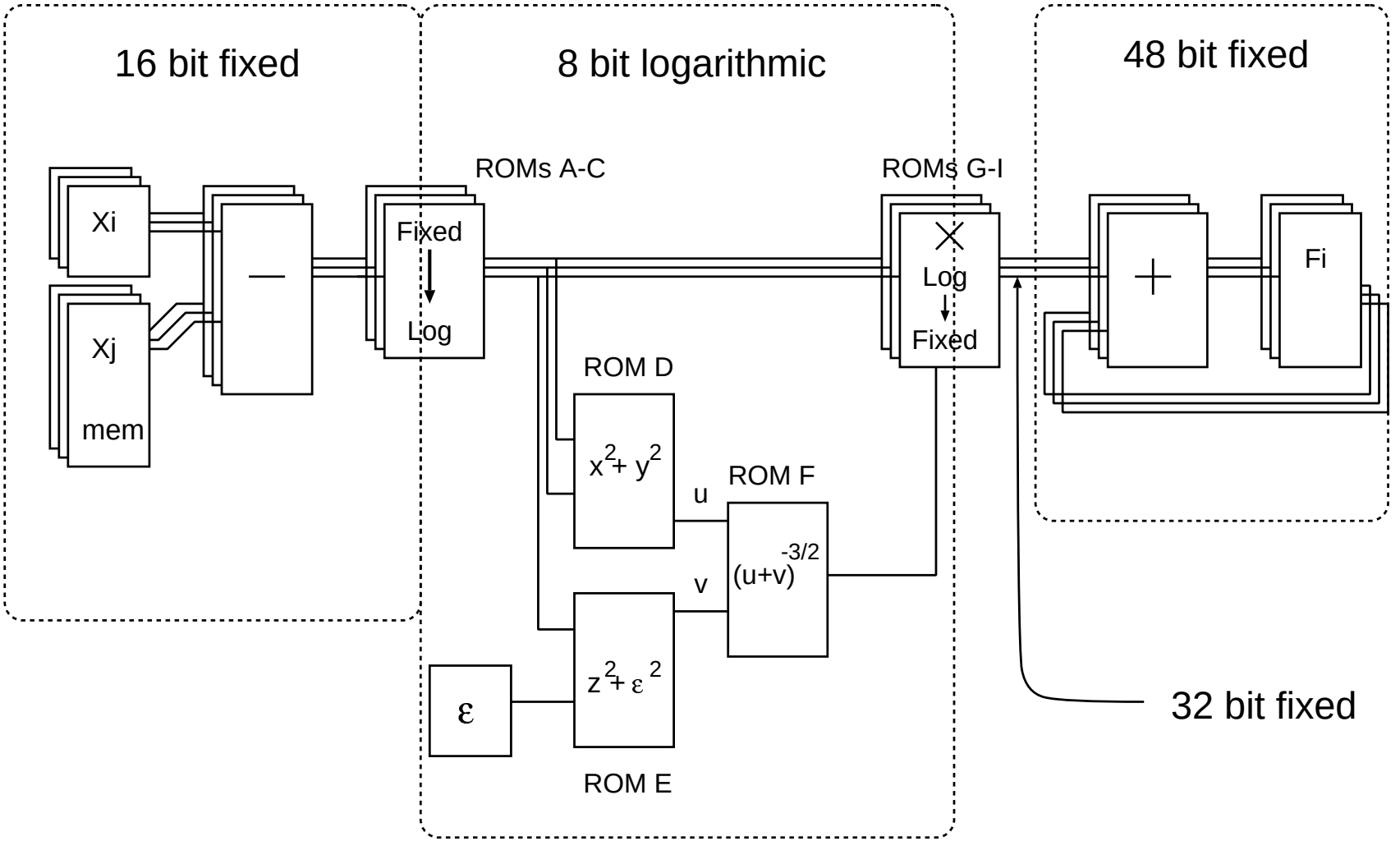
GRAPE-1 internals

"Digital Circuit for the beginners"

Initial goal

- Make something like a force pipeline
- Connect to the host and evaluate performance
- Do not care much if it is useful for real calculation

GRAPE-1 pipeline



Troubles during development

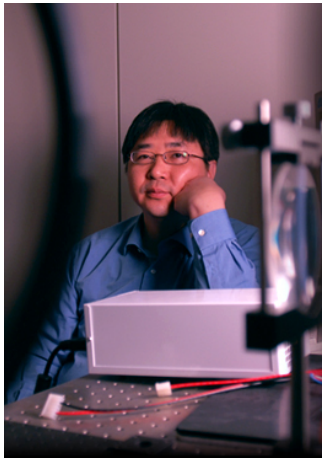
Hardware seemed to be completed without much problem (since Ito did the work, not me)

Performance problem:

Initially we used one MS-DOS PC (NEC PC-98). It was fine

We moved to a Unix workstation (Sony NEWS): Communication became very slow
We had to hack the operating system...

Tomoyoshi Ito

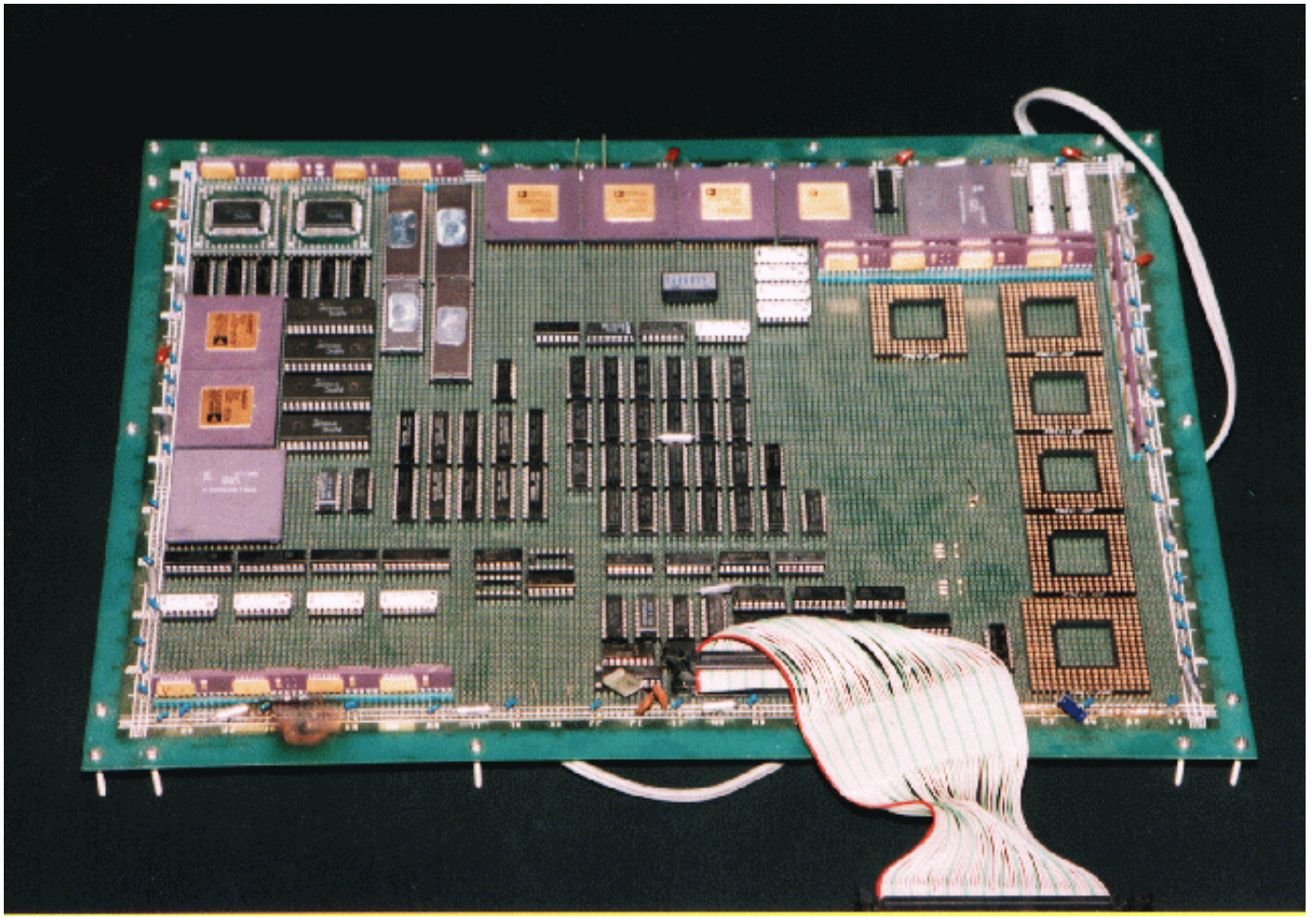


Might be better known as the author of the comic series
“Eiko-naki tensai tachi”
(Geniuses without fame)
Now professor of EE at Chiba Univ.

