Challenges: Star Clusters

Globular Star Clusters contain Millisecond Pulsars, „Blue Stragglers" (probably merger remnants), neutron star binaries

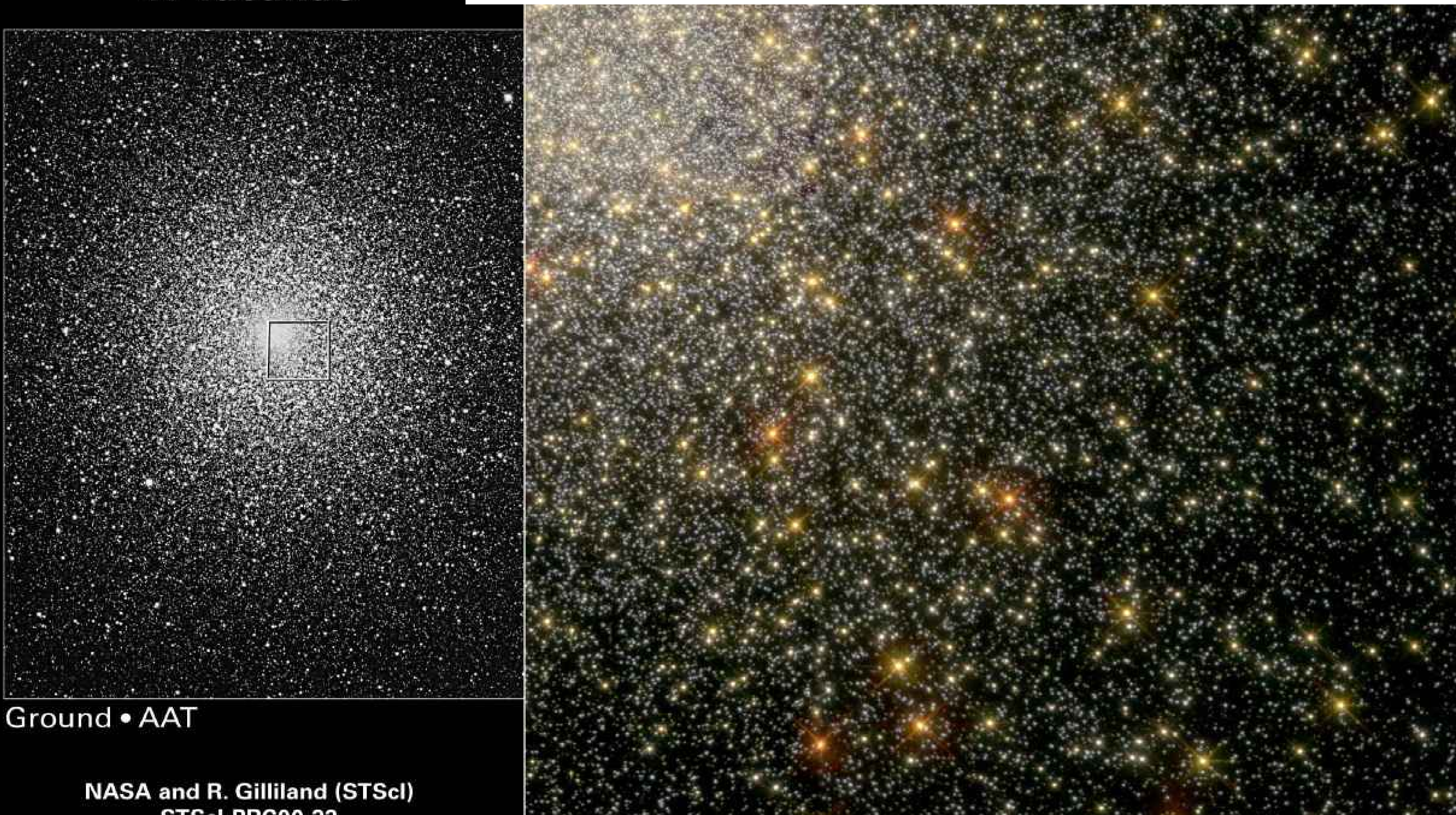
Dynamic range in time scales 10^{18} !

(Density Range in Star Formation 10^{24} !)

Scales are coupled in complex way!

$$\vec{a}_0 = \sum_j G m_j \frac{\vec{R}_j}{R_j^3} \quad ; \quad \dot{\vec{a}}_0 = \sum_j G m_j \left[\frac{\vec{V}_j}{R_j^3} - \frac{3(\vec{V}_j \cdot \vec{R}_j)\vec{R}_j}{R_j^5} \right]$$

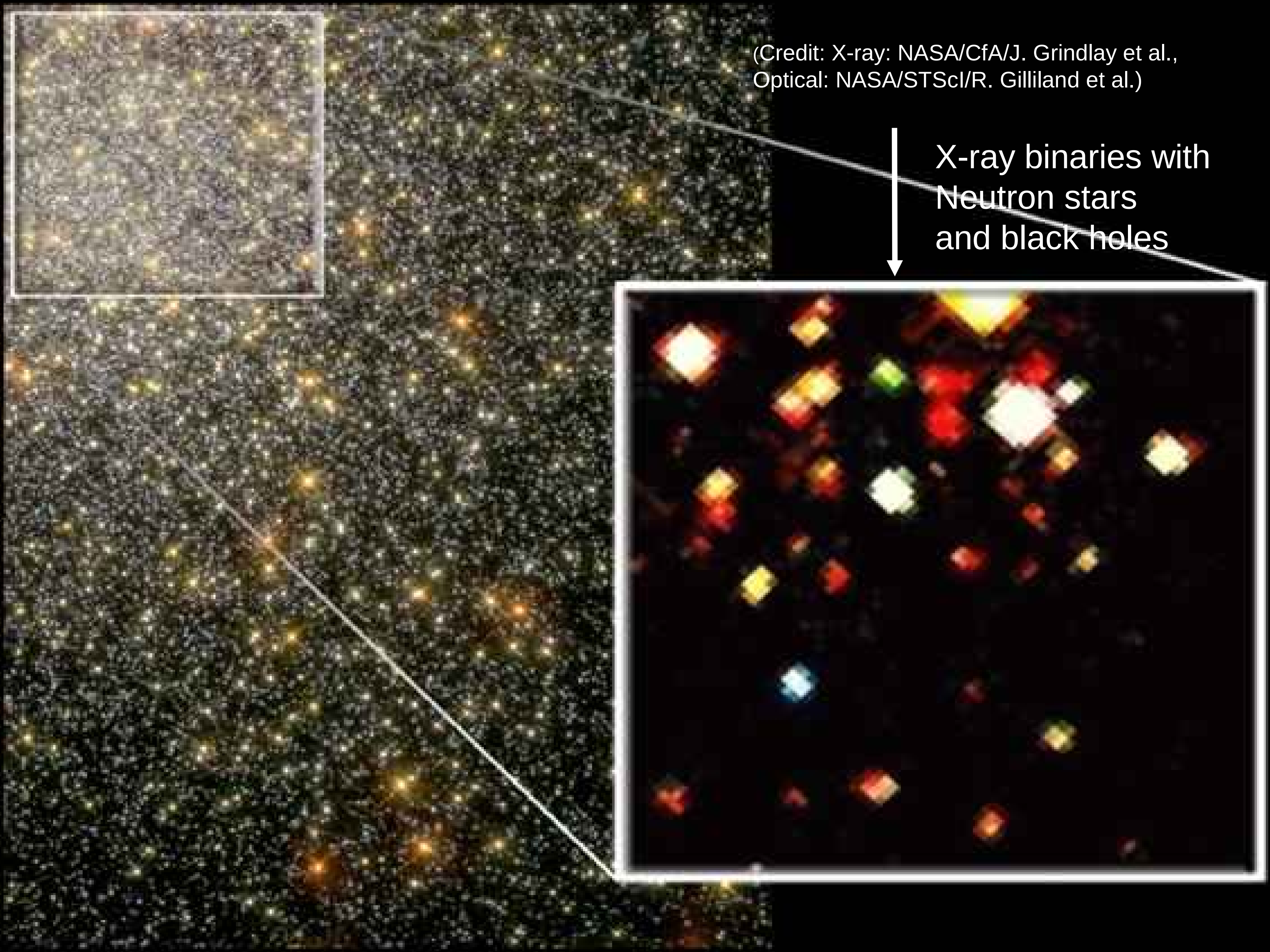
Globular Cluster 47 Tucanae



Ground • AAT

Hubble Space Telescope • WFPC2

NASA and R. Gilliland (STScI)
STScI-PRC00-33

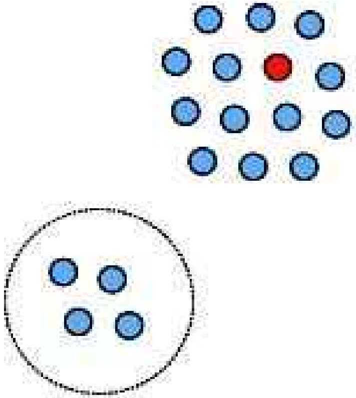

(Credit: X-ray: NASA/CfA/J. Grindlay et al.,
Optical: NASA/STScI/R. Gilliland et al.)
X-ray binaries with
Neutron stars
and black holes

You cannot shield gravity...

