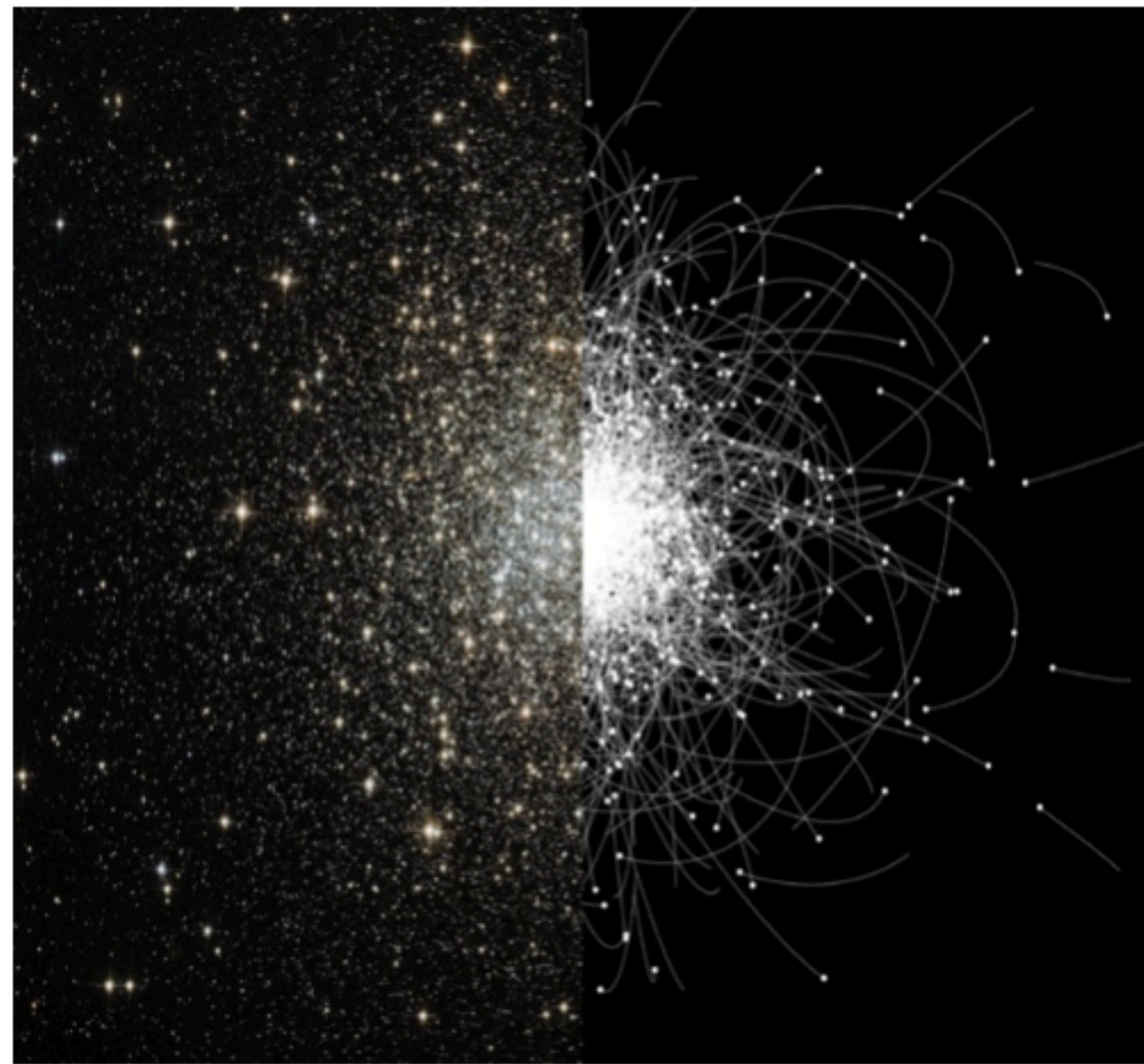


Star Cluster Dynamics and Evolution



Geoplanet Doctoral School Lecture Course (Spring 2024)

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 **MOCCA**

BH GROWTH
★★★★ Growing Black Holes in Star Clusters ★★★★★



Reminder: What do we need to integrate?

The equations of motion to be integrated are

$$\ddot{\mathbf{r}}_i = -G \sum_{j=1, j \neq i}^N m_j \frac{\mathbf{r}_i - \mathbf{r}_j}{|\mathbf{r}_i - \mathbf{r}_j|^3}$$

These can be written in the equivalent form

$$\dot{\mathbf{r}}_i = \mathbf{v}_i$$

$$\dot{\mathbf{v}}_i = \mathbf{a}_i = - \sum_{j=1, j \neq i}^N Gm_j \frac{\mathbf{r}_i - \mathbf{r}_j}{|\mathbf{r}_i - \mathbf{r}_j|^3}$$

where \mathbf{r}_i , \mathbf{v}_i are the position and velocity of the i th particle.

- To solve the ordinary differential equations (2 coupled ODEs)
- Accurate time integration of close encounters is the most difficult part of collisional N -body methods
- For collisionless N -body methods force softening alleviates this problem substantially.

Recap: Implementation of direct N -body codes for collisional dynamics

- **Direct summation N -body approach; “brute force”**

- NBODYX series of codes: <https://people.ast.cam.ac.uk/~sverre/web/pages/nbody.htm> (Aarseth 2003)
- NBODY6++GPU (Wang, Spurzem et al. 2015; 2016): <https://github.com/nbody6ppgpu>

- **Integration Scheme:**

- Since close encounters and interactions between stars are important in star clusters → integrator must be high accuracy even on short times scales → 4th order accuracy
- Expand Taylor series solution for the position and velocities to fourth order in an interval → Hermite integrator
$$\mathbf{r}_i(t + \Delta t) = \mathbf{r}_i(t) + \Delta t \mathbf{v}_i(t) + \frac{1}{2}(\Delta t)^2 \mathbf{a}_i(t) + \frac{1}{6}(\Delta t)^3 \mathbf{j}_i(t) + \dots$$

Euler method Algorithm:

$$r(t + \Delta t) = r(t) + v(t)\Delta t$$

$$v(t + \Delta t) = v(t) + a(t)\Delta t$$

Leapfrog algorithm

$$v\left(t + \frac{\Delta t}{2}\right) = v(t) + a(t)\frac{\Delta t}{2}$$

$$r(t + \Delta t) = r(t) + v(t)\Delta t + \frac{1}{2}a(t)\Delta t^2$$

$$v(t + \Delta t) = v\left(t + \frac{\Delta t}{2}\right) + a(t + \Delta t)\frac{\Delta t}{2}$$

New position is calculated using an extra term proportional to Δt^2

Velocity updated in 2 steps - first half of the time step is taken using the current acceleration and second is taken using the new acceleration

Recap: Hermite Integration: 4th order predictor-corrector

- The algorithm consists of a prediction step:

$$r_p = r(t) + v(t)\Delta t + \frac{1}{2}a(t)\Delta t^2 + \frac{1}{6}j(t)\Delta t^3$$

$$v_p = v(t) + a(t)\Delta t + \frac{1}{2}j(t)\Delta t^2$$

Taylor series evaluation

- a correction step that makes use of the initial coordinates and the predicted coordinates:

$$r(t + \Delta t) = r(t) + \frac{1}{2} (v(t) + v_p) \Delta t + \frac{1}{12} (a(t) - a_p) \Delta t^2$$

$$v(t + \Delta t) = v(t) + \frac{1}{2} (a(t) + a_p) \Delta t + \frac{1}{12} (j(t) - j_p) \Delta t^2$$

- $j(t)$ is the jerk which is the time derivative of the acceleration
- a_p is the acceleration calculated using the predicted positions

Calculating the Jerk:

$$\mathbf{a}_i = -G \sum_{j=1, \neq i}^N m_j \frac{\mathbf{r}_i - \mathbf{r}_j}{|\mathbf{r}_i - \mathbf{r}_j|^3}$$

$$\mathbf{j}_i \equiv \dot{\mathbf{a}}_i = -G \sum_{j=1, \neq i}^N m_j \left(\frac{\mathbf{v}_i - \mathbf{v}_j}{|\mathbf{r}_i - \mathbf{r}_j|^3} - 3 \frac{(\mathbf{v}_i - \mathbf{v}_j) \cdot (\mathbf{r}_i - \mathbf{r}_j)}{|\mathbf{r}_i - \mathbf{r}_j|^5} (\mathbf{r}_i - \mathbf{r}_j) \right)$$

Hermite interpolation which approximates the higher accelerating terms by another Taylor series
 Trick: Instead of doing more derivatives of jerk, use derivative of predicted values



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Taylor series evaluation

Calculating the Jerk:

$$a_i = -G \sum_{j=1, \neq i}^N m_j \frac{\mathbf{r}_i - \mathbf{r}_j}{|\mathbf{r}_i - \mathbf{r}_j|^3}$$

- a correction step

4th order Hermite predictor-corrector scheme is 3 step:

- 1. predictor step: predicts positions and velocities at 3rd order**
- 2. calculation step: calculates acceleration and jerk for the predicted positions and velocities**
- 3. corrector step: corrects positions and velocities using the acceleration and jerk calculated in 2**

$$\frac{(\mathbf{v}_i - \mathbf{v}_j) \cdot (\mathbf{r}_i - \mathbf{r}_j)}{|\mathbf{r}_i - \mathbf{r}_j|^5} (\mathbf{r}_i - \mathbf{r}_j)$$

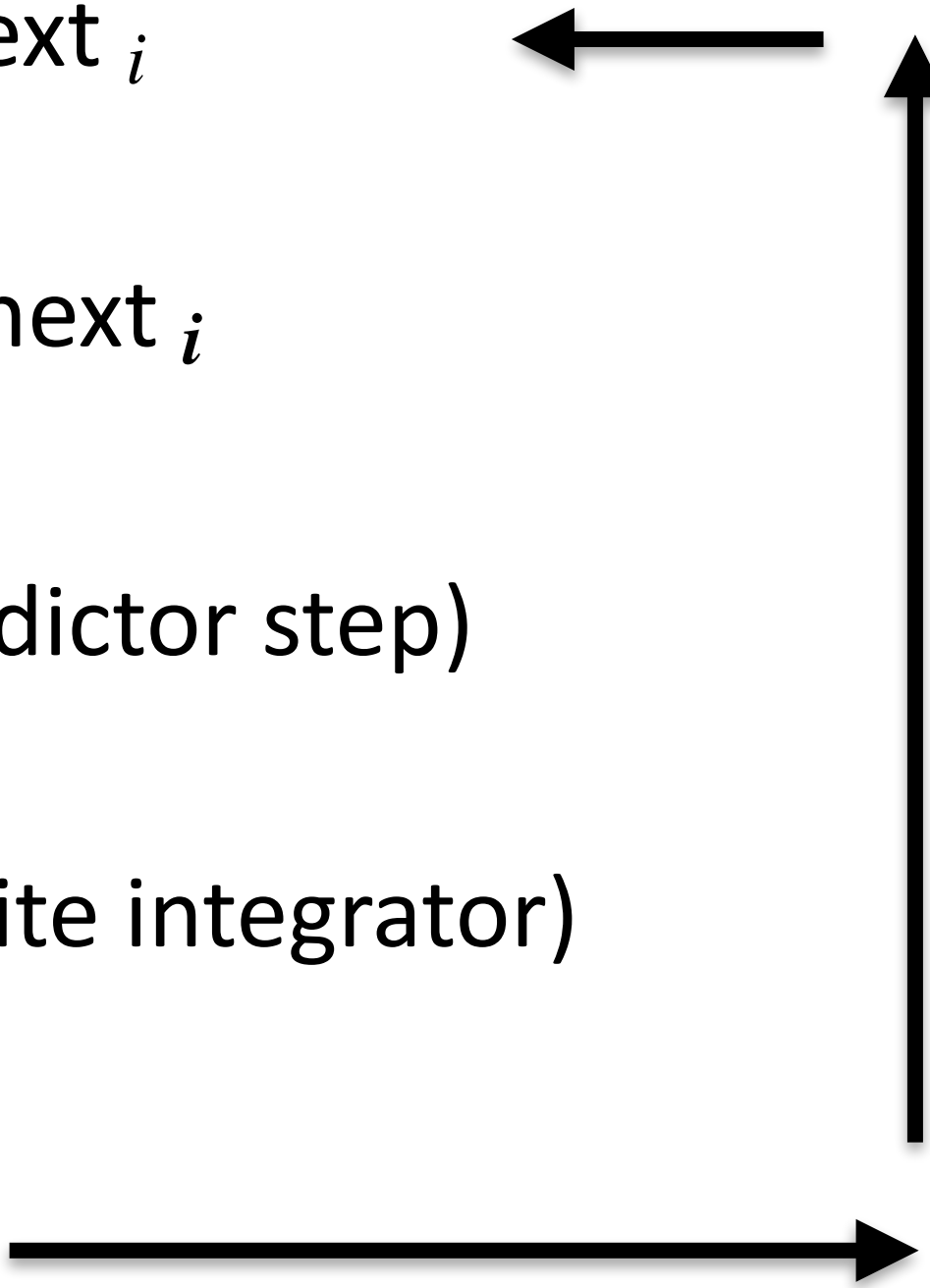
$$r(t + \Delta t) = r(t) + \frac{1}{2} (v(t) + v_p)$$

$$v(t + \Delta t) = v(t) + \frac{1}{2} (a(t) + a_p)$$

interpolation which
 the higher accelerating
 other Taylor series
 TRICK: instead of doing more derivatives
 of jerk, use derivative of predicted values

- $j(t)$ is the jerk which is the time derivative of the acceleration
- a_p is the acceleration calculated using the predicted positions

Recap: Basic structure of an N -body code

1. Initialisation of $\mathbf{r}_i, \mathbf{v}_i, t_{\text{next } i}$ (update time $t_i + \Delta t_i$), $\mathbf{a}_i, \dot{\mathbf{a}}_i$ for all i
 2. Choose i minimising $t_{\text{next } i}$
 3. Extrapolate all $\mathbf{r}_j, \mathbf{v}_j$ to $t_{\text{next } i}$
 4. Compute new $\mathbf{a}_i, \dot{\mathbf{a}}_i$ (Predictor step)
 5. Correct new $\mathbf{r}_i, \mathbf{v}_i$ (Hermite integrator)
 6. Compute new $t_{\text{next } i}$
- 

Note: This is the basic structure of NBODY6, except for the absence of block time steps

Recap: Basic structure of an N -body code and time step issues

1. Initialisation of $\mathbf{r}_i, \mathbf{v}_i, t_{\text{next } i}$ (update time $t_i + \Delta t_i$), $\mathbf{a}_i, \dot{\mathbf{a}}_i$ for all i

$$\Delta t_i = \eta \frac{a_i}{j_i}$$

2. Choose i minimising $t_{\text{next } i}$



3. Extrapolate all $\mathbf{r}_j, \mathbf{v}_j$ to $t_{\text{next } i}$

4. Compute new $\mathbf{a}_i, \dot{\mathbf{a}}_i$ (Predictor step)

5. Correct new $\mathbf{r}_i, \mathbf{v}_i$ (Hermite integrator)

6. Compute new $t_{\text{next } i}$



- Time step issues:
 - Same time step for all particles?
 - Expensive because a few particles undergo close encounters
→ force changes more rapidly for them
 - Ideally:
 - Longer time steps for 'unperturbed' particles
 - Shorter for particles that undergo close encounters
 - Different Δt_i for each particle is expensive and systems lose coherence
 - Block time step scheme: group particles by replacing their individual time steps such that $t/\Delta t_{i,b}$ is an integer (good for synchronization):
Group together particles which have very similar update times. The extrapolation is shared among them.

Check out Aarseth, Tout & Mardling (eds): *The Cambridge N-Body Lectures* (2008) for details

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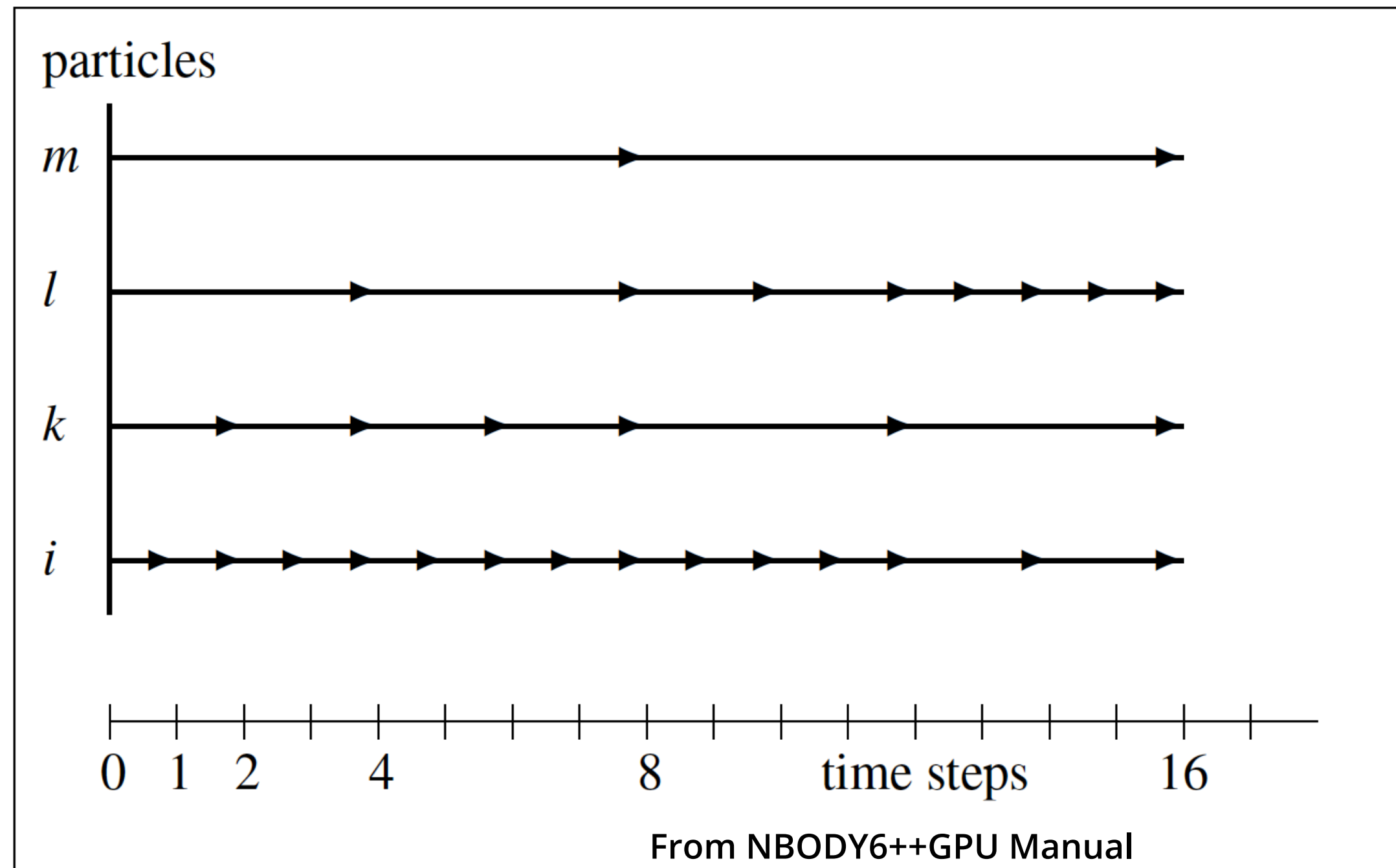