Lessons learned

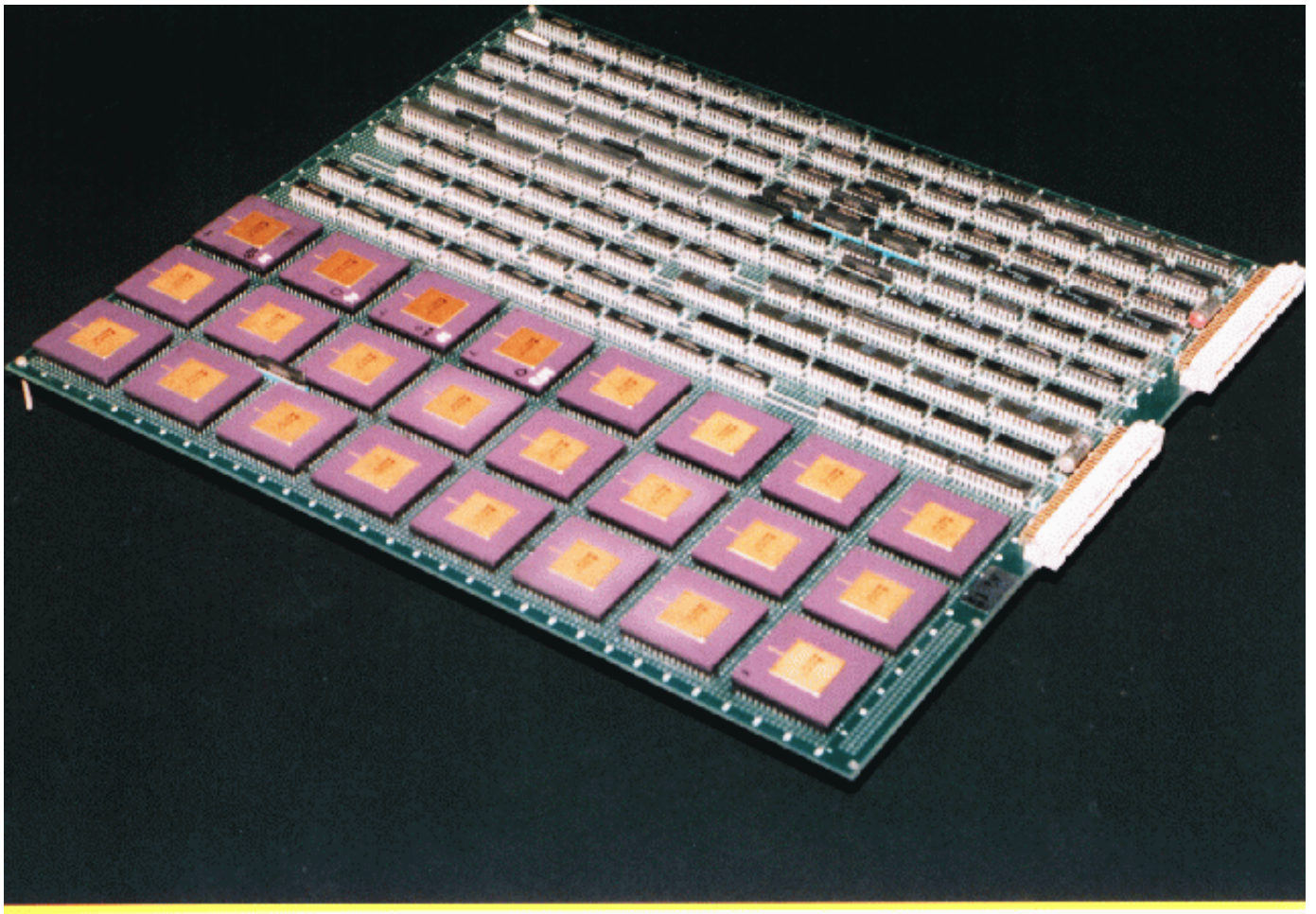
- Communication software is difficult
- "Recommended" or usual methods in textbook does not necessarily give good result
- Good result justifies whatever approach used

GRAPE-2

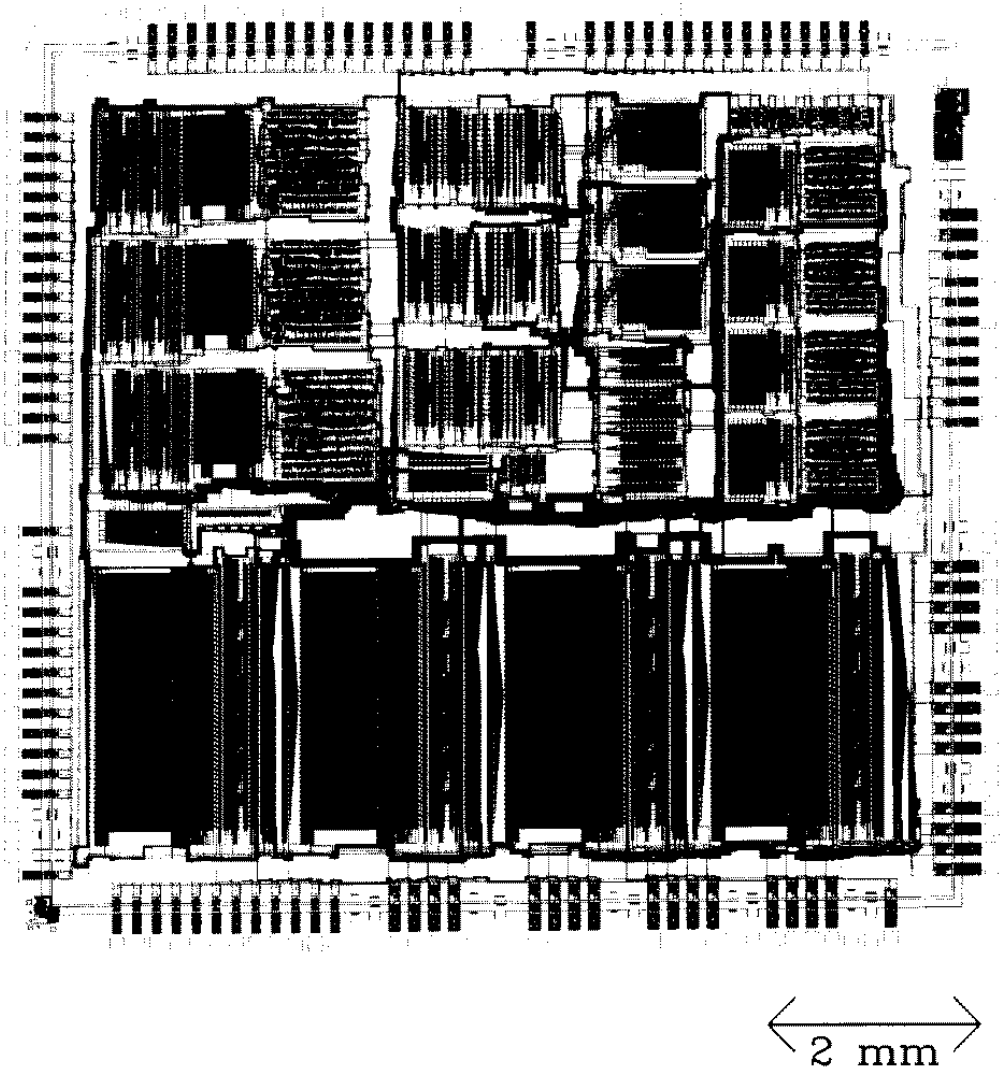


x

GRAPE-3



GRAPE-3 Custom LSI



GRAPE-3 chip design

- Specification, behavior simulation: JM
- Detailed logic design: Fuji-Xerox
- SCS Genesil design tool
- National Semiconductor. 1μm

How the chip-making affect your health?

We never had the budget for "respin", or redesign of the chip

Division of the responsibility

- If the test pattern did not get through, that is manufacturer's fault
- If other faults found, that's my fault...

In theory, if we can prepare perfect test pattern, there will be no problem.

In practice...

GRAPE-4

GRAPE-6

- Design principle
- Processor chip
- Overview

Design principle

Goal of the project (when we got budget)

— achieve the world's best performance

Our real goal:

To build a machine which can do real sciences.