Newton's law of gravity

$$\vec{a}_i = \sum_{i=1}^{N} \frac{Gm_j}{\left|\vec{x}_j - \vec{x}_i\right|^3} \cdot \left(\vec{x}_j - \vec{x}_i\right)$$

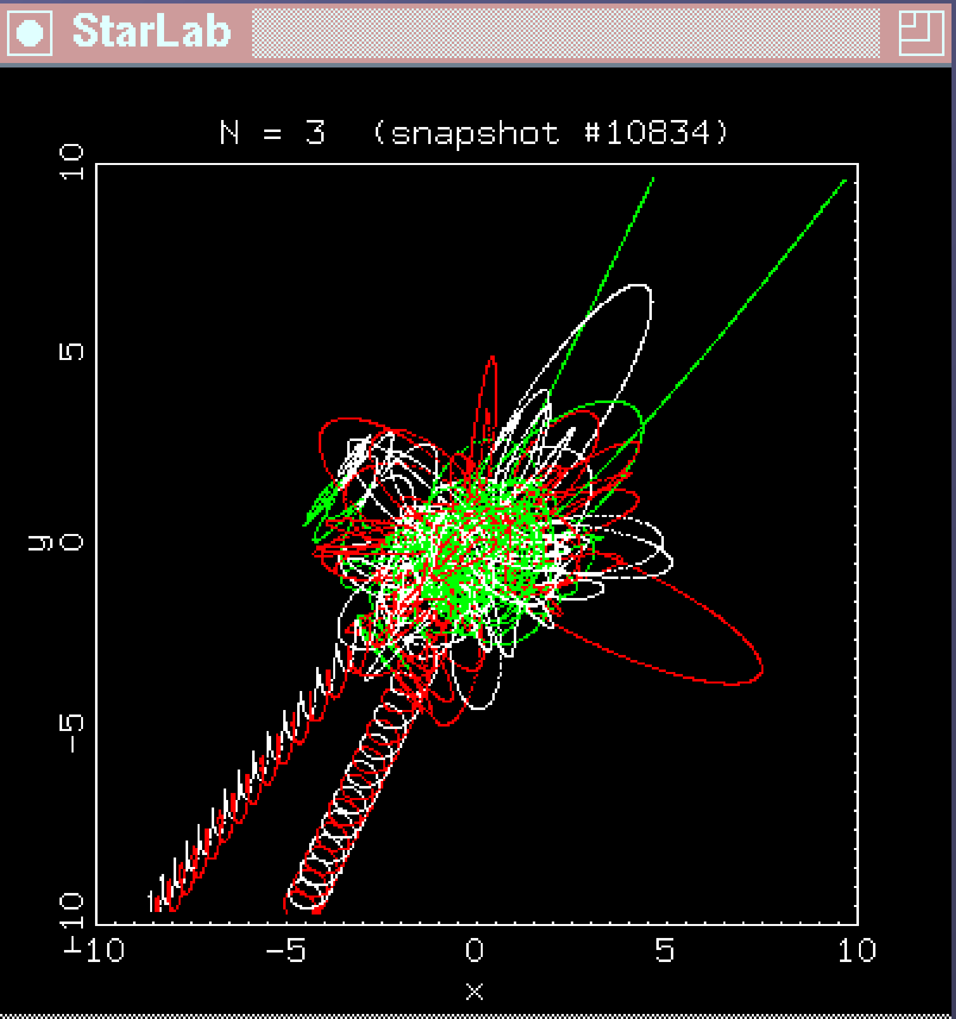
full problem scales with O(N^2)
caveat: hierarchical time-steps



- hardware accelerators
- approximation methods (O(N log$N$))
- or both !!

HITS

Challenges: Star Clusters



Resonant 3-Body Encounter

Starlab Simulation by S.L.W. McMillan

http://www.physics.drexel.edu/~steve/
-> Three-Body-Problem

Challenges: Star Clusters

Chaos in the 3-Body Problem
(by S.L.W. McMillan)

1 pixel in image = 1 simulated 3-body encounter

X-axis: initial phase of binary

Y-axis: impact parameter

Colour: angle by which escaping star leaves the system.

Fortunately there exist statistical averages for cross sections

Challenges: Star Clusters

So we need (among others):

- 2-body Regularization (Kustaanheimo & Stiefel 1965)
- 3-body Regularization (Aarseth & Zare 1974)
- Hierarchical Subsystems (Chain, Aarseth & Mikkola)

Quaternions....

Physical and Numerical Methods: Modelling the Dynamics

$$\vec{a}_0 = \sum_j G m_j \frac{\vec{R}_j}{R_j^3} \quad ; \quad \dot{\vec{a}}_0 = \sum_j G m_j \left[\frac{\vec{V}_j}{R_j^3} - \frac{3(\vec{V}_j \cdot \vec{R}_j)\vec{R}_j}{R_j^5} \right]$$

- $N = \infty$

negative specific Heat

gravothermal Collapse

gravothermal Oscillations

- $N = 3$ $(N = 2, \ldots, \approx 100)$

History

Exponential Instability

Chaos and Resonance

Regularisation

- $N = 10^6$ $(N = 10^4, 10^5)$

Post-Kollaps-Evolution

Binaries

Globular Clusters

Physical and Numerical Methods: Modelling the Dynamics

Why N-body Simulations?

1. N too small for safe thermodynamics

2. $\lambda \gg R$

Why "brute force"?

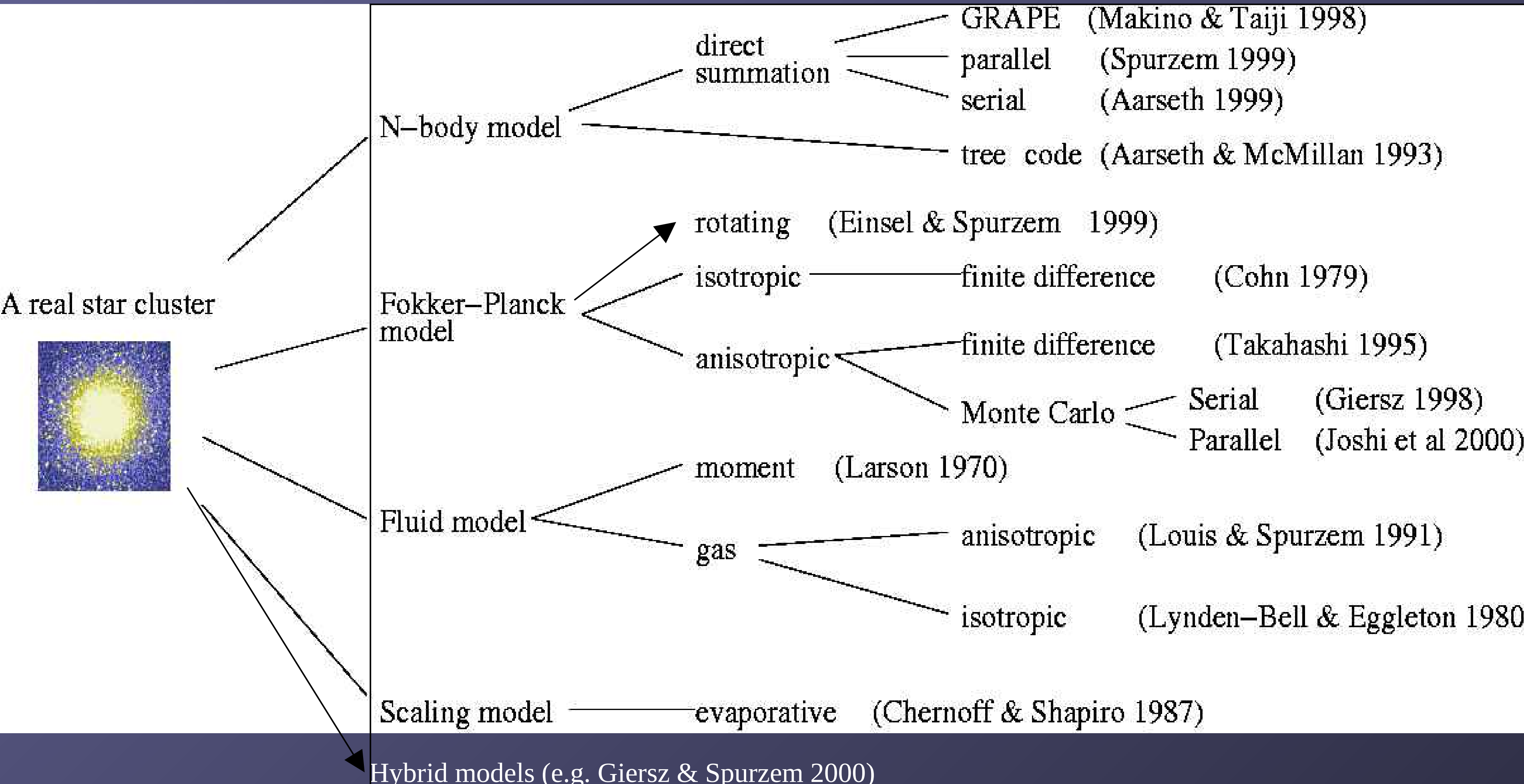
1. Multiple Time Scales

2. Granularity of Potential

3. Special Purpose Hardware

Physical and Numerical Methods: Modelling the Dynamics

Some methods for studying the evolution of globular clusters (by D.C.Heggie)