Figure 9.1: Block time steps exemplary for four particles.

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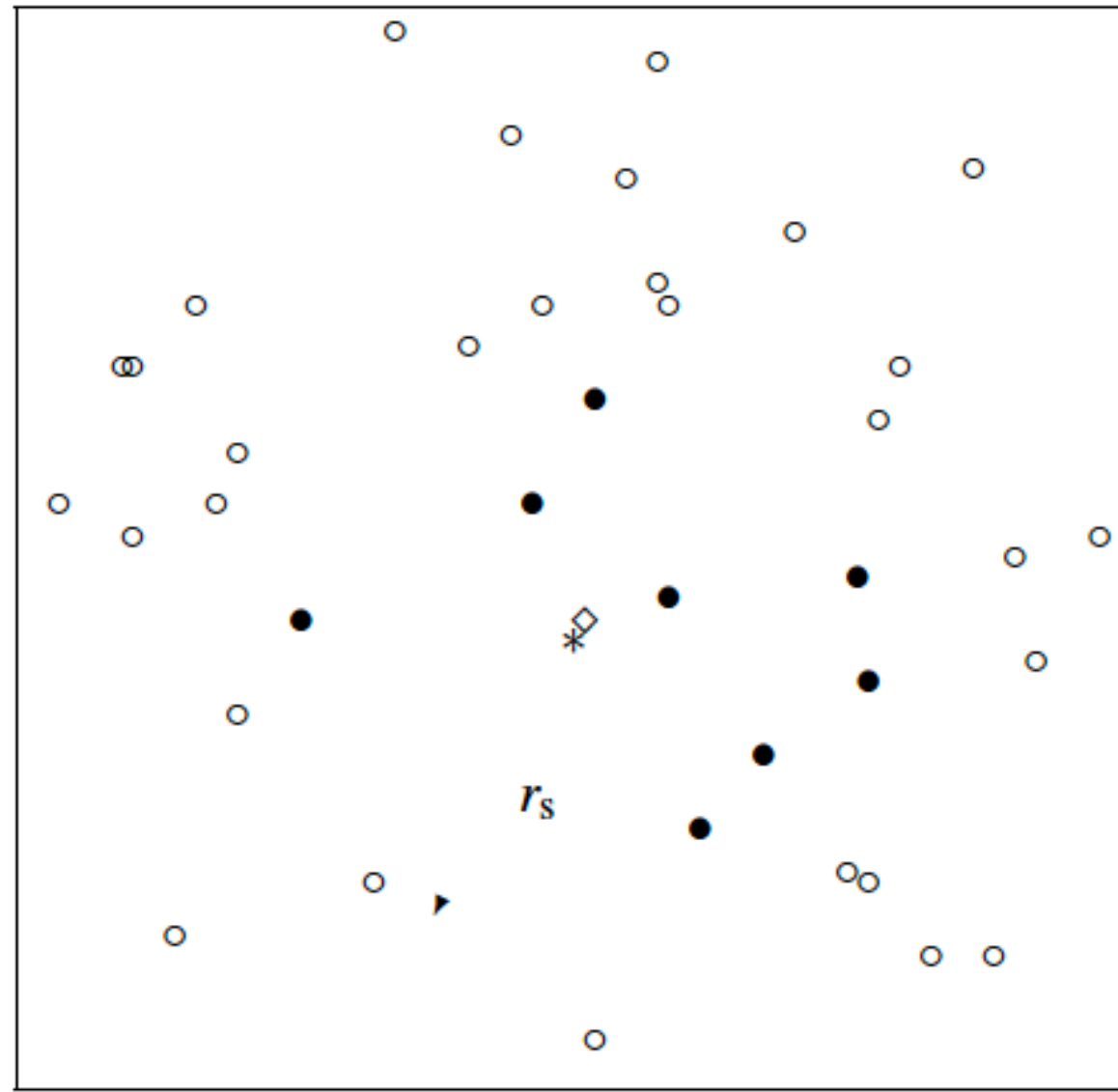


Figure 10.1: Illustration of the neighbour scheme for particle i marked as the asterisk (after [2]).

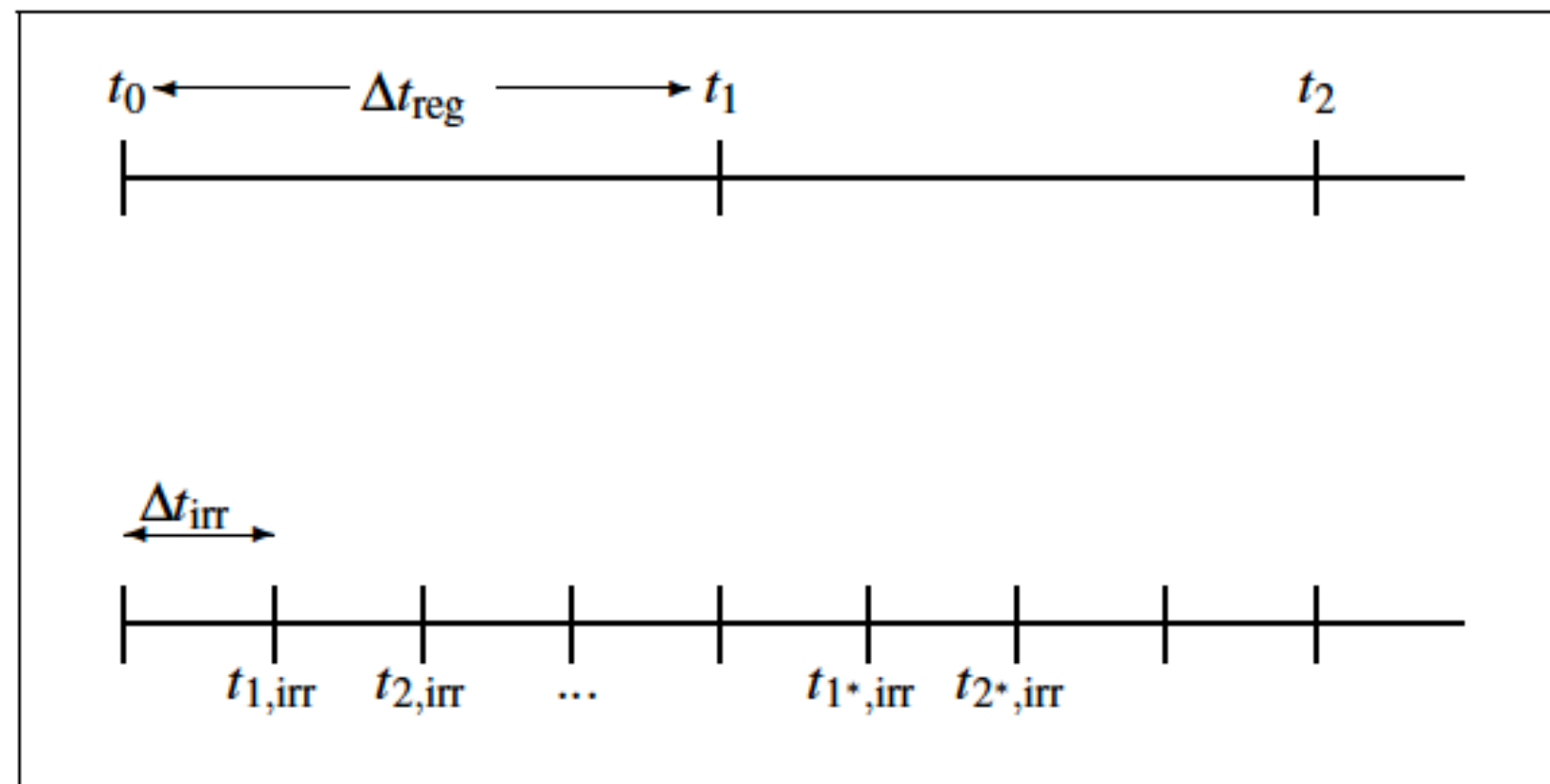


Figure 10.2: Regular and irregular time steps (after [22]).