Boundary condition

- **Budget: 500MJYE (Earth Simulator 50BJYE, ASCI Q 200MUSD**

Target performance: 200Tflops (5 times that of ES)

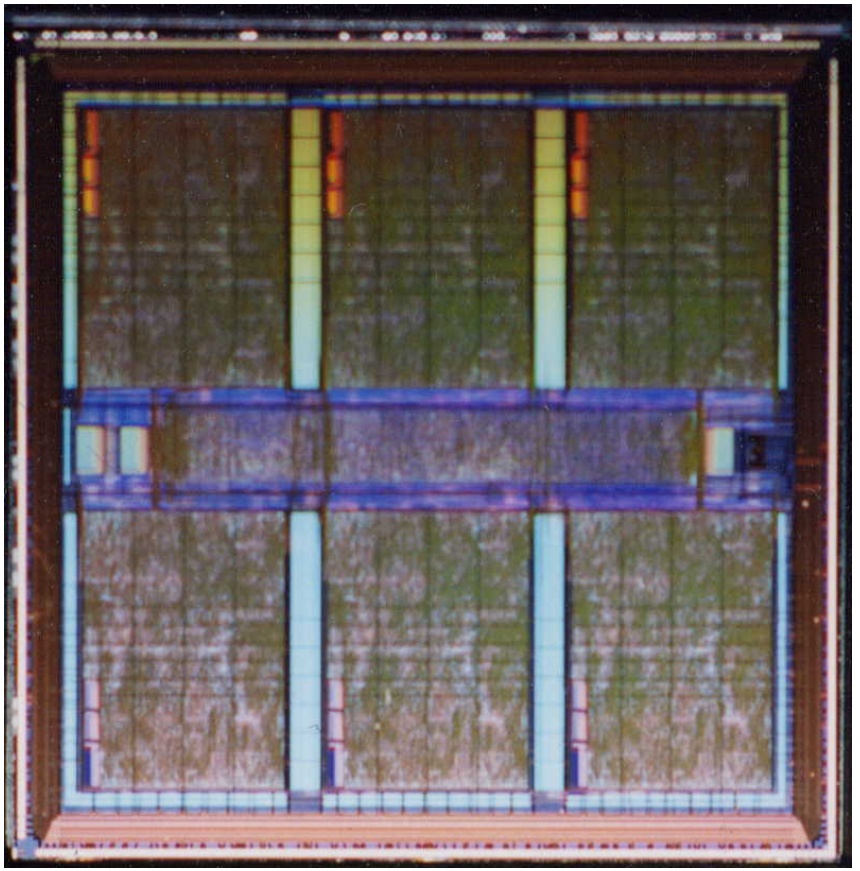
Performance prediction for GRAPE-6

Prediction: Extrapolation from GRAPE-4

	G4	G6 (pred)	G6 (real)
Design	1μm	0.25μm	0.25μm
Clock	32 MHz	125 MHz	90MHz
Pipelines	1/3	5-10	6
Performance	600Mflops	36-72 Gflops	31 Gflops
Initial Cost	25M	70M	More than 100M
Chip cost	8000K	10-20K	30K

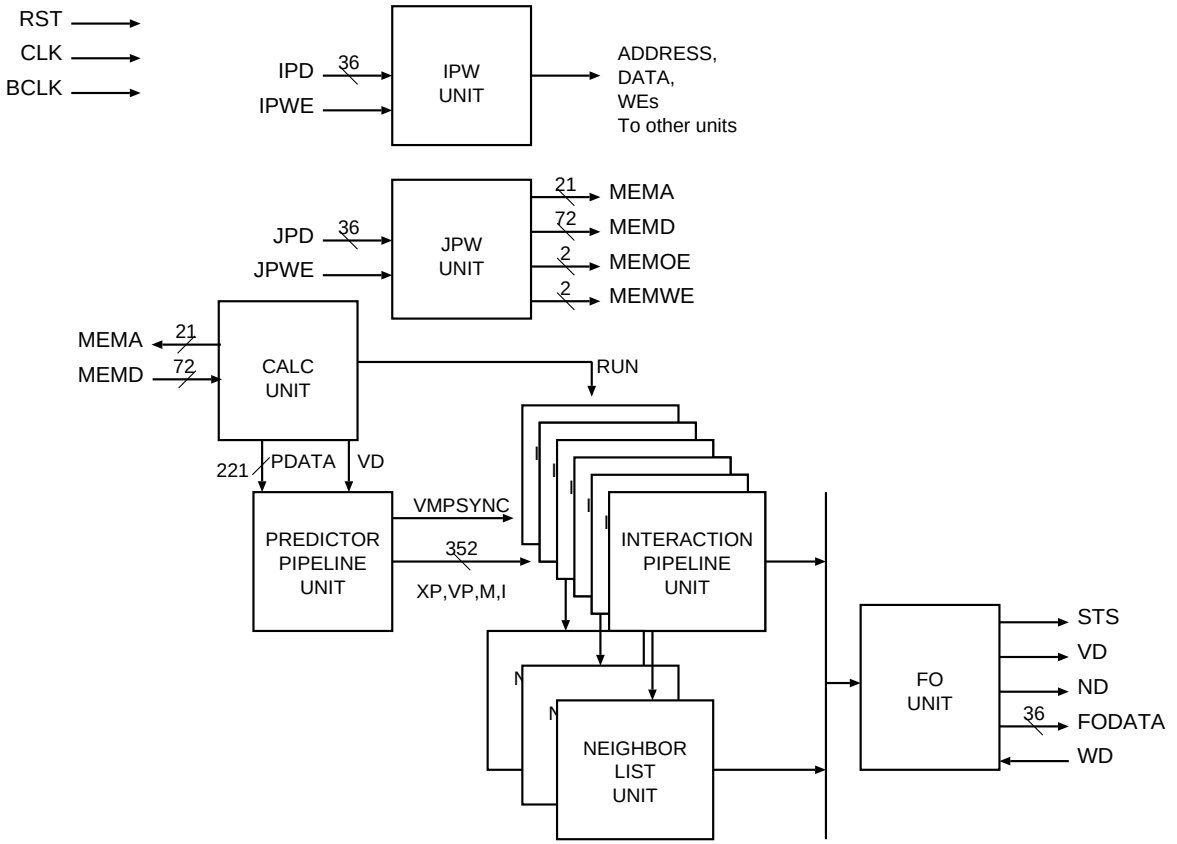
Accurate except for the cost estimate...

Pipeline chip



- 0.25 μm (Toshiba TC-240, 1.8M gates)
- 90 MHz Clock
- 6 pipelines
- 31 Gflops

Details of LSI



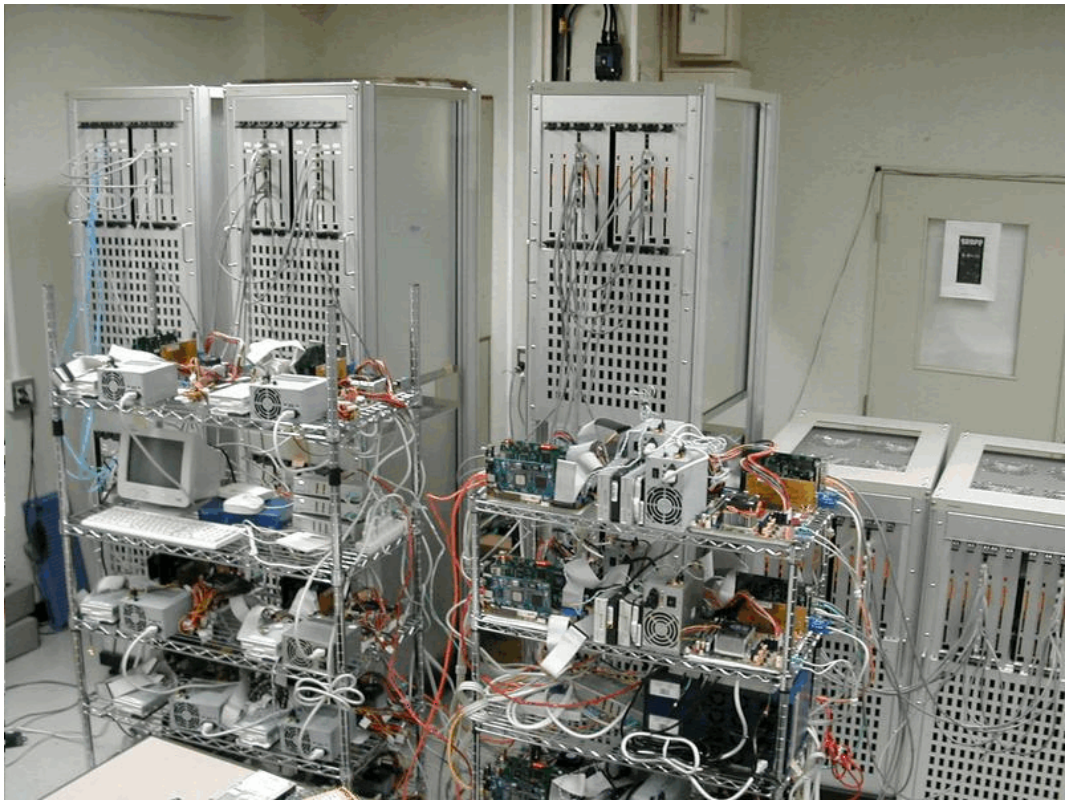
Equivalent to single GRAPE-4 board

- Host IF
- Memory IF
- Pipelines
- Controls

GRAPE-6 processor board

- 32 chips/board
- LVDS interface(350MHz clock, 4 wires, about 1Gbps)