Physical and Numerical Methods: Direct Simulations

The Hermite Scheme: 4th Order on two time points

$$\vec{a}_0 = \sum_j Gm_j \frac{\vec{R}_j}{R_j^3} \quad ; \quad \dot{\vec{a}}_0 = \sum_j Gm_j \left[\frac{\vec{V}_j}{R_j^3} - \frac{3(\vec{V}_j \cdot \vec{R}_j)\vec{R}_j}{R_j^5} \right] ,$$

$$\vec{x}_p(t) = \frac{1}{6}(t - t_0)^3 \dot{\vec{a}}_0 + \frac{1}{2}(t - t_0)^2 \vec{a}_0 + (t - t_0)\vec{v} + \vec{x} ,$$

$$\vec{v}_p(t) = \frac{1}{2}(t - t_0)^2 \dot{\vec{a}}_0 + (t - t_0)\vec{a}_0 + \vec{v} ,$$

Repeat Step 1 at $t_1$using predicted x,v → $a_{1,}$ å$_1$

Physical and Numerical Methods: Direct Simulations

$$\frac{1}{2}\vec{a}^{(2)} = -3\,\frac{\vec{a}_0 - \vec{a}_1}{(t-t_0)^2} - \frac{2\dot{\vec{a}}_0 + \dot{\vec{a}}_1}{(t-t_0)}$$

$$\frac{1}{6}\vec{a}^{(3)} = 2\frac{\vec{a}_0 - \vec{a}_1}{(t-t_0)^3} - \frac{\dot{\vec{a}}_0 + \dot{\vec{a}}_1}{(t-t_0)^2}\ ,$$

The Hermite Step

Get Higher Derivatives

$$\vec{x}(t) = \vec{x}_p(t) + \frac{1}{24}(t-t_0)^4\vec{a}_0^{(2)} + \frac{1}{120}(t-t_0)^5\vec{a}^{(3)}\ ,$$

$$\vec{v}(t) = \vec{v}_p(t) + \frac{1}{6}(t-t_0)^3\vec{a}_0^{(2)} + \frac{1}{24}(t-t_0)^4\vec{a}_0^{(3)}\ .$$

The Corrector Step – this is not time symmetric!

Physical and Numerical Methods: Direct Simulations

P(EC)^n Scheme, n=1, Kokubo et al. 1998, Hut et al. 1995

$$\boldsymbol{x}_{\mathrm{p},j} = \boldsymbol{x}_j + \boldsymbol{v}_j(t-t_j) + \frac{\boldsymbol{a}_j}{2}(t-t_j)^2 + \frac{\dot{\boldsymbol{a}}_j}{6}(t-t_j)^3,$$

$$\boldsymbol{v}_{\mathrm{p},j} = \boldsymbol{v}_j + \boldsymbol{a}_j(t-t_j) + \frac{\dot{\boldsymbol{a}}_j}{2}(t-t_j)^2,$$

1 higher order in x-prediction

$$\boldsymbol{x}_1 = \boldsymbol{x}_0 + \frac{1}{2}(\boldsymbol{v}_1 + \boldsymbol{v}_0)\Delta t - \frac{1}{10}(\boldsymbol{a}_1 - \boldsymbol{a}_0)\Delta t^2 + \frac{1}{120}(\dot{\boldsymbol{a}}_1 + \dot{\boldsymbol{a}}_0)\Delta t^3$$

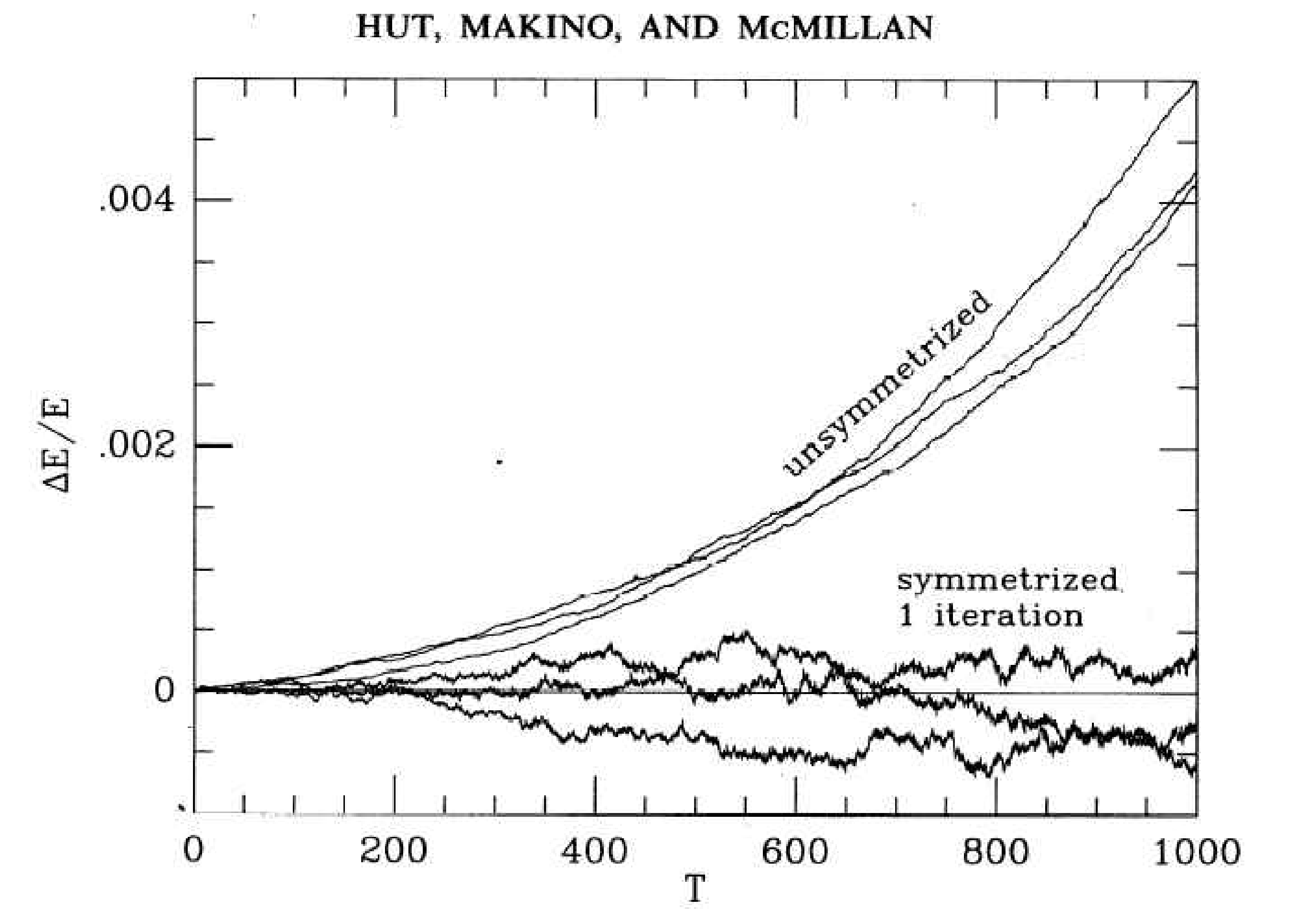
$$\boldsymbol{v}_1 = \boldsymbol{v}_0 + \frac{1}{2}(\boldsymbol{a}_1 + \boldsymbol{a}_0)\Delta t - \frac{1}{12}(\dot{\boldsymbol{a}}_1 - \dot{\boldsymbol{a}}_0)\Delta t^2.$$

This is time-symmetric (exchange 0,1, change sign(v),sign(å))!

(But pred/corr diff. in x,v of field particles neglected)

By iteration n>1 it improves further.