From NBODY6++GPU Manual

- Neighbour Scheme (Ahmad & Cohen 1973)
- Time step determined by nearest neighbour
- Few near neighbours \rightarrow force due to them can be computed frequently with little effort (the "irregular force")
- force due to the more numerous non-neighbours (the "regular force") fluctuates more slowly, and can be computed with a longer time step
- Requires keeping a list of neighbours

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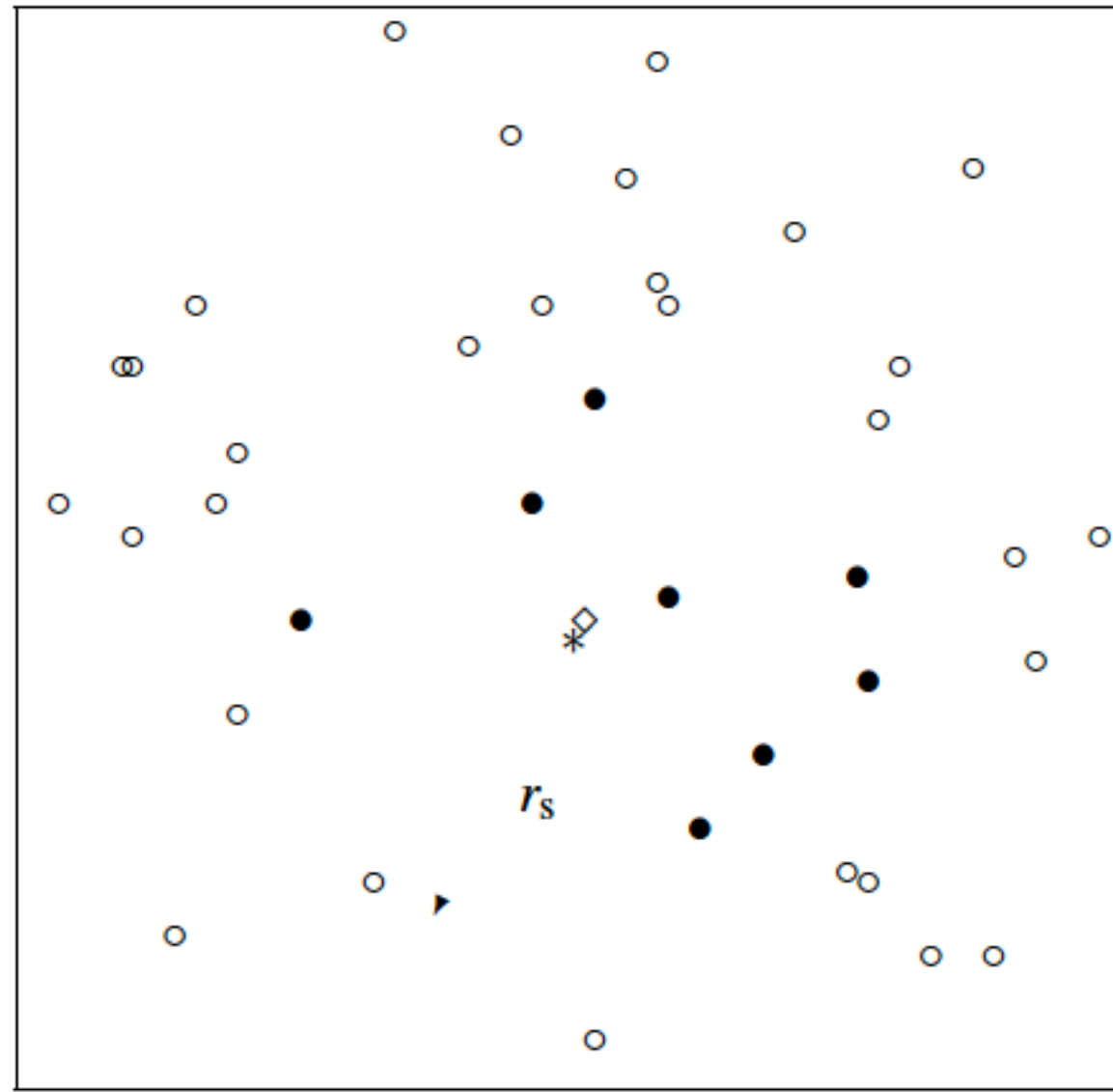


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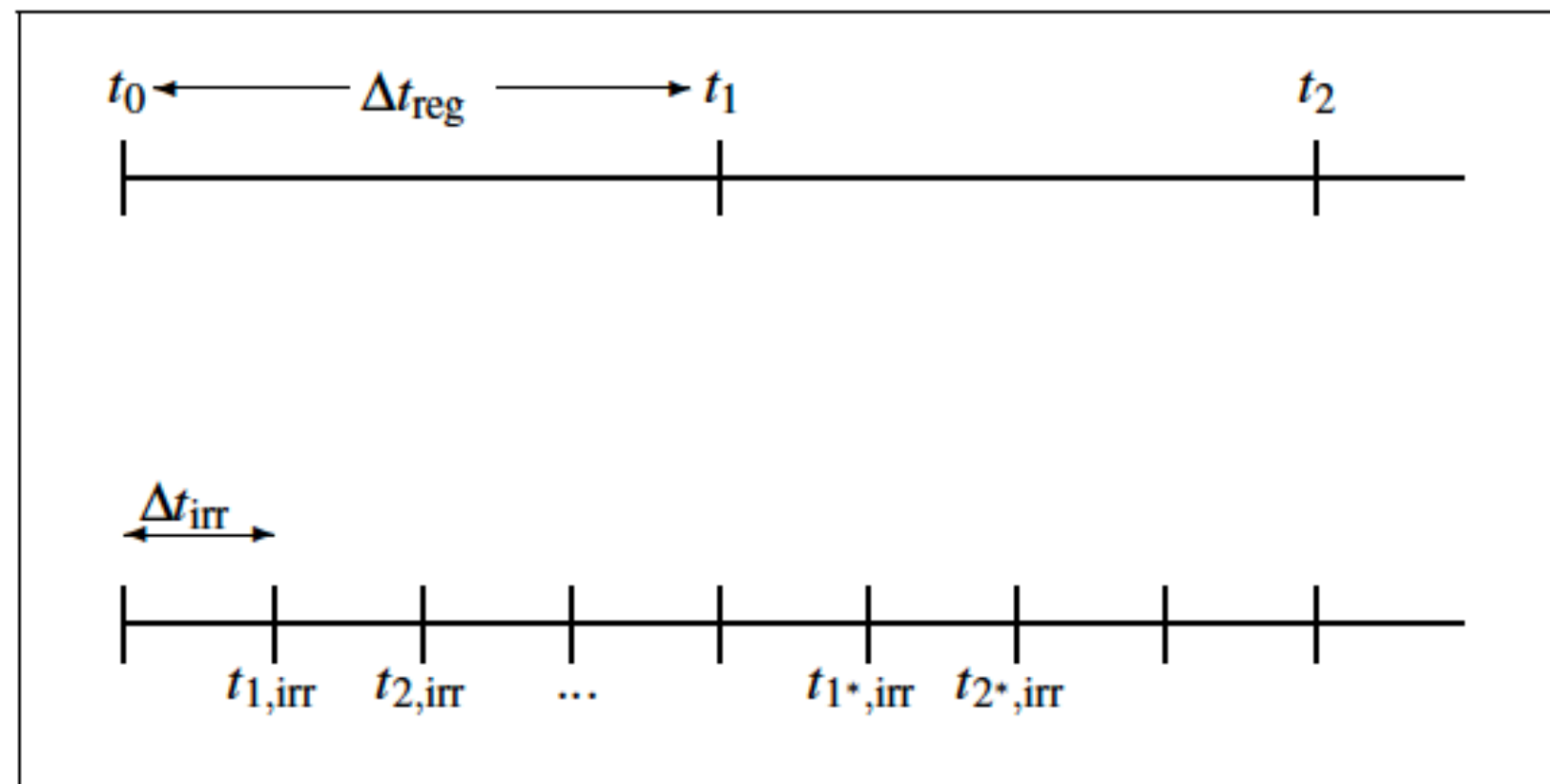


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The **irregular forces** are those fast-changing forces from nearby particles inside the neighbour sphere

$$\mathbf{a}_i = \mathbf{a}_{i, \text{irr}} + \mathbf{a}_{i, \text{reg}}$$

The **regular forces** are from the distant particles outside of the neighbour sphere, which change more slowly