The 64-Tflops GRAPE-6 system

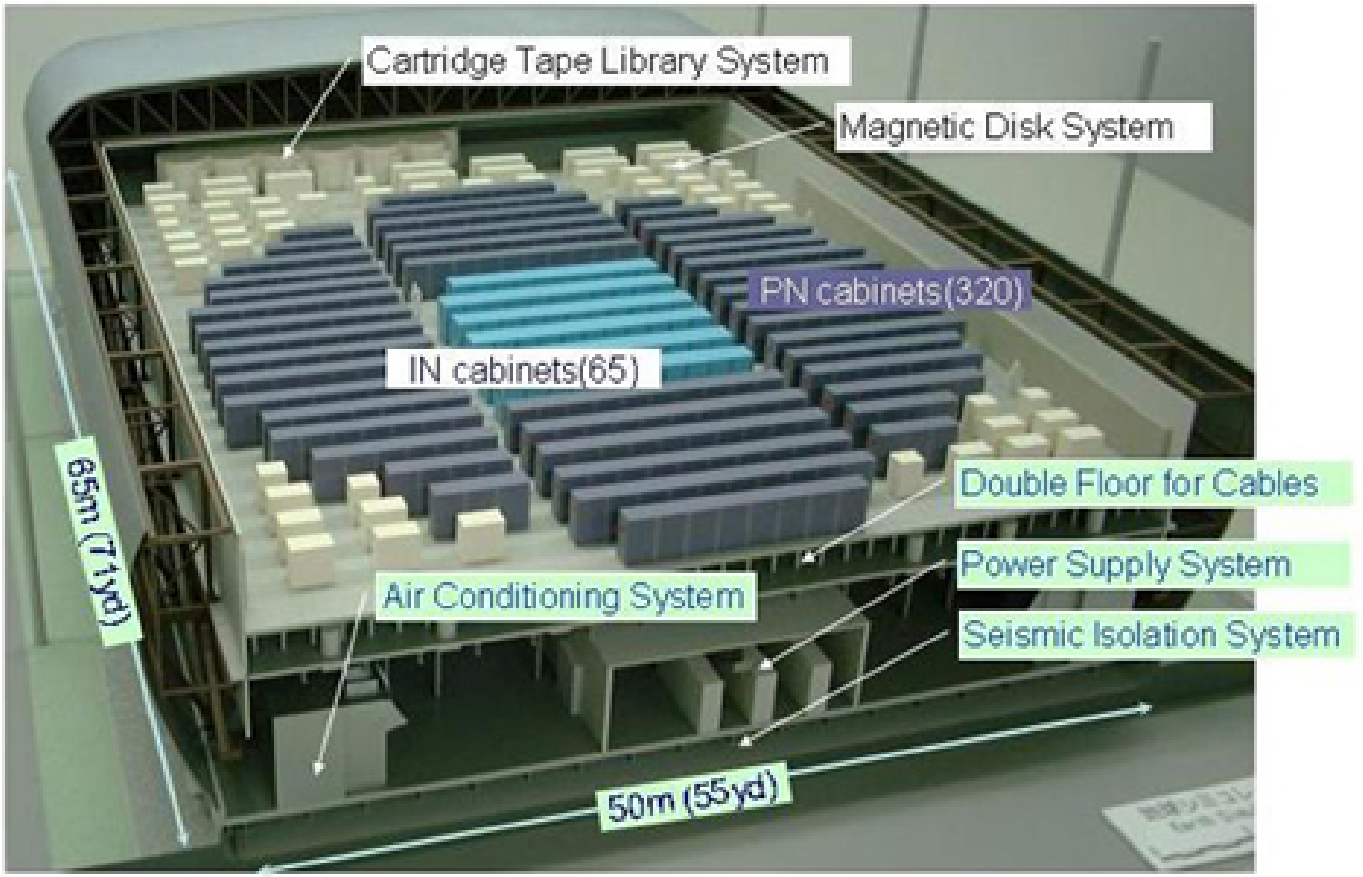


64-Tflops system.

4 blocks with 16 host computers.

In one room in Building 3, Asano-area of UT

The 40-Tflops Earth Simulator



Comparison with a recent Intel processor

	GRAPE-6	Intel Xeon X7460
Year	1999	2008
Design rule	250nm	45nm
Clock	90MHz	2.66GHz
Peak speed	32.4Gflops	64Gflops
Power	10W	130 W
Perf/W	3.24Gflops	0.49 Gflops

Even after 10 years...

"Problem" with GRAPE approach

- Chip development cost becomes too high.

Year	Machine	Chip initial cost	process
1992	GRAPE-4	200K$	1μm
1997	GRAPE-6	1M$	250nm
2004	GRAPE-DR	4M$	90nm
2008?	GDR2?	$\sim$ 10M$	65nm?

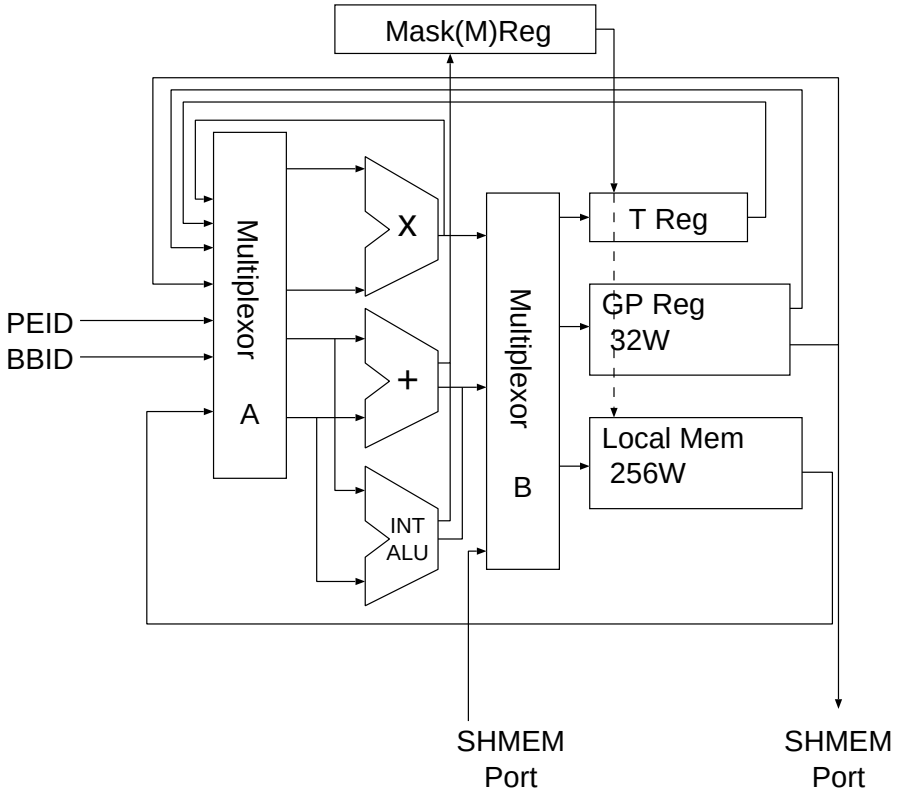
Initial cost should be 1/4 or less of the total budget.

How we can continue?

Next-Generation GRAPE — GRAPE-DR

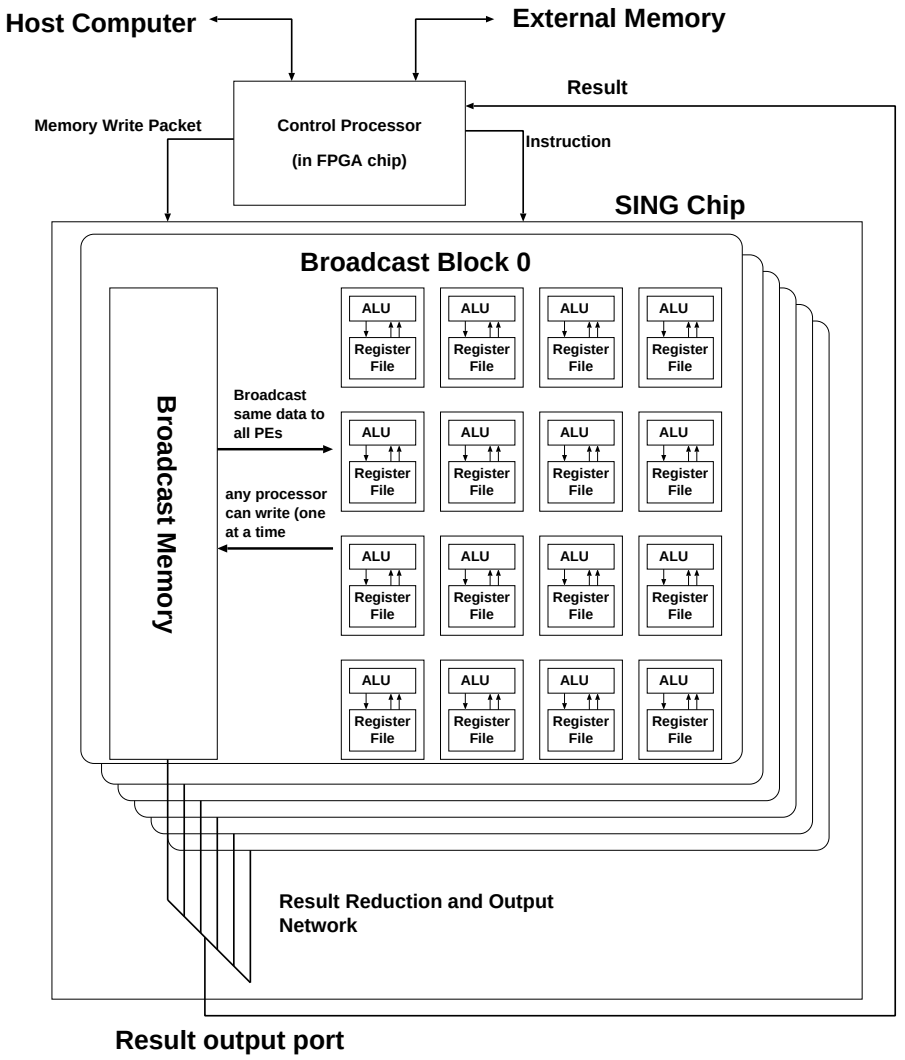
- Planned peak speed: 2 Pflops
- New architecture — wider application range than previous GRAPEs
- primarily to get funded
- No force pipeline. SIMD programmable processor
- Planned completion year: FY 2008 (early 2009)