Physical and Numerical Methods: Direct Simulations



1995

N=100

1000
orb.times

Physical and Numerical Methods: Direct Simulations

Kokubo et al. 1998

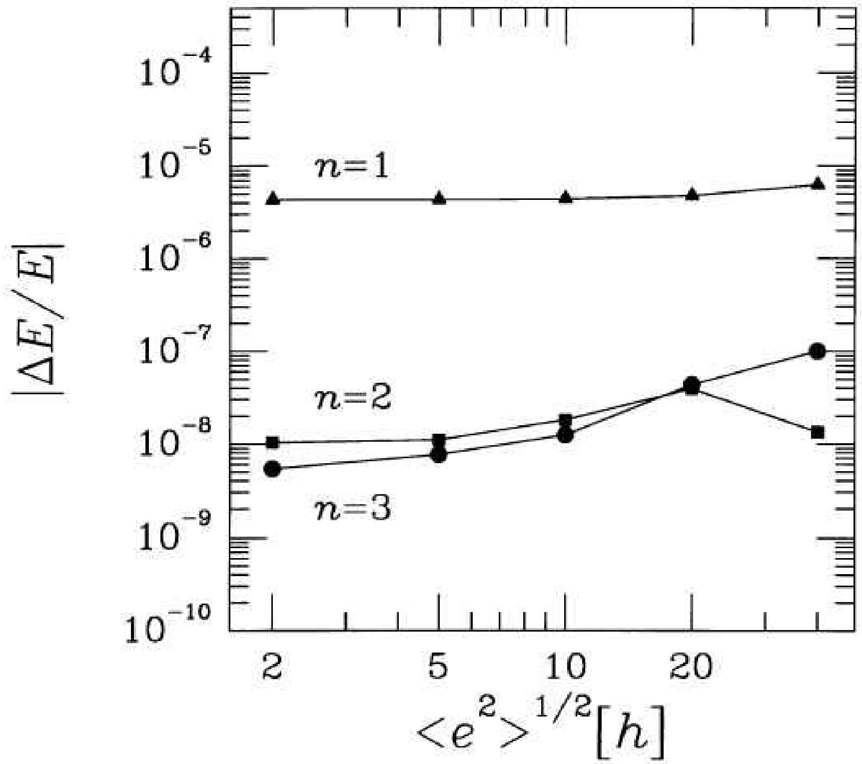
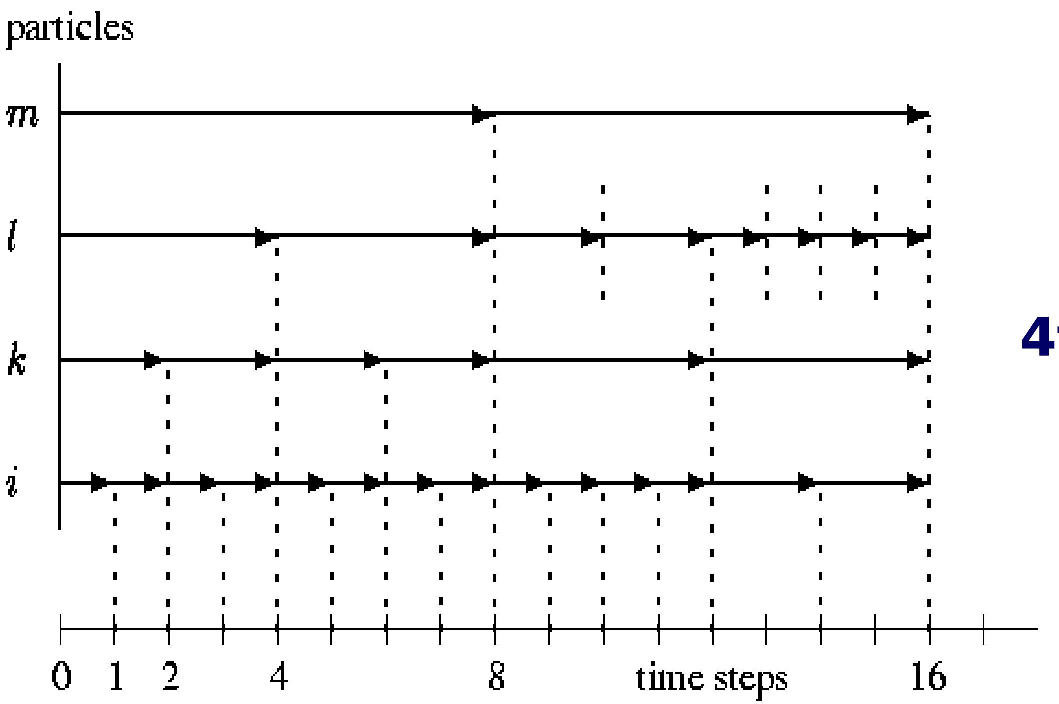


Figure 4. The relative error of the total energy of a planetesimal system that consists of 100 equal-mass ($m = 10^{25}$ g) bodies after $1000T_K$ as a function of the initial $\langle e^2 \rangle^{1/2}$ for the $P(EC)^n$ ($n = 1, 2, 3$) Hermite schemes with the hierarchical time-step scheme. The triangles show the result of the $n = 1$ scheme, the squares $n = 2$ and the circles $n = 3$.

Presently used GPU (GRAPE) N-body code

Harfst, Berczik, Merritt, Spurzem et al, NewA, 12, 357 (2007)
Spurzem et al., Comp. Science Res. & Dev. 23, 231 (2009)

Hierarchical Individual Block Time Steps

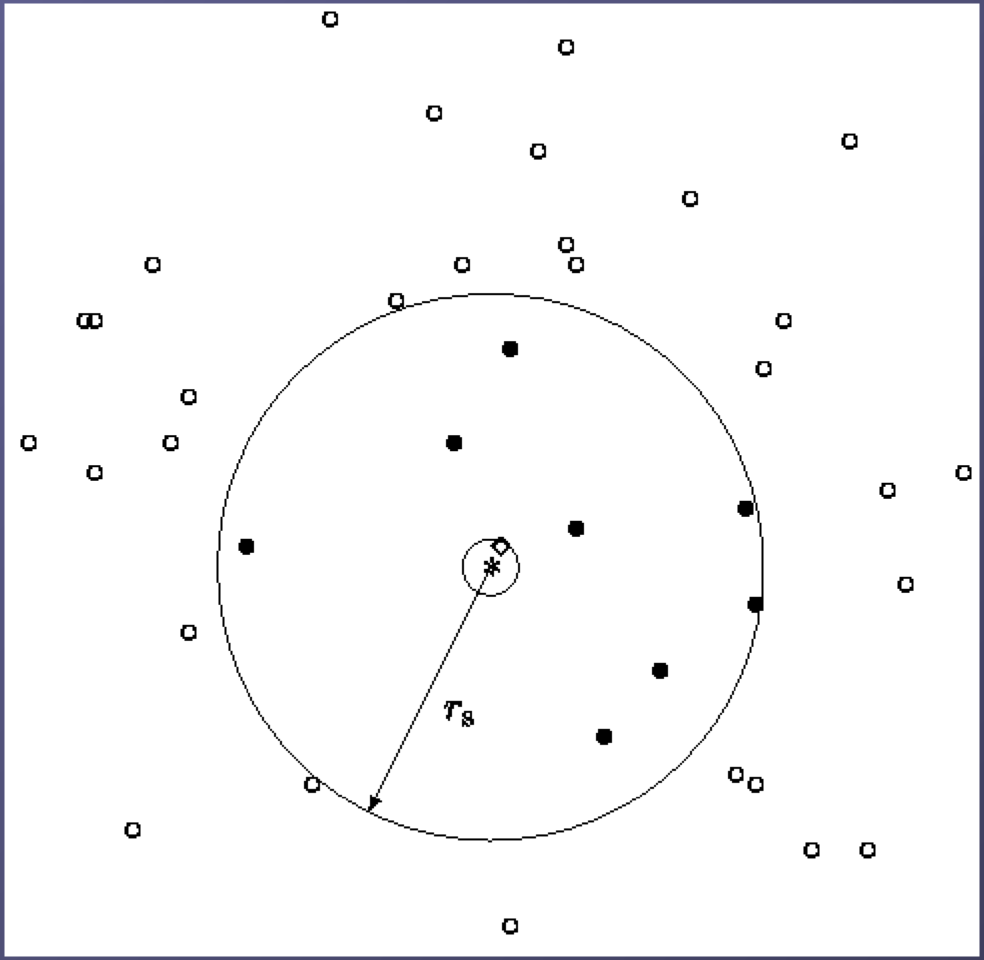


$$\Delta t = \sqrt{\eta \frac{|\vec{a}||\vec{a}^{(2)}| + |\dot{\vec{a}}|^2}{|\dot{\vec{a}}||\vec{a}^{(3)}| + |\vec{a}^{(2)}|^2}} \, .$$

4th order Hermite scheme

$$\frac{d^2 \vec{r}_i}{dt^2} = \vec{a}_i$$

Physical and Numerical Methods: Direct Simulations



Ahmad-Cohen Neighbour Scheme

(Double Volume for Incoming Particles)

Special Care for fast Particles

New Developments in progress!