Recap: Basic structure of an N -body code and time step issues

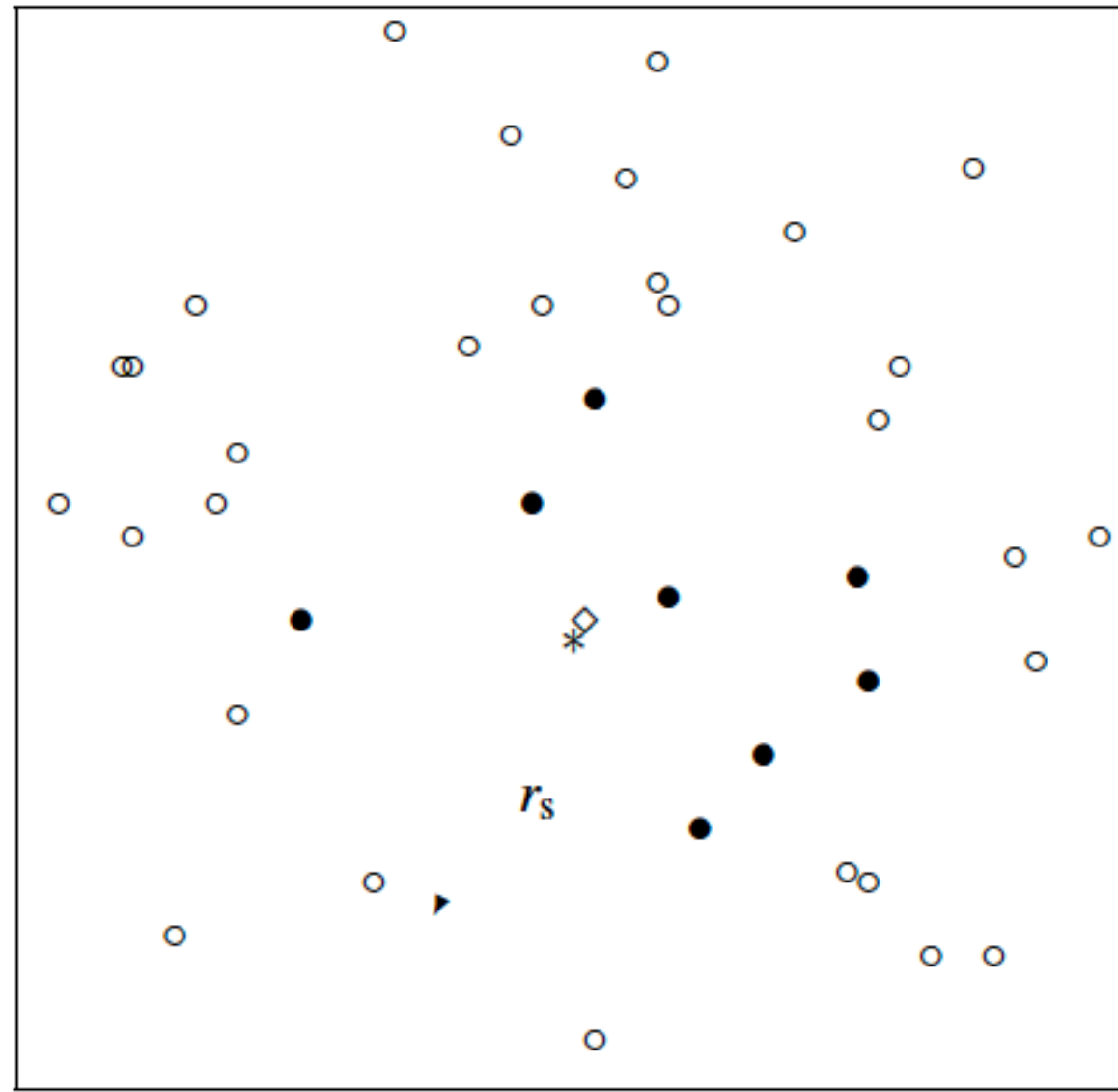


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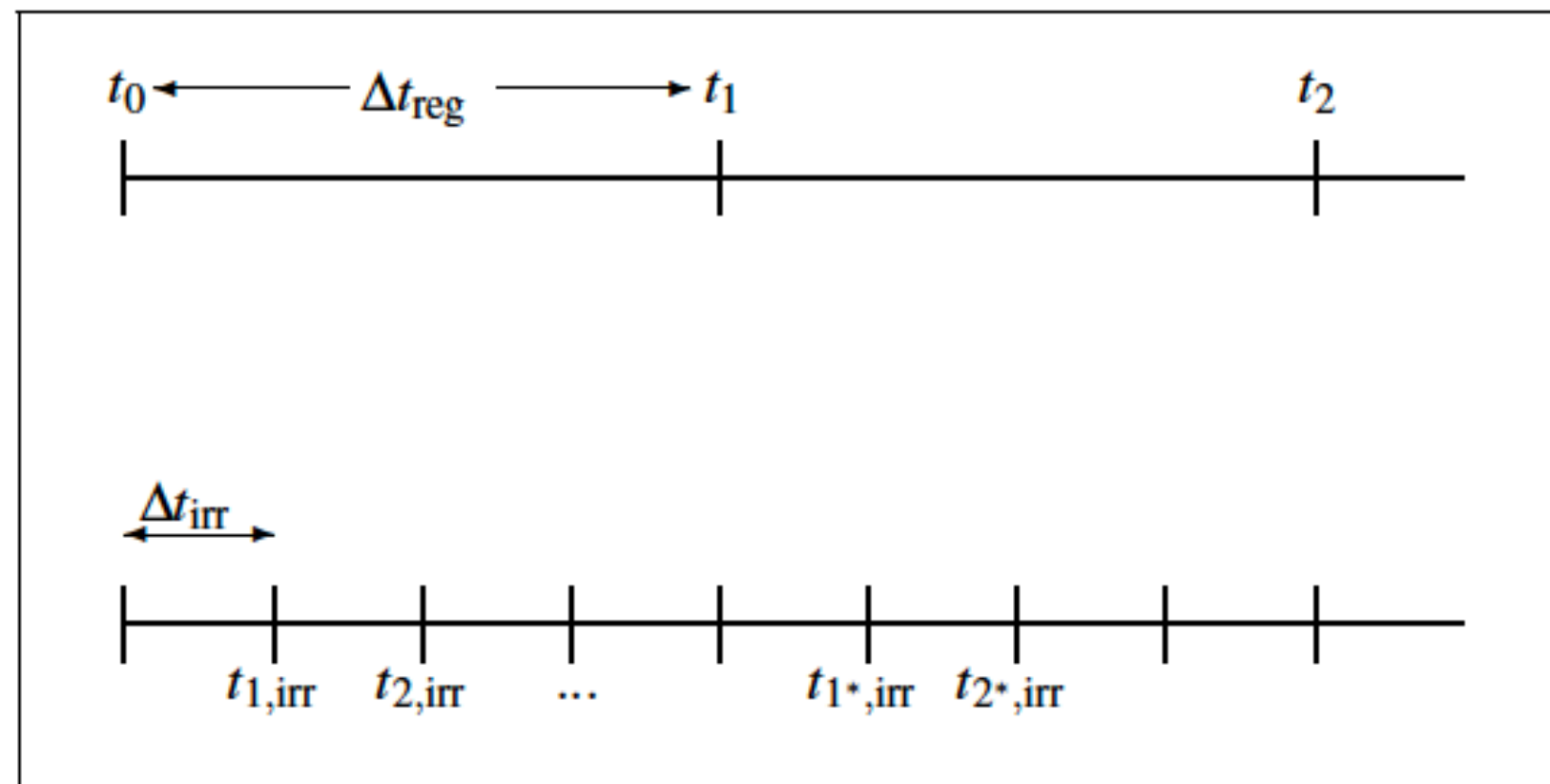


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Summary: Neighbour scheme and hierarchical time-step scheme

- Both have in common that they are centered on one particle i
- Both distinguish between nearby and remote stars, and they save computational time
- What is the fundamental difference between them?
- Neighbour scheme is a spatial hierarchy, which avoids a frequent force calculation of the remote particles \rightarrow their totality provides a smooth potential which does not vary so much \rightarrow potential is superposed by fluctuating peaks of close-by stars (irregular force)
- Time step scheme exhibits the temporal behaviour of the intervals for re-calculation of the full force in order to maintain the exactness of the trajectory; time steps chosen too small slow down the advancing calculation losing the computer's efficiency