Processor architecture



- Float Mult
- Float add/sub
- Integer ALU
- 32-word registers
- 256-word memory
- communication port

Chip structure



Collection of small processors.

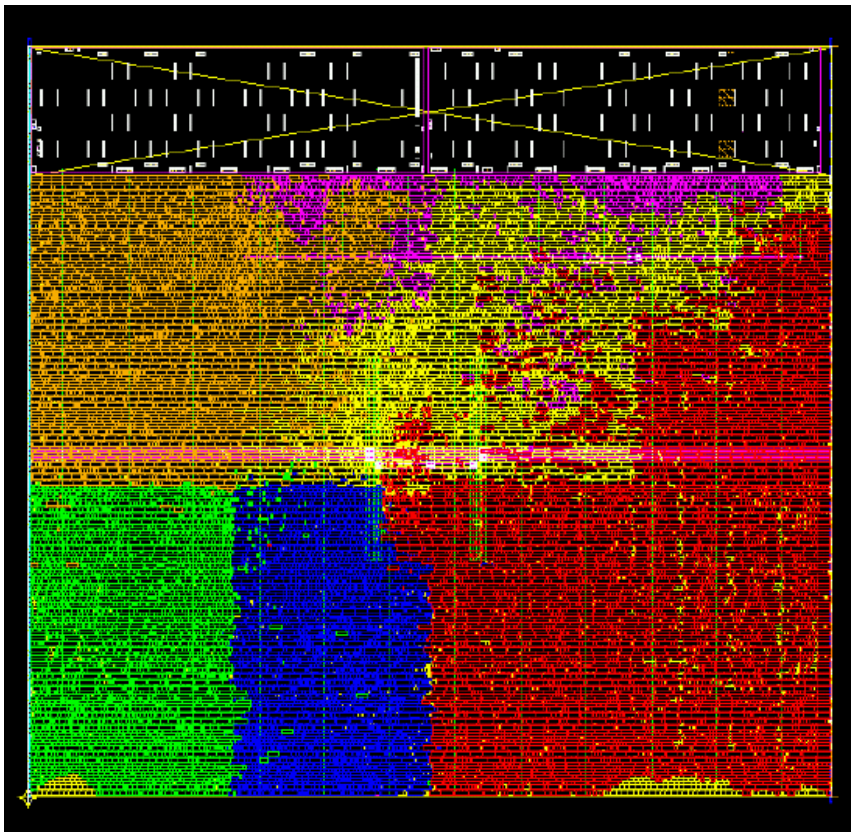
512 processors on one chip
500MHz clock

Peak speed of one chip: 0.5 Tflops (20 times faster than GRAPE-6).

Why we changed the architecture?

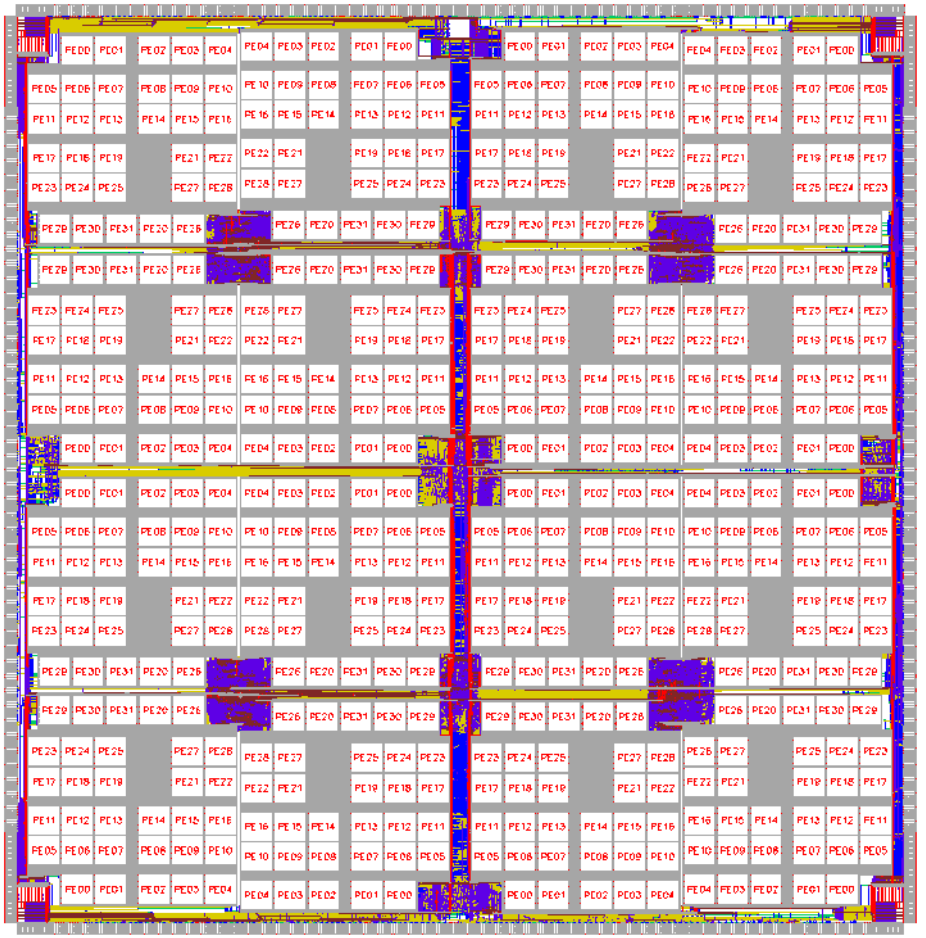
- To get budget (N-body problem is too narrow...)
- To allow a wider range of applications
  - Molecular Dynamics
  - Boundary Element method
  - Dense matrix computation
  - SPH
- To allow a wider range of algorithms
  - FMM
  - Ahmad-Cohen
  - ...

PE Layout



0.7mm by 0.7mm
Black: Local Memory
Red: Reg. File
Orange: FMUL
Green: FADD
Blue: IALU