Parallelization and Software

Acronym	Algorithm	Scaling	Comments
PM	Particle Mesh	$N\ n_c^3 \log_2 n_c^3$ (1)	fixed geometry
FMP	Fast Multipole	$N\ nlm$	req. equal Δt
SCF	Self-Consistent Field	$N\ nlm$	series evaluation (2)
NBODY1	Aarseth	N^2	ITS, softening
NBODY1++	Hermite	N^2	HTS, softening
NBODY2	Aarseth, AC	$N N_n + N^2/\gamma$	ITS, softening, (3)
NBODY3	Aarseth	N^2	ITS, KS-reg.
NBODY4	Hermite	N^2	HTS, KS-reg.
NBODY5	Aarseth, AC	$N N_n + N^2/\gamma$	ITS, KS-reg., (3)
NBODY6	Hermite, AC	$N N_n + N^2/\gamma$	HTS, KS-reg., (3)
NBODY6++	parallel NBODY6	$N N_n + N^2/\gamma$	HTS, KS-reg., (3,4)
KIRA	Hermite	N^2	HTS, (5)
TREE	TREE-code	$N \ln N$	N^2 for high accuracy
P^{3}M	Part.-Part. PM	$N_n^2\ n_c^3 \log_2 n_c^3$ (1)	fixed geometry (6)

φGRAPE/φGPU
P. Berczik, T.Hamada,...

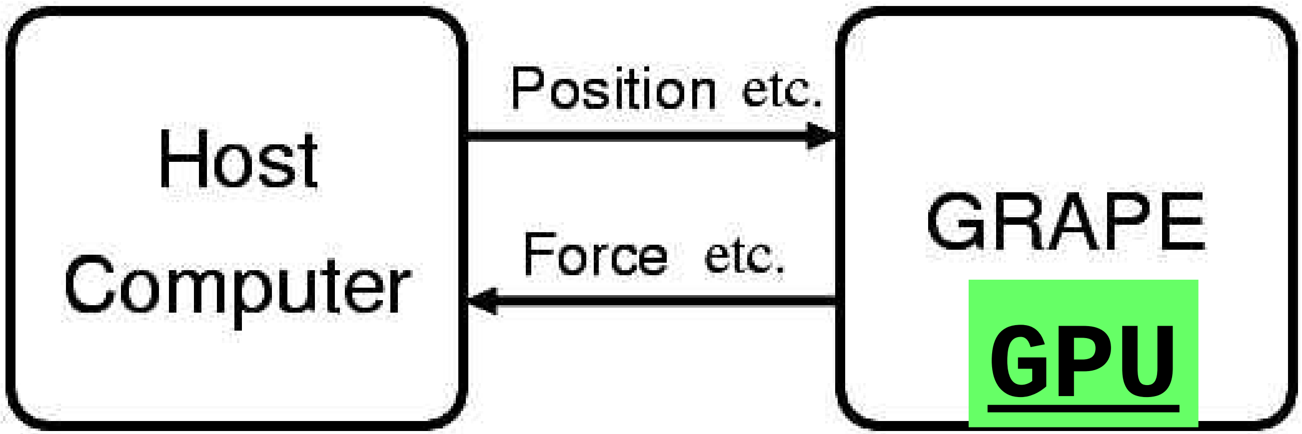
NBODY6-single GPU
NBODY6++ - MPI parallel
R. Spurzem, S. Aarseth,...

(Spurzem 1999)
Journ. Comp. Appl. Maths.

softening: singularity in pairwise potential removed by softening parameter ε
ITS: Individual Time Step Scheme
HTS: Hierarchical Block Time Step Scheme
KS-reg.: KS regularization of perturbed two- and hierarchical N-body motion [48,68]
AC: Ahmad-Cohen neighbour scheme [5]
(1) Discrete FFT on regular 3D mesh with n linear mesh points assumed
(2) Sufficient Accuracy requires appropriate basis function set [37]
(3) γ: ratio of regular to irregular time step
(4) speedup by parallel execution not contained in scaling, see [81]
(5) New high accuracy Hermite code based on STARLAB [64,75]
(6) with hierarchically nested adaptive grids used for cosmological simulations [73]

Our own φGRAPE/GPU N-body code

~N



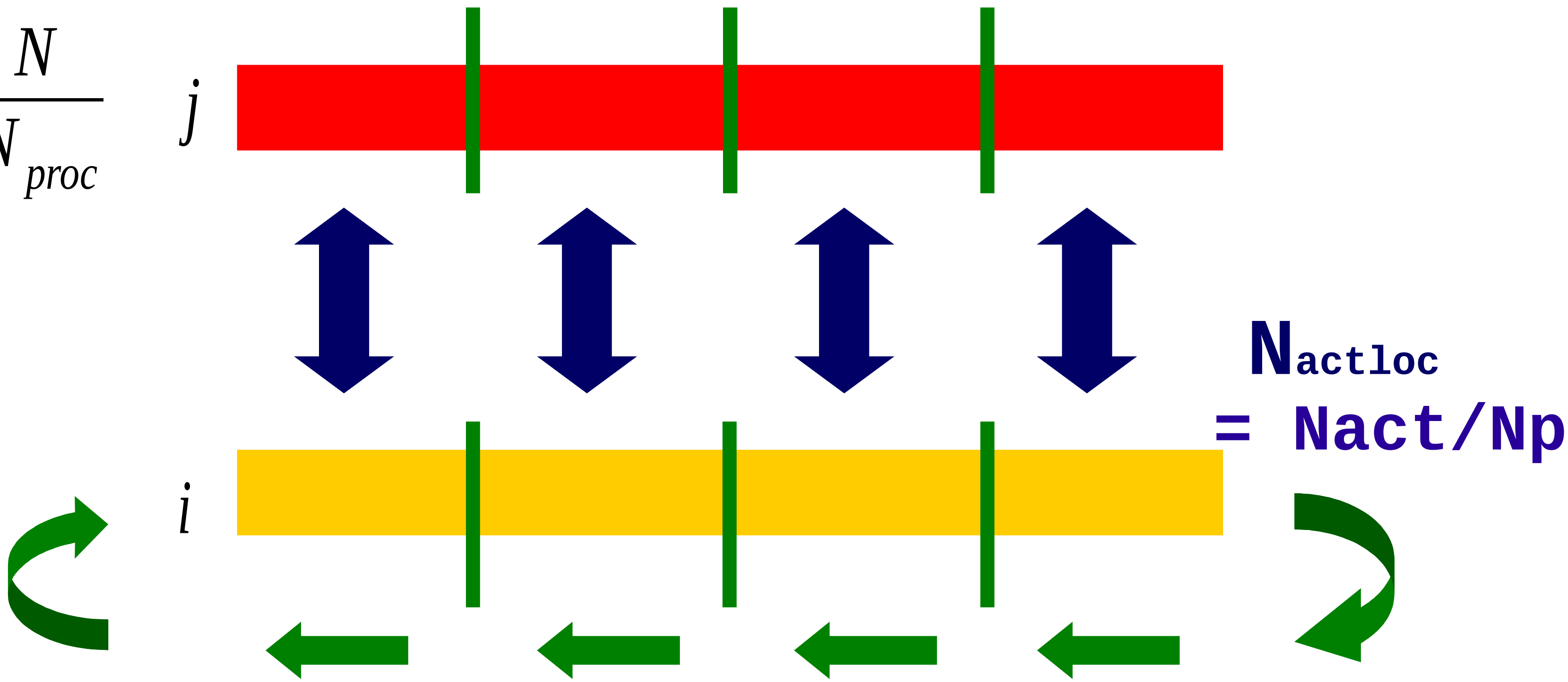
~N^2

$$\vec{a}_i = \sum_{j=1;j\neq i}^{N} \vec{f}_{ij} \qquad \vec{f}_{ij} = -\frac{G \cdot m_j}{\left(r_{ij}^2 + \varepsilon^2\right)^{3/2}} \vec{r}_{ij}$$

Basic idea of parallel N-body code

$$i,j-particle$$

$$N_{loc}=\frac{N}{N_{proc}}$$



Some communication scheme...

Parallelization and Software

Non-blocking systolic communication.... But only simple code yet...

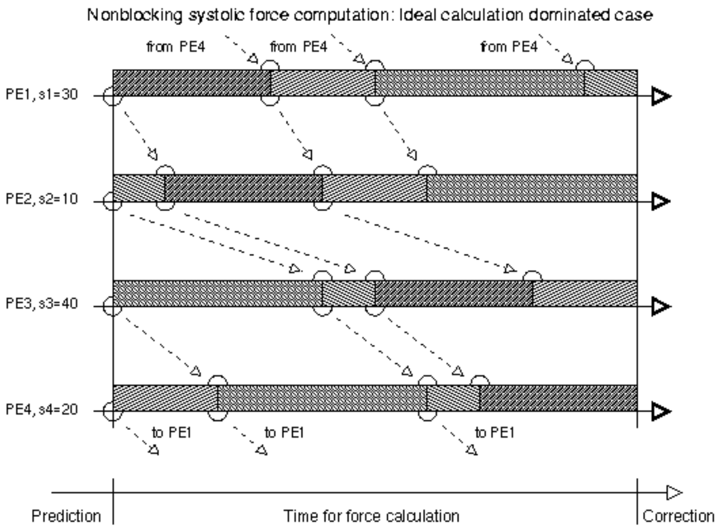


FIG. 1. **Workflow diagram for an ideal, calculation-dominated nonblocking systolic force computation.** Time increases to the right; the bold-faced arrows represent the work of each of the computing nodes, assumed here to be four. The dashed arrows indicate the flow of the position information between the nodes. Circles indicate the points when each processor switches from computing the partial forces from one subgroup to the next subgroup, including the time to finalize one communication thread and initialize the next one. Vertical lines represent barriers which can only be passed when all processes reach the same state of execution.