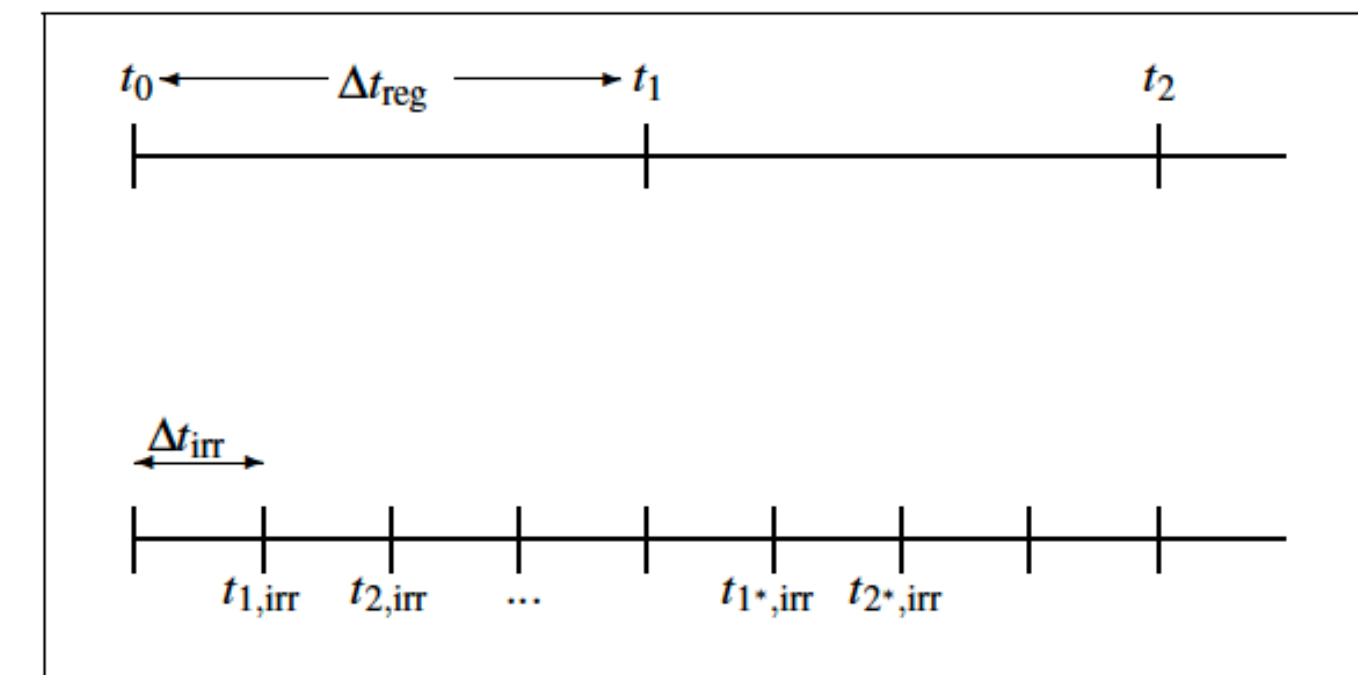


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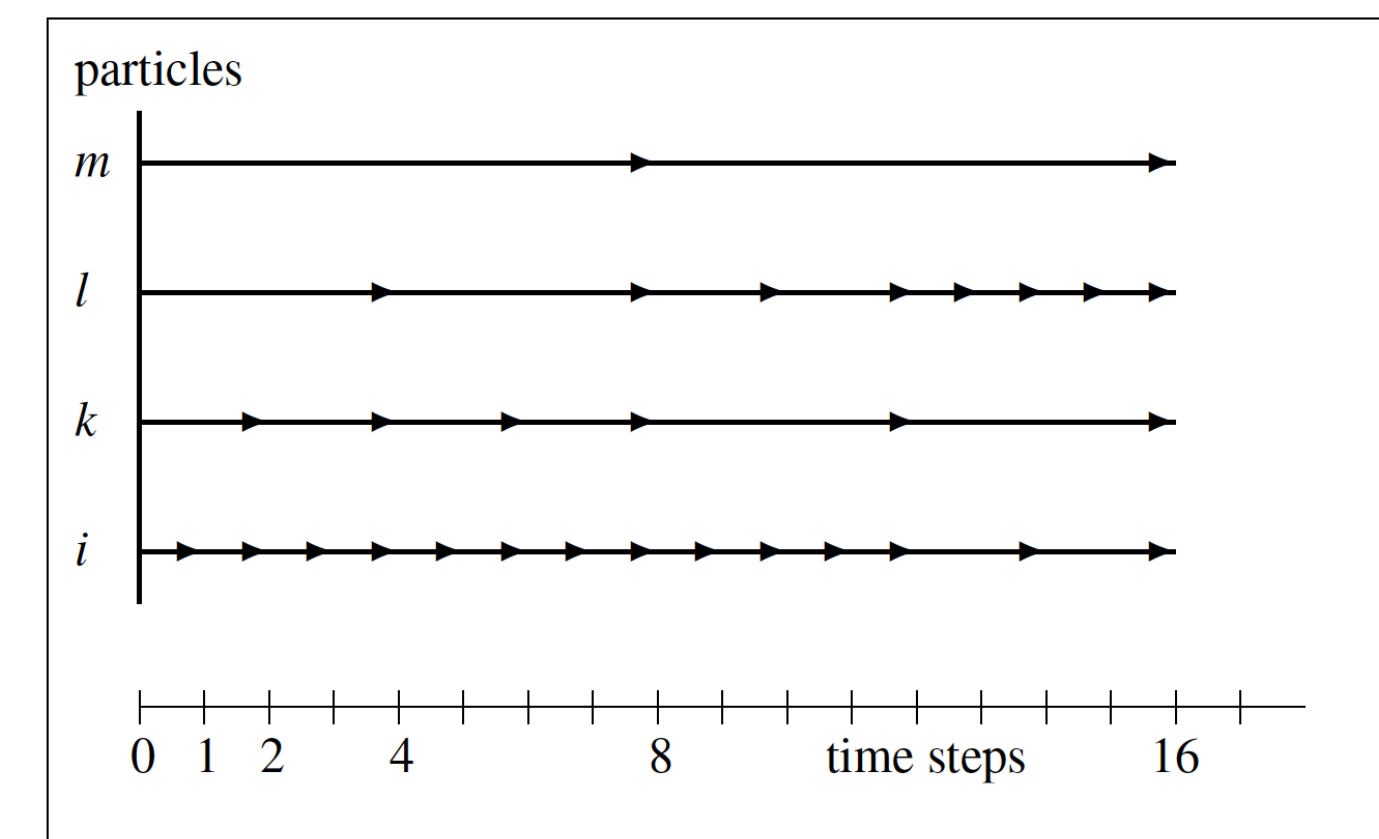


Figure 9.1: Block time steps exemplary for four particles.

Regularization

- Stellar systems are characterized by a huge dynamical range in distance and time scales.
- The time scale varies e.g. in a star cluster from orbital periods of binaries of some hours/days up to the relaxation of a few hundred million years, or even billions of years.
- A key problem when modelling collisional dynamics is dealing with the divergence in the force for $\mathbf{r}_i \rightarrow \mathbf{r}_j$

$$\ddot{\mathbf{r}}_i = -G \sum_{j=1, \neq i}^N m_j \frac{\mathbf{r}_i - \mathbf{r}_j}{|\mathbf{r}_i - \mathbf{r}_j|^3}$$

Recap: Softening

- The equation of motion is

$$\ddot{\mathbf{r}}_i = -G \sum_{j=1, \neq i}^N m_j \frac{\mathbf{r}_i - \mathbf{r}_j}{|\mathbf{r}_i - \mathbf{r}_j|^3}$$

- Singularity as $|\mathbf{r}_i - \mathbf{r}_j| \rightarrow 0 \rightarrow$ can cause very small time steps

- Replace denominator with $\left(|\mathbf{r}_i - \mathbf{r}_j|^2 + \epsilon^2\right)^{3/2}$

$$\mathbf{F}_i = \sum_{i \neq j} \frac{Gm_i m_j}{|\mathbf{r}_i - \mathbf{r}_j|^2 + \epsilon^2}$$

- ϵ is a small constant: softening parameter

- This approximation may be justifiable if close encounters between particles are unimportant (e.g., galaxy dynamics)**

- Not necessarily good for modelling star clusters \rightarrow physically eliminates formation of binaries with $r < \epsilon$**

- Hard binaries (very small separation) are an important source of energy in clusters**

Regularization: binaries/close encounters in N -body codes for collisional dynamics

- Stellar systems are characterized by a huge dynamical range in distance and time scales.
- The time scale varies e.g. in a star cluster from orbital periods of binaries of some hours/days up to the relaxation of a few hundred million years, or even billions of years.

- A key problem when modelling collisional dynamics is dealing with the divergence in the force for $\mathbf{r}_i \rightarrow \mathbf{r}_j$

$$\ddot{\mathbf{r}}_i = -G \sum_{j=1, \neq i}^N m_j \frac{\mathbf{r}_i - \mathbf{r}_j}{|\mathbf{r}_i - \mathbf{r}_j|^3}$$

- Hermite 4th order behaviour: Time step reduction
- smaller $\Delta t \rightarrow$ more steps to reach the same time \rightarrow larger numerical errors
- To avoid this problem, collisional N -body codes introduce regularisation for particles that move on tightly bound orbits or for when $\mathbf{r}_i \rightarrow \mathbf{r}_j$