Chip layout

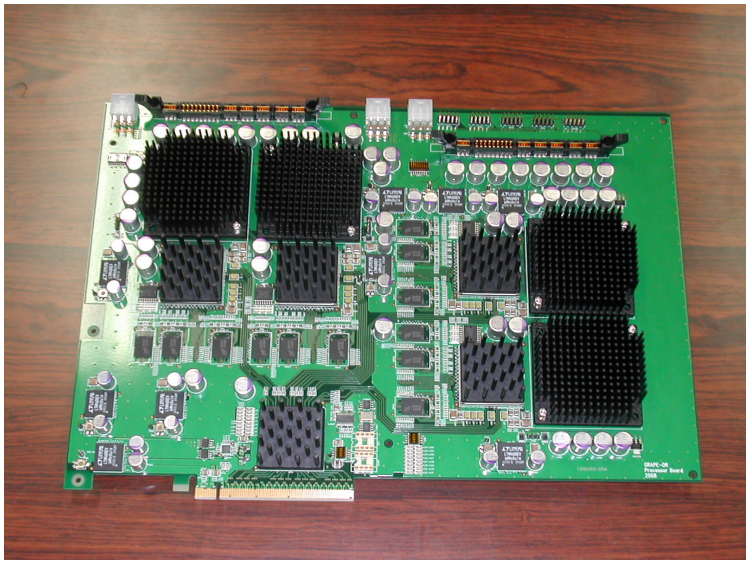


- 32PEs in 16 groups
- 18mm by 18mm

The processor chip

Sample chip delivered May 2006

Processor board

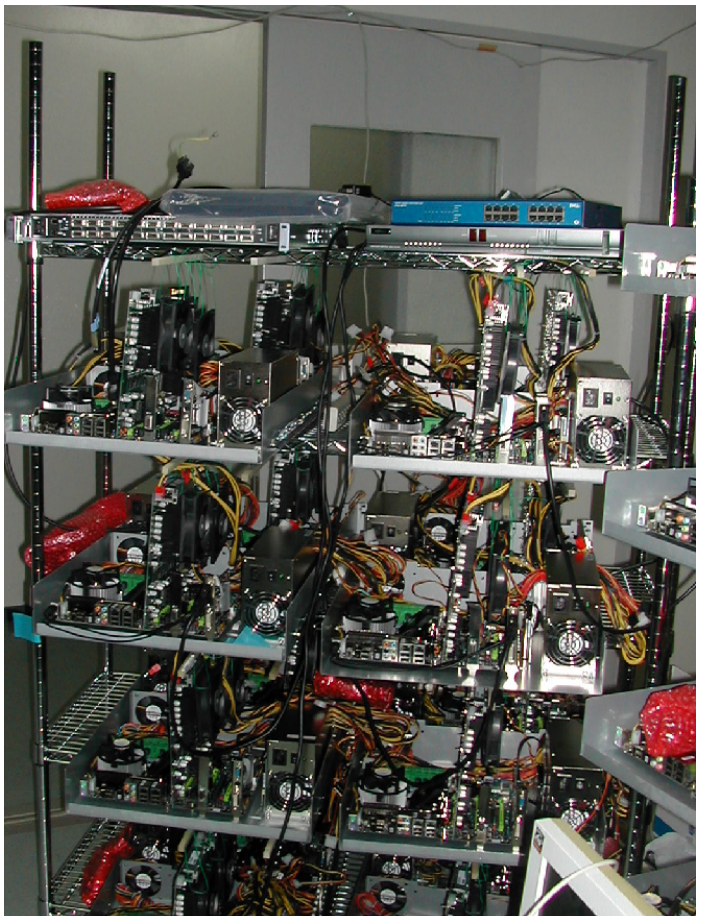


PCIe x16 (Gen 1) interface
Altera Arria GX as DRAM controller/communication interface

- Around 250W power consumption
- Not quite running at 500MHz yet... (FPGA design not optimized yet)
- 900Gflops DP peak (450MHz clock)
- Available from K&F Computing Research

GRAPE-DR cluster system

Just to show that the system exists...



Host computer: Intel Core 2 Quad Q6600 with nVidia 780i chipset

8GB memory

Network: IB (4x DDR)

HPC Linpack passed (not tuned yet....)

The system and (preliminary) performance numbers submitted to TOP500

Major concern: Effective host memory bandwidth

GDR cluster in 2009

- Nehalem with 3way DDR3 memory should resolve bandwidth problem.
- IB network
- 800T-1P DP peak range.

Japan's Next-generation Supercomputer Project

- FY 2006-2012
- Total budget: 110 BJYE (about 80 times that of GRAPE-DR)
- Peak speed: 10Pflops (about 10 times that of GRAPE-DR)
- Vector (like ES) + Scalar (???) hybrid

Summary

- GRAPEs seems to be fairly successful
- However, we cannot continue...
- With GRAPE-DR, we moved to new architecture
- We'll see if this was the right move or not.

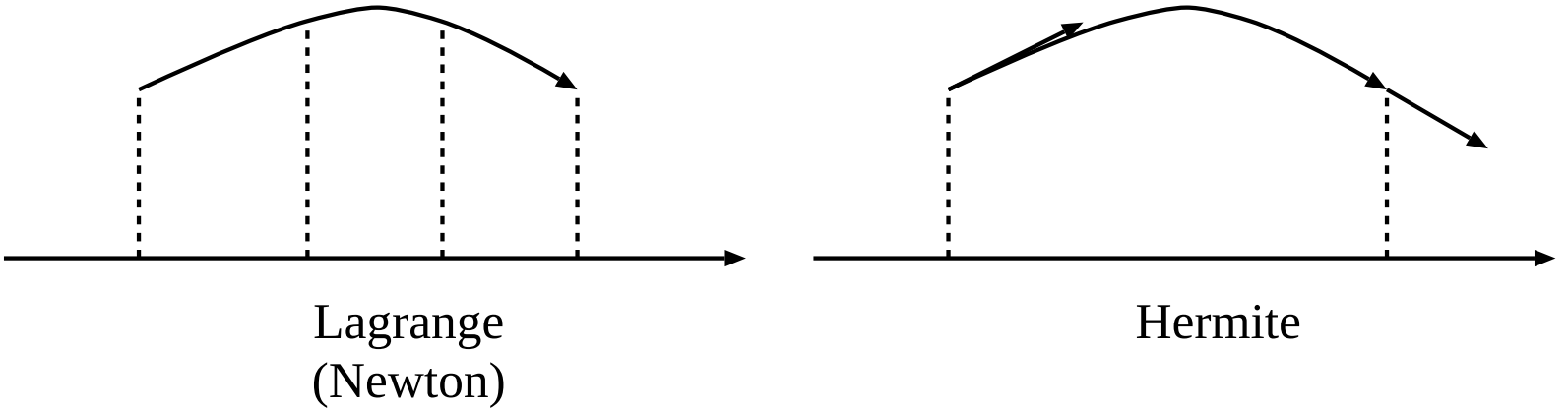
Integration scheme

Integration order: "4th the best" (JM 1990)

6-8th seems better: (Nitadori and JM 2007)

- **Aarseth scheme (Aarseth 1963): Adams scheme, PEC mode, 4th**
- **Hermite scheme (JM 1990): Hermite interpolation with direct calculation of the first time derivative of the force**

Aarseth scheme and Hermite scheme



Left: Aarseth scheme with Newton interpolation

Right: Hermite scheme

Hermite scheme is much simpler to implement and faster

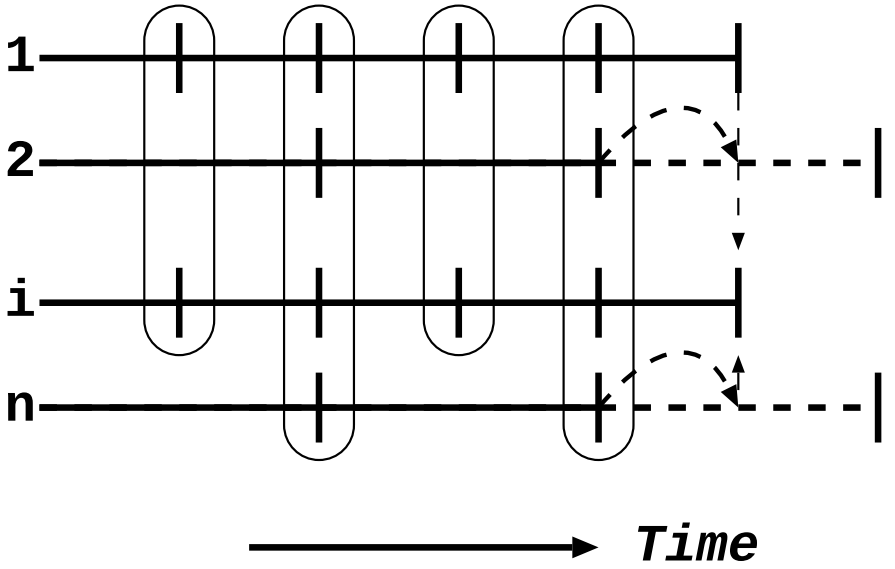
High-order Hermite schemes

Nitadori and JM 2007

- **Direct calculation of second derivative: 6th**
- **Direct calculation of third derivative: 8th**
- **Predictor requires the values at previous steps (for 4th order scheme previous value was not needed)**

Block individual timesteps

(McMillan 1986) improvement for parallel computers



- Limit timesteps to 2^{-k}
- stars with the same $t_i + \Delta t_i$ (even with different Δt_i) integrated in parallel

$O(N_c^{2/3})$ stars (N_c: number of stars in the core)

Initial plan

- ROM table for arithmetic, 8-bit data
- GPIB (IEEE-488) communication

Calculation/communication: Designed to use with 10,000 particles or around

5 MHz clock = can use around 1 ms for one particle communication

$<$ 100 bytes data per particle $\rightarrow$ communication speed 100KB/s

RS-232C too slow

SCSI too difficult to design

Design change

It turned out that, even if the accuracy of the pairwise force is low, if we do

- **first subtraction of positions**
- **final accumulation of the force**

in high accuracy, we can achieve the accuracy better than treecode.

First sub: 16bit, final acc:48bit, both fixed point

Personal feeling...

It seems rather difficult to build something like GRAPE
Understandings of

- **Target problem**
- **Algorithm, accuracy**
- **Computer architecture**
- **Digital logic design**
- **Physical design (packaging, cooling....)**
- **OS, device driver etc**

need to be integrated, ideally in a single person.

(Digital Orrery: G. Sussman had all of this)

Not necessary the world best understanding, though.
Something reasonable is okay.