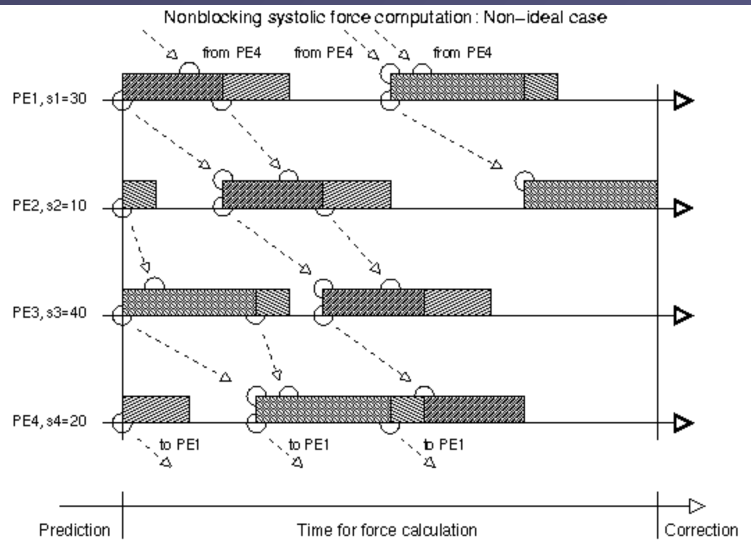
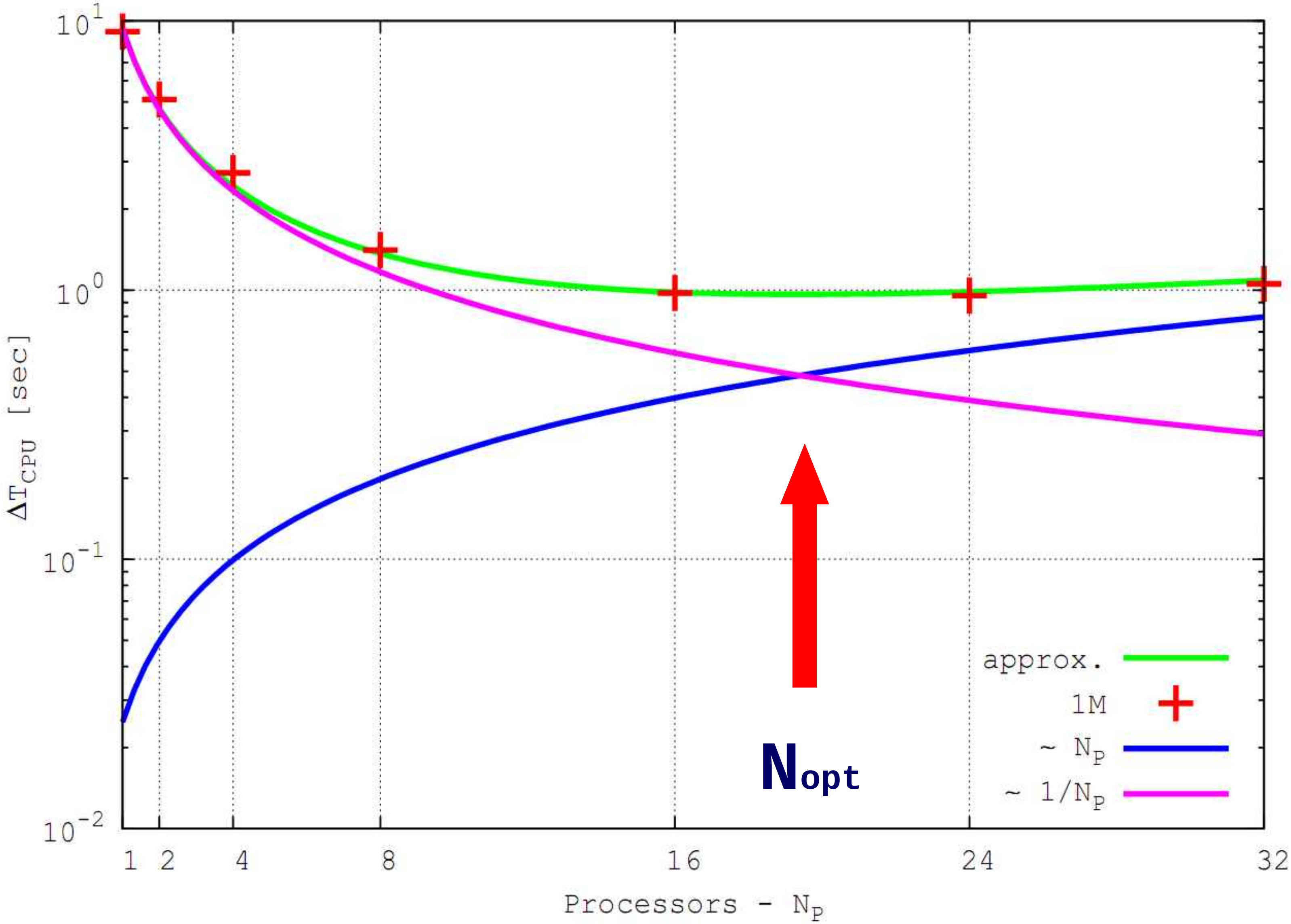


FIG. 2. **Workflow diagram for a mixed communication- and calculation-dominated systolic force calculation.** In this example we have chosen the communication time to be a linear function of the calculation time with $t_{c,i} = t_{f,i}$ and $\tau_1 = 0$. The hatched blocks symbolize times when the processors perform the force calculations. The circles at the lower ends of these blocks denote times when the communication of positional data is initiated. The ones at the upper end denote the times when the communication has completed. The dashed arrows show the dataflow. In order to simplify this graph, the communication of partial forces is omitted.

Dorband, Hemsendorf, Merritt, 2003, Jl. Comp. Phys., astro-ph/0112092

Parallel code on cluster



Parallelization and Software

•**Copy Algorithm**: parallelize work over block members
replicate all data on all processors

Example: NBODY6++, for regular and irregular forces
experimental: for binaries
(Spurzem 1999)

•**Ring Algorithm:** domain decomposition
partial forces shifted
blocking or non-blocking, systolic or hyper-systolic
(Gualandris et al. 2005, Dorband et al. 2003)

•**Mixed Algorithm**: φGRAPE – domain decomposition on GRAPE memories, copy algorithm for active particles (Harfst el al. 2006)

All scaling: $O(N\ p) + O(N^2/p)$

Note: Special hypersystolic quadratic algorithm (Makino 2002):
$O(N/sqrt(p)) + O(N^2/p)$

Software

NBODY4, NBODY6, S.J.Aarseth, S. Mikkola, ...
(ca. 20.000 lines, since 1963):