Regularization: a way of handling binaries/close encounters

- Mathematical trick → remove the singularity in the Newtonian law of gravitation for two particles which approach each other arbitrarily close
 - change of variables
 - without affecting the physics (different from softening)
- Kustaanheimo-Stiefel (KS) regularization: for binaries and 3-body encounters
 - Change from coordinates to offset coordinates: CM and relative particle
 - Kepler orbit is transformed into a harmonic oscillator
 - Significantly reduces the number of steps needed to integrate the orbit and reduces round-off error

$$x_{CM} = \frac{m_1 x_1 + m_2 x_2}{m_1 + m_2} \quad x_{rel} = x_1 - x_2$$

One dimensional regularization

- Consider unperturbed binary motion:

$$\ddot{r} = -\frac{1}{r^2}$$

- where we have scaled to units such that $G(m_i + m_j) = 1$. Introduce new variables z, τ (transformed coordinate and time) such that

$$r = z^2$$
$$\frac{dt}{d\tau} = r$$



Since $r = z^2, \dot{r} = 2z\dot{z}$

Since $dt/d\tau = r,$

$$\dot{r} = 2zz' \frac{d\tau}{dt} \text{ where } , \text{ means } d/d\tau$$

$$= \frac{2zz'}{r} \text{ since } dt/d\tau = r$$

$$= \frac{2z'}{z}.$$

Derivation based on 'Computation and astrophysics of the N -body problem' by Douglas Heggie

One dimensional regularization

$$\dot{r} = \frac{2z'}{z}$$

$$\ddot{r} = -\frac{1}{r^2}$$

$$r = z^2$$
$$\frac{dt}{d\tau} = r$$

- Differentiating again with respect to time gives similarly

$$\begin{aligned}\ddot{r} &= \frac{2z''}{z^3} - 2\frac{z'^2}{z^4} \\ &= -\frac{1}{r^2} \text{ (equation of motion)} \\ &= -\frac{1}{z^4}\end{aligned}$$



We have

$$\frac{2z''}{z^3} - 2\frac{z'^2}{z^4} = -\frac{1}{z^4}$$

Hence

$$\begin{aligned}z'' &= \frac{z'^2}{z} - \frac{1}{2z} \\ &= \frac{1}{2}z \left(\frac{2z'^2}{z^2} - \frac{1}{z^2} \right) \\ &= \frac{1}{2}z \left(\frac{1}{2}\dot{r}^2 - \frac{1}{r} \right) \\ &= \frac{1}{2}hz\end{aligned}$$

$$h = \frac{1}{2}\dot{r}^2 - \frac{1}{r}$$

One dimensional regularization

- Now

$$h = \frac{1}{2}\dot{r}^2 - \frac{1}{r}$$

is the energy of the binary (per unit [reduced] mass); the kinetic energy is $\dot{r}^2/2$, the potential energy is $-1/r$. Thus in the transformed equation of motion

$$z'' = \frac{1}{2}hz$$

the coefficient of z is constant. This is the simple harmonic oscillator equation

- Transformed the one-dimensional Kepler problem (which is singular at $r = 0$) into the simple harmonic oscillator equation, which is regular everywhere.

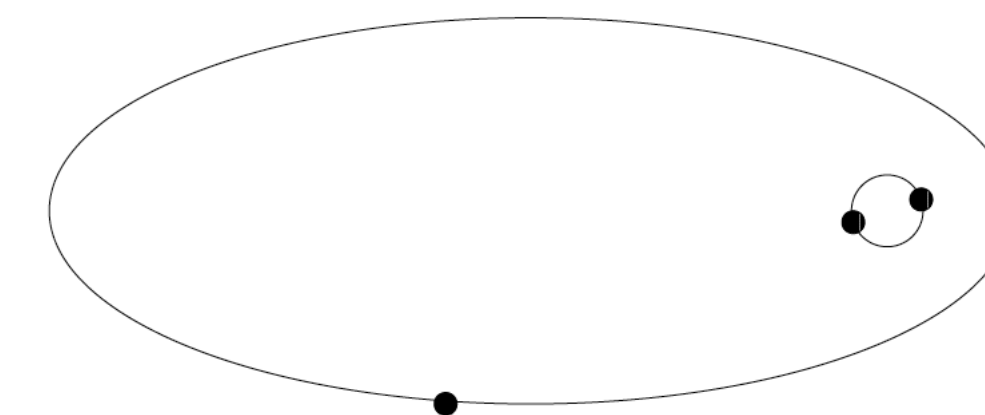
$$\ddot{r} = -\frac{1}{r^2} \qquad z'' = \frac{1}{2}hz$$

- 3D version of this is called KS regularisation

See Heggie & Hut (2003), chapter 15 for more details

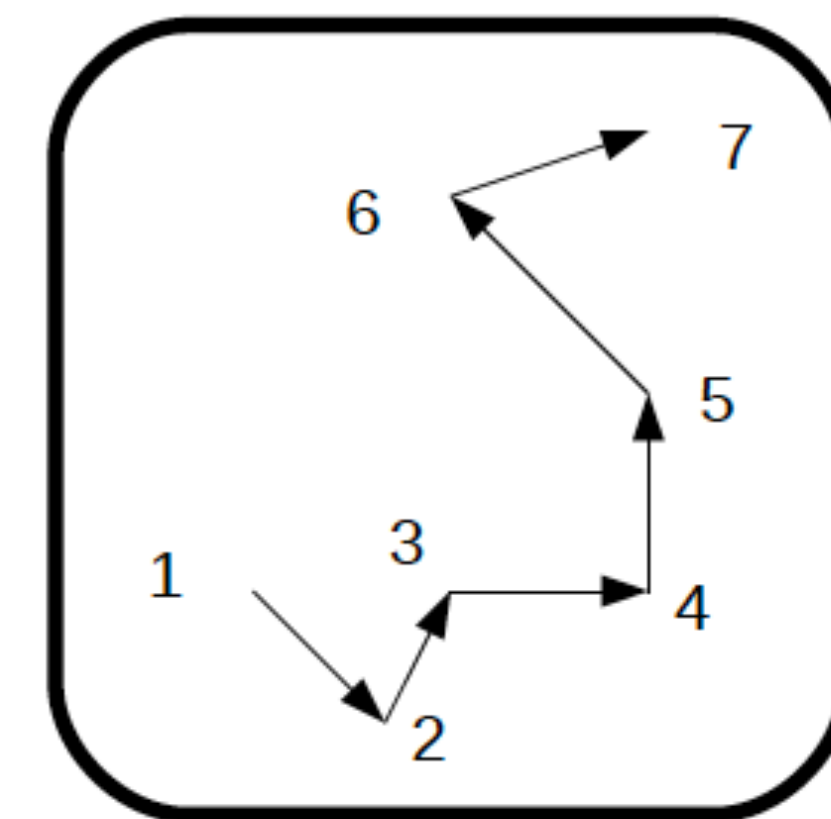
Regularization: a way of handling close encounters

- Hierarchical triples are binaries constantly perturbed by a third body: there is a procedure called “slow-down” which follows secular perturbations with (much) larger time step



Credit: Lecture slides from Douglas Heggie

- CHAIN regularization (Mikkola & Aarseth 1993: for small N-body systems (non-hierarchical triples, quadruples)
- Calculate distances between an active object (e.g. binary) and the closest neighbours
- find vectors that minimize the distances → use these vectors (“chain coordinates”)
- to change coordinates and make suitable changes of time coordinates → calculate forces with new coordinates



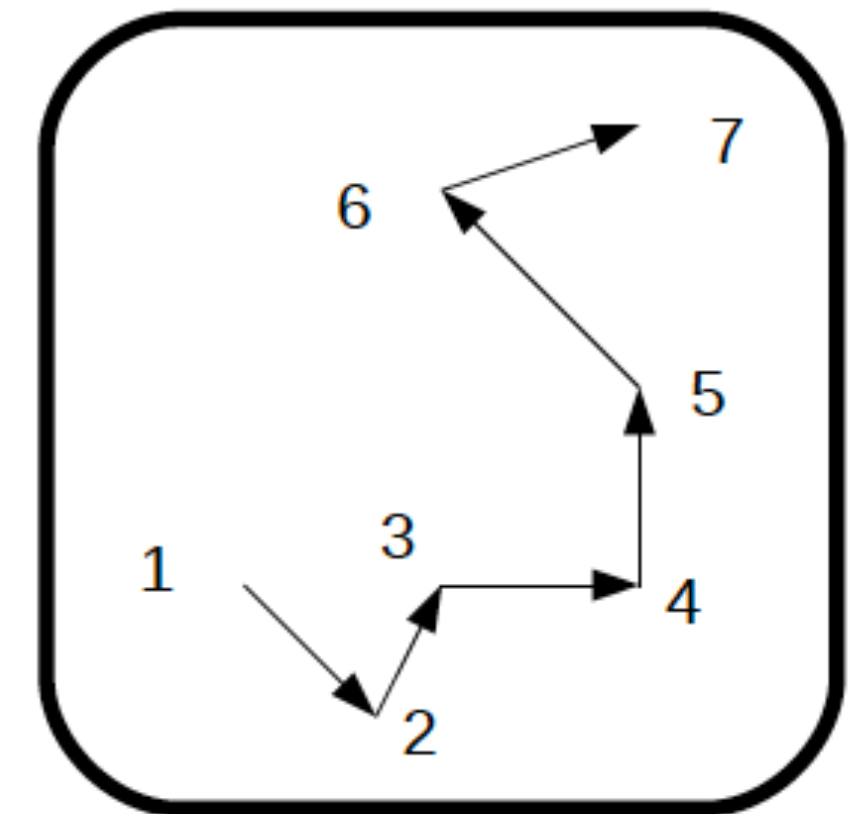
Credit: Mapelli lectures on *N*-body techniques in astrophysics