Compared to general purpose computer

With general-purpose computer you don't have to worry about

- **Target problem**
- **Algorithm, accuracy**

really?

- **Other things:**

You need the best.

Are special-purpose computers difficult?

Rather few successful examples.

Particle systems: two approaches

Pipelined processors

- DMDP (Delft)
- FASTRUN
- GRAPE
- MD-Engine
- MDM

Programmable Parallel machines

- Digital Orrery
- Transputer-based projects...
- HaMM
- Many others

Why failures?

Two reasons:

1. **Machine could not be used**
2. **Machine too slow when completed**

Second one is much more common.

Problem with development time

Almost everybody (including myself) is too optimistic.
Essential problem:
In the case of special-purpose computer, a project which loses meaning with 1-2 years of delay should not be started.
Roughly speaking, when you start, if the price performance is better by

- 1000 — okay
- 100 — getting difficult
- 10 — should not start

If we assume five-year development time and five-year lifetime of the hardware.

A few more words on software

- The right way to separate the task between host CPU and (GRAPE, GRAPE-DR, GPU, FPGA) is the same
- The right way to make efficient use of large number of processors on (GRAPE, GRAPE-DR, GPU, FPGA, CPU) is the same

We should develop a common software platform for different hardwares

Preliminary data for first commercial version

- Prototype board working
- 1 Chip on a board (0.5Tflops peak)
- PCI-Express x4 interface
- 80W ...
- $\sim$ 5K USD ...

Dynamical time

For a stellar system with mass M, typical radius R, we have the Virial Theorem

$$E = -K = W/2$$

E: total energy ($K + W$), K: total kinetic energy, W: total potential energy,

$$W = \sum_{i<j} G\frac{m_i m_j}{|x_i - x_j|}$$

$$K = \sum_i \frac{1}{2} m_i v_i^2$$

Dynamical time (2)

For R, we have

$$W \sim -\frac{GM^2}{R}$$

and for K

$$K = -\frac{Mv^2}{2}$$

and we have $v \sim \sqrt{GM/R}$, and

$$T = R/v = \sqrt{\frac{R^3}{GM}}$$

Nonexistence of the thermal equilibrium

Thermal equilibrium, if exists, must be described by the Maxwell-Boltzmann statistics.

This is however impossible for a stellar system.

Reason:

Energies of all stars in the system cannot exceed the potential energy at the infinity (otherwise they go to infinity).

Therefore, there must be an upper cutoff in the energy distribution function.

Final state of stellar systems

Essentially the same as $N = 3$.

If high-energy stars are generated through gravitational scattering, they escape from the system.n

In other words, from the equilibrium statistical mechanics we can conclude:

> **Every gravitational many-body system will evaporate, if we wait long enough**

This is certainly true, but not too useful for the understanding of existing stellar systems.

We do need non-equilibrium statistical mechanics.

Principle of the individual timestep

Each star has its own time t_i and timestep Δt_i

1. **Select the star with minimum $t_i + \Delta t_i$**
2. **Integrate its orbit to its new time $t_i + \Delta t_i$**
3. **determine its new timestep**
4. **go back to step 1.**

We need high-accuracy position prediction for other stars at time $t_i + \Delta t_i$.

Predictor-corrector type schemes are used.

Calculation cost and accuracy

Simple estimate:

$$error \propto \theta^{(p+1)}$$

$$cost \propto \theta^{-3} p^2 N \log N$$

p: expansion order

$\log N$: tree level

θ^3: number of cells in one level which interact with one particle

In reality...

Actual behavior: rather complex

- **Accuracy is better than the estimate in the previous slide**
- **Calculation cost shows weaker dependence on θ**

Calculation cost for thermal evolution

- per step: N^2
- number of orbits: $N/\log N$
- steps per orbit: $> N^{1/3}$
- In total:

$$\frac{N^{10/3}}{\log N}$$

- $N \sim 2 \times 10^5$ is the current limit with fastest computers available

Numerical integration over thermal timescale

- Very costly
- Do we need to do such expensive calculations?
- Can't we rely on some statistical approach, if the system is statistical anyway?

I do not have a short answer...

Summary of a long answer

- **Thermal equilibrium does not exist**
- **Small-N effects alway become important**

As a result:

Reliable statistical methods are very difficult to construct

Numerical methods

Let me discuss the techniques for numerical integration.

Very naively, it is important to do calculations

- **with large N**
- **with high accuracy**
- **for long time**

since that helps to develop the better understanding.

How we can do better calculations?

Basic idea: If we can do the same calculation faster, that means we could use larger N or achieve higher accuracy, if we use the same amount of the computer time

Impact on the calculation cost

Simple variable timestep would cost too much

Reason: Power-law distribution of timesteps

Calculation cost increases as some power of N

Structure formation: $O(N^{1.3})$ or around

Two-body scattering: $O(N^{1/3})$

Solution:

- **Assign different timesteps to different stars (individual timestep)**
- **Two-body collision, binaries: Coordinate transformation**

Memory bandwidth requirement

Reduction of communication

Host — GRAPE: N stars, N^2 calculation

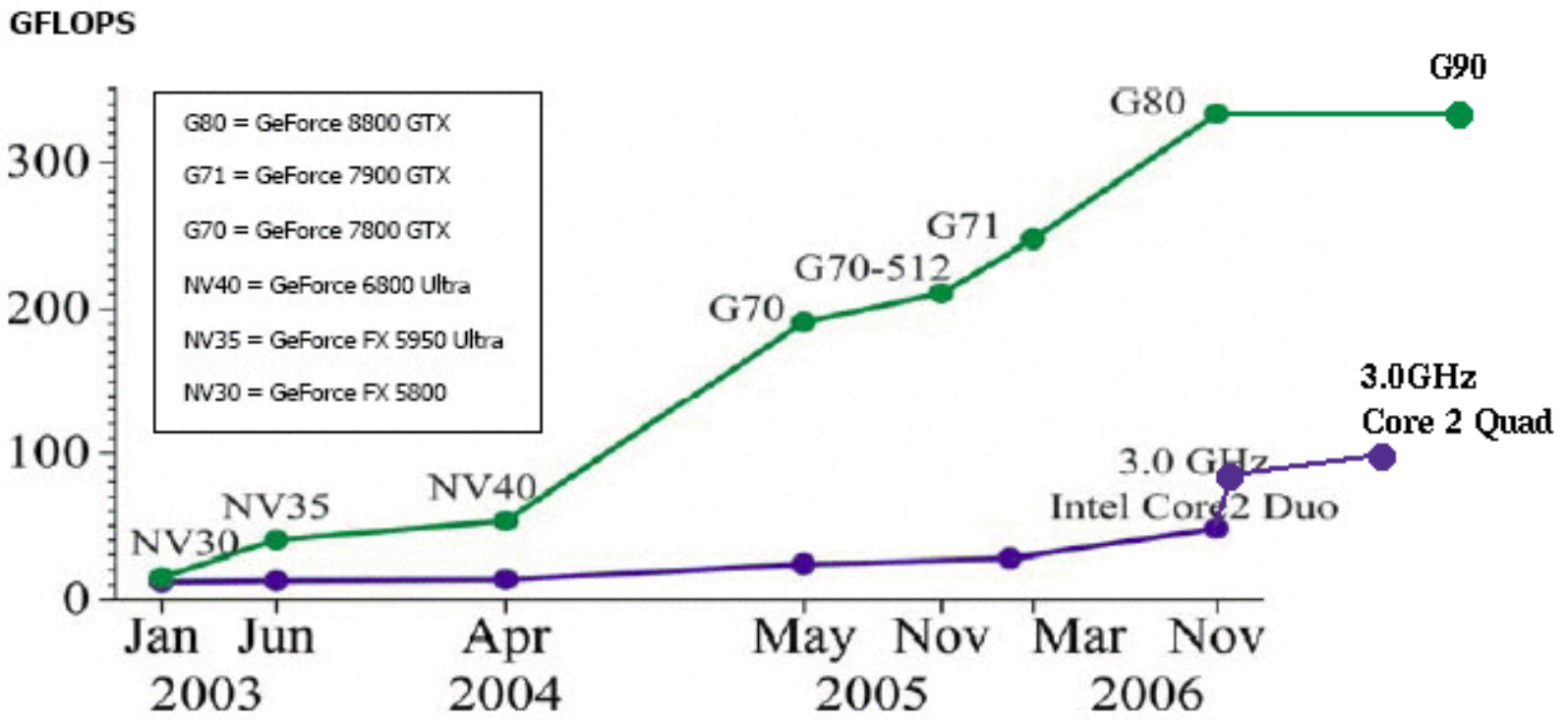
Board/chip level:

- **Multiple pipelines calculate the force from same particle to different particles**
- **Virtual multiple pipeline: One pipeline calculates the forces on several particles**

Comparison with FPGA

- much better silicon usage (ALUs in custom circuit, no programmable switching network)
- (possibly) higher clock speed (no programmable switching network on chip)
- easier to program (no VHDL necessary; assembly language and compiler instead)

GPGPUs —Today



Hmm...