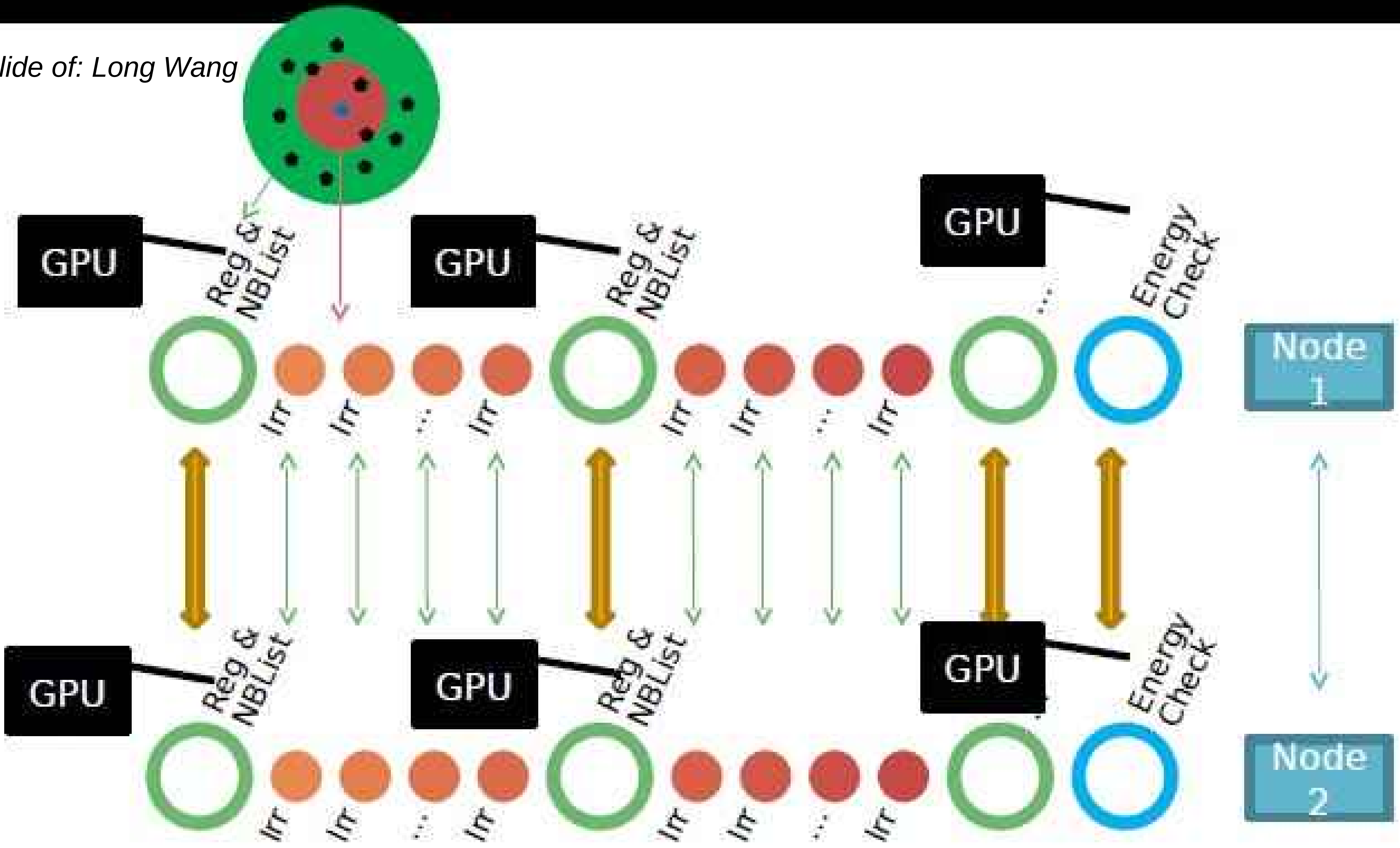
- Hierarchical Individual Time Steps (HITS)
- Ahmad-Cohen Neighbour Scheme (ACS)
- Kustaanheimo-Stiefel and Chain-Regular. (KSREG)
  for bound subsystems of N<6 (Quaternions!)
- 4th order Hermite scheme (pred/corr), Bulirsch-Stoer (for Chain)
- Stellar Evolution (single/binary) (w Hurley)

- *NBODY6++, φGPU, R. Spurzem, P. Berczik, T. Hamada, K. Nitadori,...*
- *(massively parallel codes, since 1999):*

- NBODY6++ (Spurzem 1999) using MPI
- Parallel φGRAPE / φGPU (Harfst et al. 2006, Spurzem et al. 2009, Berczik, Hamada et al. 2011 in prep.)
- NBODY6++/GPU-MPI (Spurzem, Aarseth, Berczik 2011 in progress...
- Parallel Binary Integration in Progress (KSREG)

Nbody6++ Structure

Slide of: Long Wang

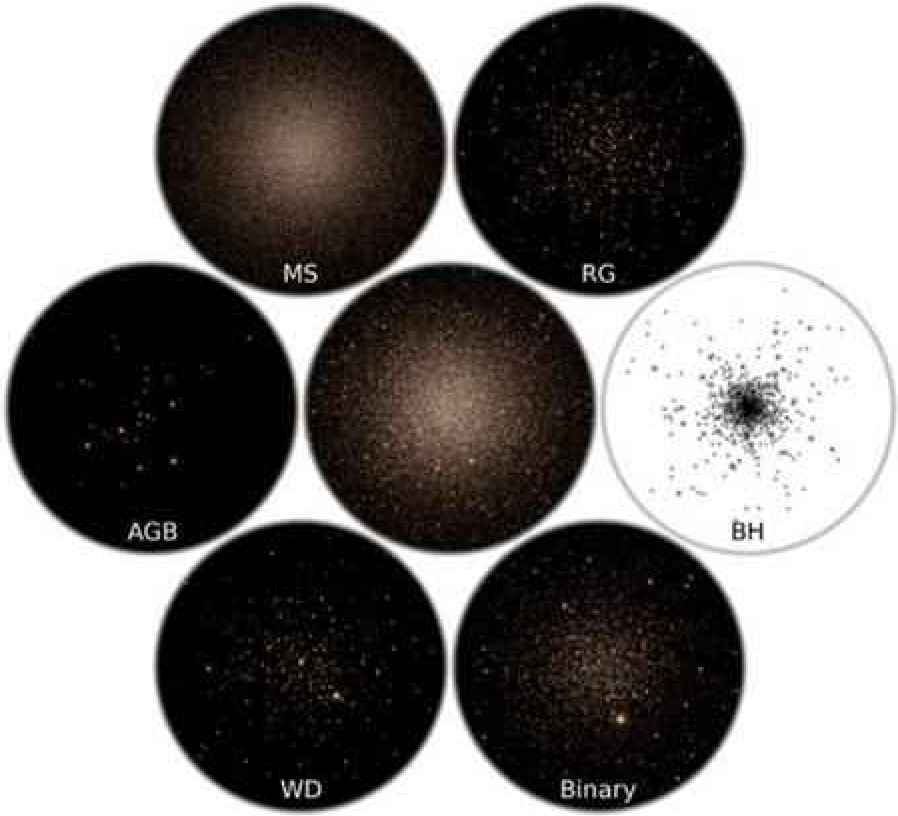


DRAGON Simulation

http://silkroad.bao.ac.cn/dragon/

One million stars direct simulation,

biggest and most realistic direct N-Body simulation of globular star clusters.
With stellar mass function, single and binary stellar evolution, regularization of close encounters, tidal field (NBODY6++GPU).
(NAOC/Silk Road/MPA collaboration).

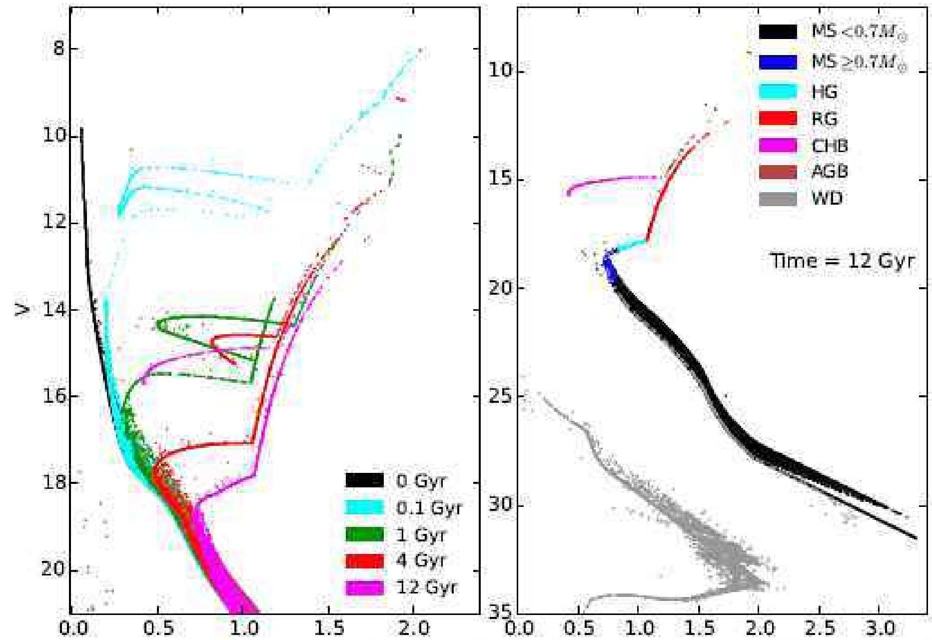


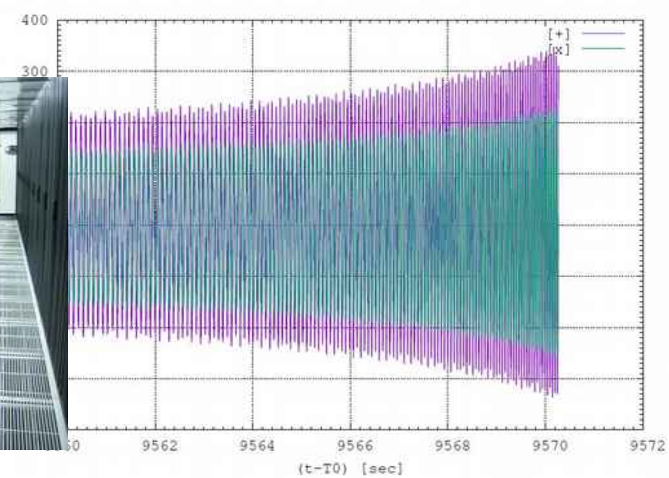
Wang, Spurzem, Aarseth, Naab et al. MNRAS, 2015
Wang, Spurzem, Aarsteh Naab, et al. MNRAS 2016

天龙星团模拟：百万数量级恒星、黑洞和引力波

Dragon Star Cluster Simulations: Millions of Stars; black holes and gravitational waves

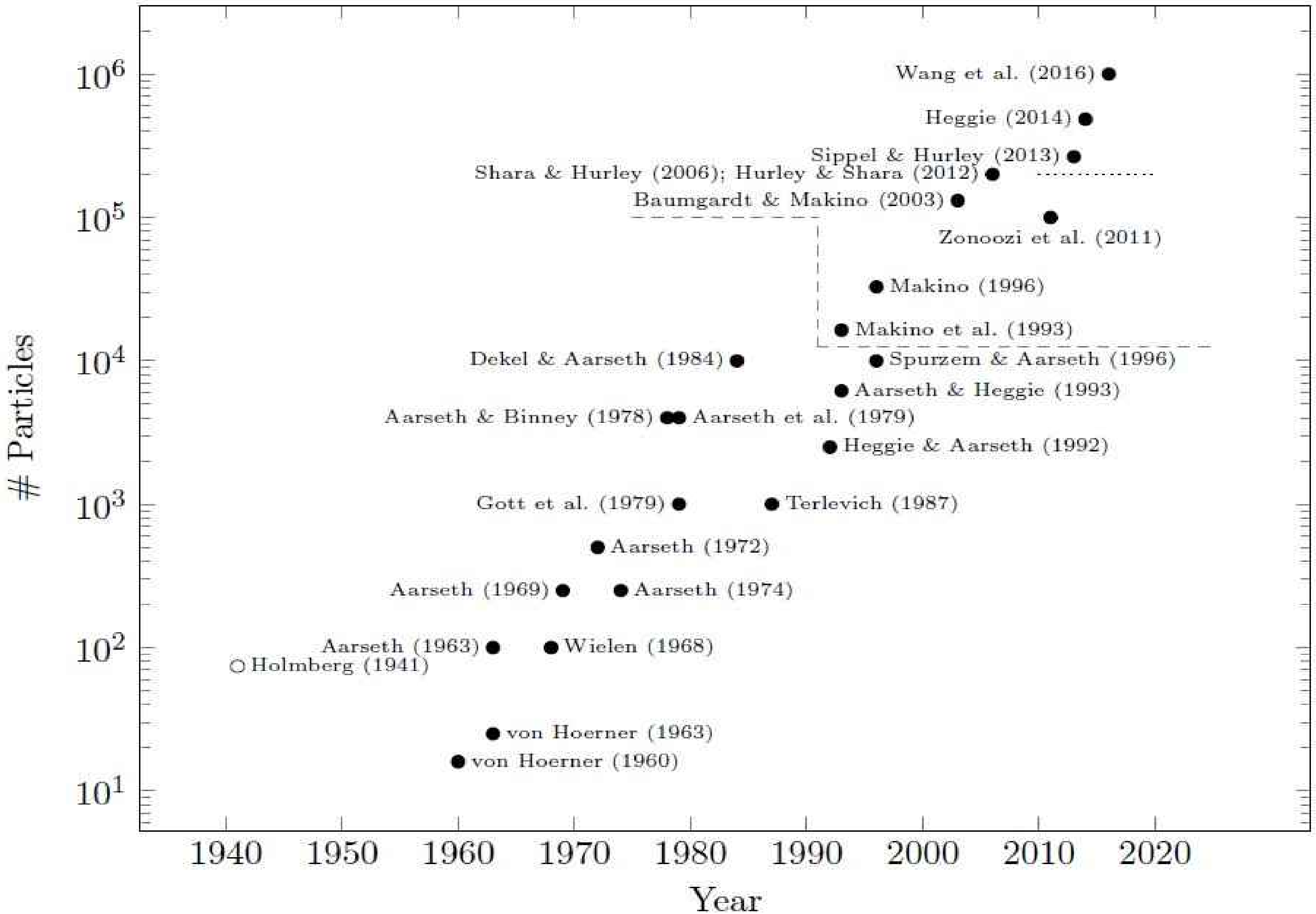
- **First realistic globular star cluster model with million stars *(Wang, Spurzem, Aarseth, …, Berczik, Kouwenhoven, … MNRAS 2015, 2016)***
- **Synthetic CMD (right side) with zero photometric errors, different ages shown**
- **Black hole binary mergers occur as observed by LIGO. Our grav. waveforms computed from simulation (right side). (Only inspiral plotted not ringdown.)**
- **GPU accelerated supercomputers laohu in NAOC and hydra of Max-Planck (MPCDF) in Germany needed!**





http://www.mpa-garching.mpg.de/328833/hl201603

"Moore's" Law for Direct N-Body



GRAPE/
GPU Clusters

GRAPE

Vector Computers

by D.C. Heggie Via added new cits. Sippel

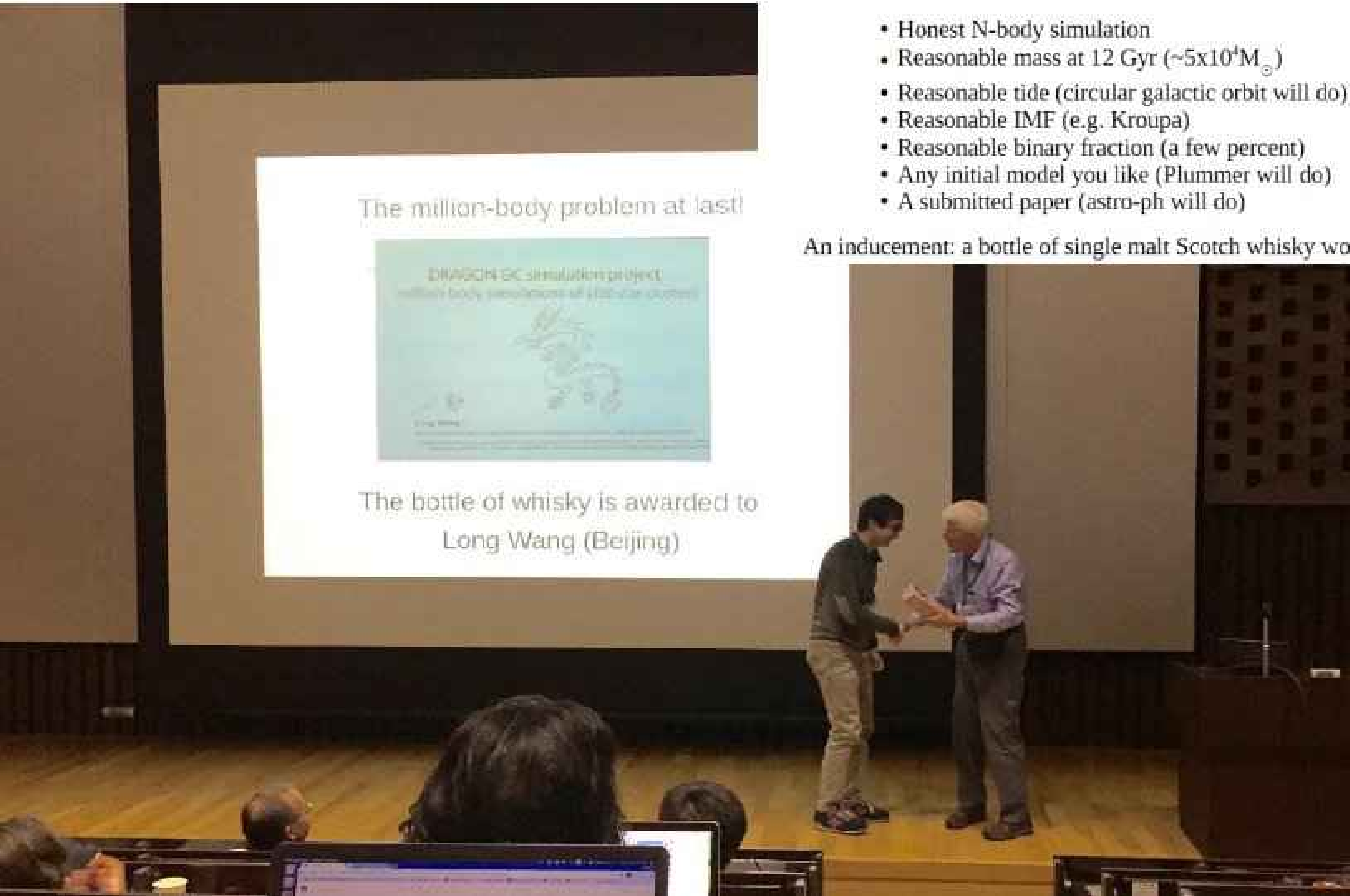
Leiden

CPU/GPU N-body6++

Key Question 1. When will we see the first star-by-star *N*-body model of a globular cluster?

- Honest N-body simulation
- Reasonable mass at 12 Gyr (~$5x10^4 M_\odot$)
- Reasonable tide (circular galactic orbit will do)
- Reasonable IMF (e.g. Kroupa)
- Reasonable binary fraction (a few percent)
- Any initial model you like (Plummer will do)
- A submitted paper (astro-ph will do)

An inducement: a bottle of single malt Scotch whisky worth €50



CPU/GPU N-body6++