How do you use it?

- GRAPE: The necessary software is now ready. Essentially the same as GRAPE-6.
- Matrix etc ... RIKEN/NAOJ will do something
- New applications:
  - Primitive Compiler available
  - For high performance, you need to write the kernel code in assembly language (for now)

Primitive compiler

(Nakasato 2006)

```
/VARI  xi, yi, zi, e2;
/VARJ  xj, yj, zj, mj;
/VARF  fx, fy, fz;
dx = xi - xj;
dy = yi - yj;
dz = zi - zj;
r2 = dx*dx + dy*dy + dz*dz + e2;
r3i= powm32(r2);
ff = mj*r3i;
fx += ff*dx;
fy += ff*dy;
fz += ff*dz;
```

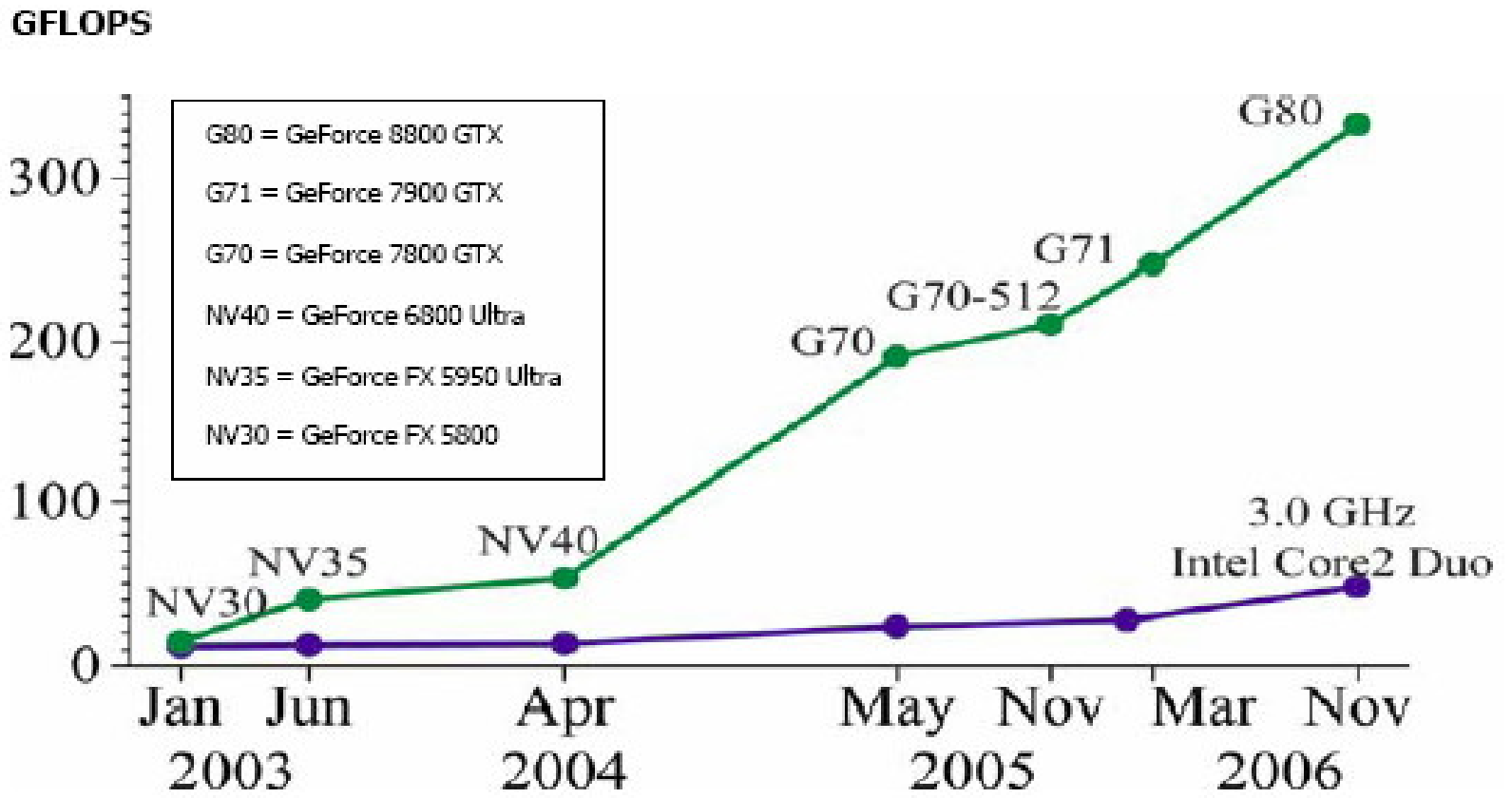
- **Assembly code**
- **Interface/driver functions**
- **SIMD parallel data distribution**
- **Data reduction**

are generated from this "high-level description".
(Can be ported to GPUs)

Interface functions

```
struct SING_hlt_struct0{
  double xi;
  double yi;
  double zi;
  double e2;
};
int SING_send_i_particle(struct SING_hlt_struct0 *ip,
                         int n);
int SING_send_elt_data0(struct SING_elt_struct0 *ip,
                        int index_in_EM);
int SING_get_result(struct SING_result_struct *rp);
int SING_grape_run(int n);
```

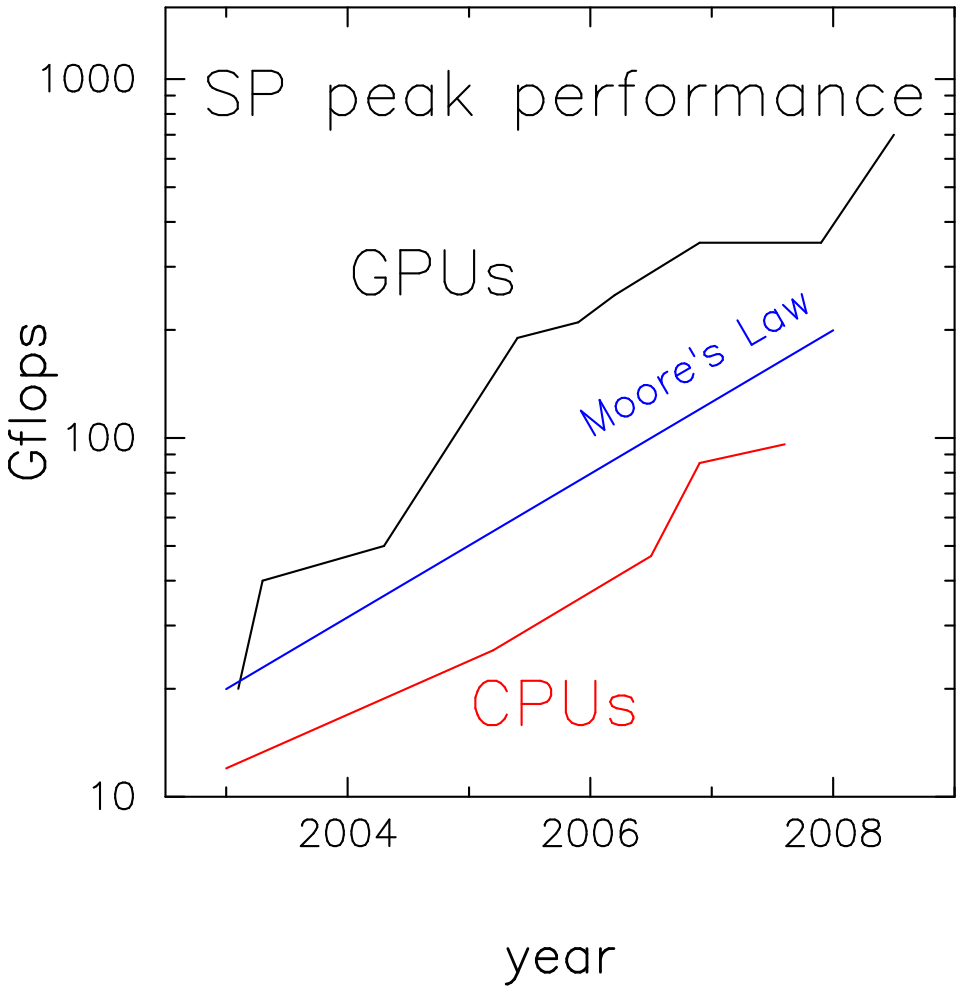
GPGPUs —What manufacturers show:



"GPUs beat Moore's Law!"

(AstroGPU, Nov 9-10, 2007, IAS, Princeton)

GPGPUs —Same data in log plot



- **Faster-than-Moore period ended in 2005**
- **Microprocessors are catching up**
- **DP performance?**
- **Design limit with memory bandwidth**

Communication overhead

NEWS was very slow

Reason: GPIB communication is through UNIX OS system call, which incurred more than 1ms overhead.

Our initial approach: Use NEC PC for buffering the data

Final solution: hack the operating system and let the application program directly manipulate the GP-IP controller LSI.