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$$x_{CM} = \frac{m_1 x_1 + m_2 x_2}{m_1 + m_2}$$

$$x_{rel} = x_1 - x_2$$



Credit: Mapelli lectures on *N*-body techniques in astrophysics

Errors and quality control

- How do we know if the results from an N-body simulation are correct?
 - No exact solutions
- Check conserved quantities
 - Total momentum
 - Total angular momentum
 - Total energy (most sensitive)
- Growth of errors is exponential
 - After a short time the positions and velocities of particles are wrong
 - Assume that the statistical properties of the simulation are correct

Basic structure of a collisional N -body code: complexity

1. Initialisation of $\mathbf{r}_i, \mathbf{v}_i, t_{\text{next } i}$ (update time $t_i + \Delta t_i$), $\mathbf{a}_i, \dot{\mathbf{a}}_i$ for all i

Done Once

2. Choose i minimising $t_{\text{next } i}$

$\propto N$

3. Extrapolate all $\mathbf{r}_j, \mathbf{v}_j$ to $t_{\text{next } i}$

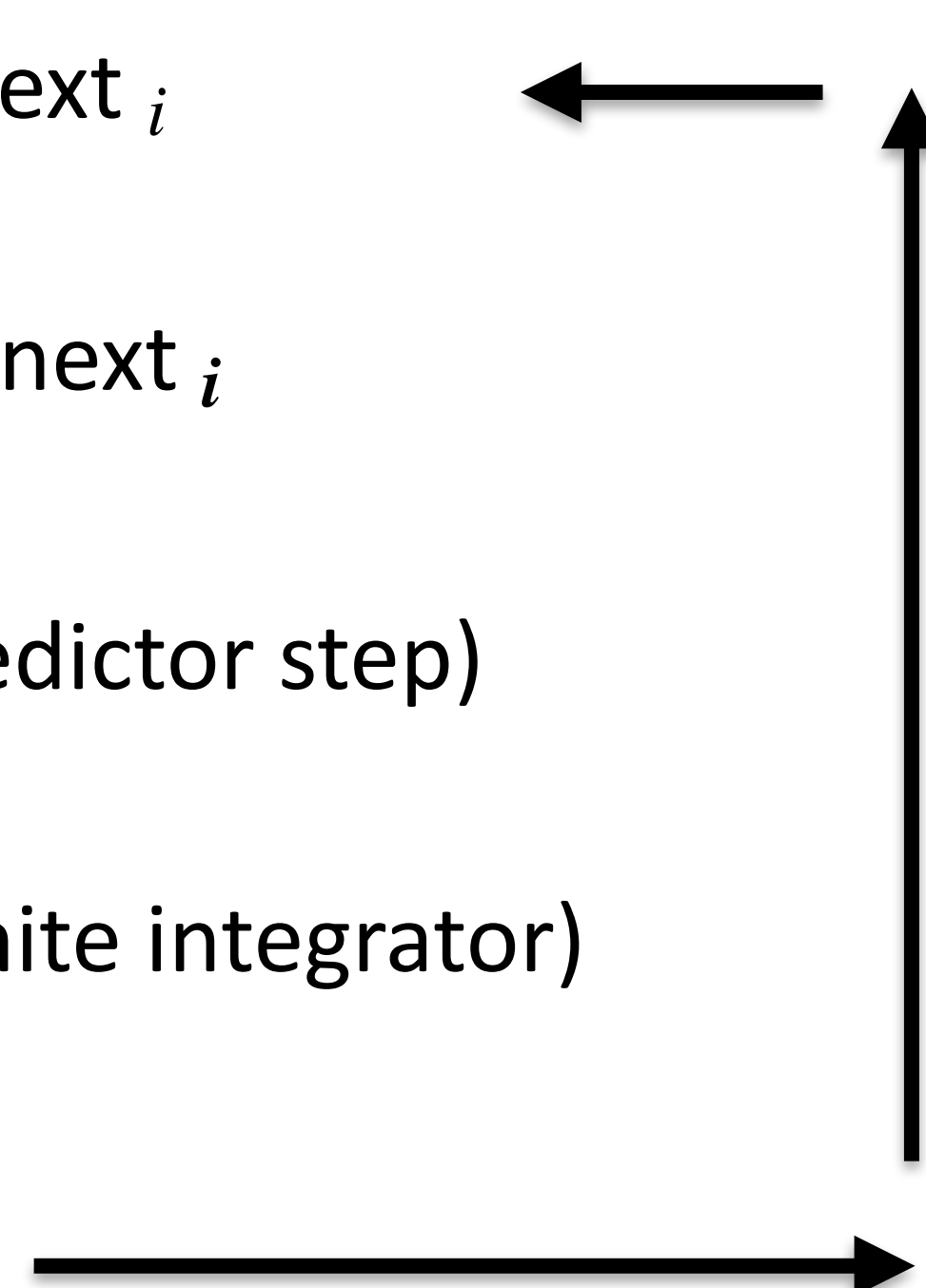
$\propto N$

4. Compute new $\mathbf{a}_i, \dot{\mathbf{a}}_i$ (Predictor step)

$\propto N$

5. Correct new $\mathbf{r}_i, \mathbf{v}_i$ (Hermite integrator)

6. Compute new $t_{\text{next } i}$



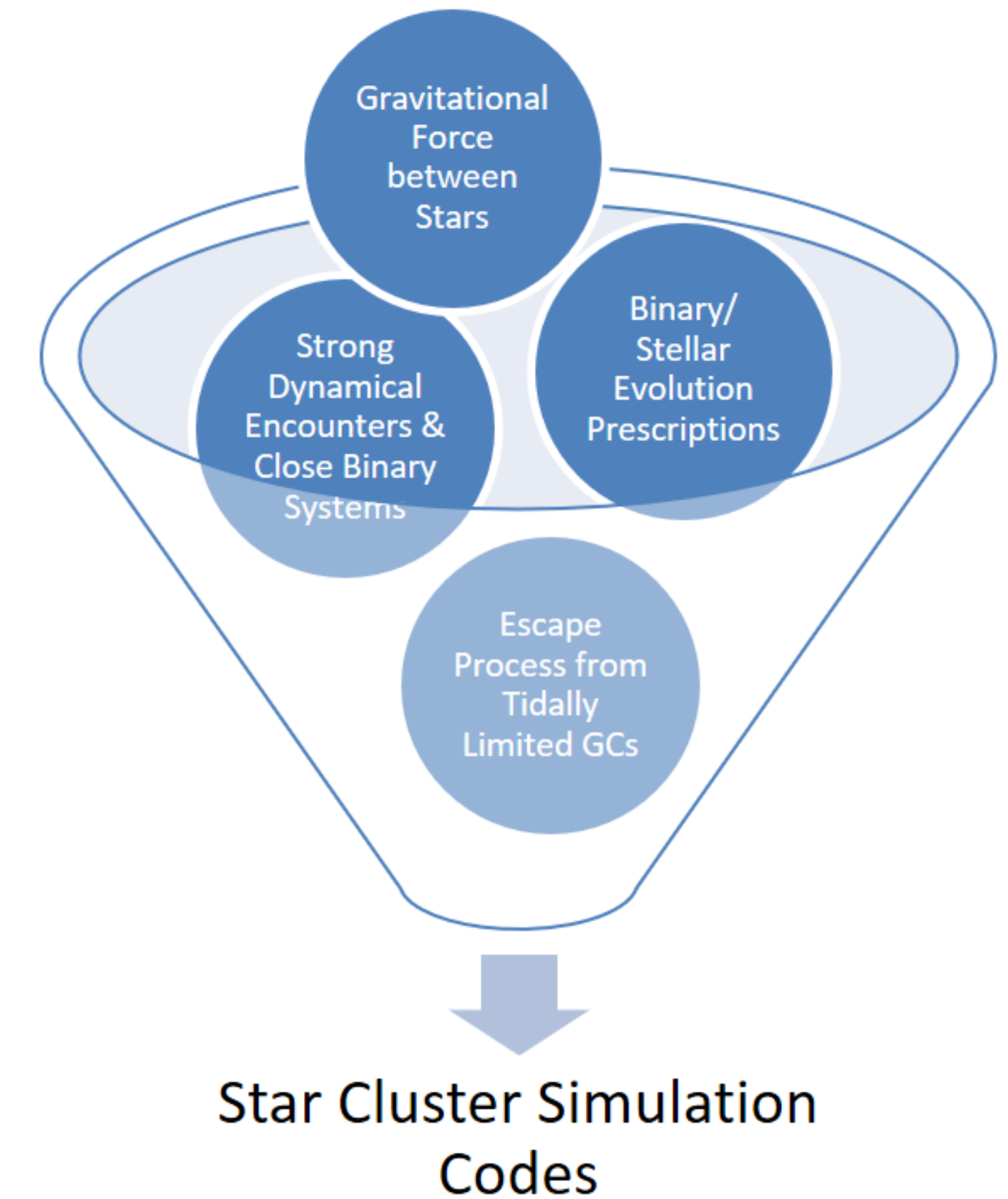
For each time step Δt , the computational effort is approximately proportional to N .

Basic structure of a collisional N -body code: complexity

- Typical time step is $\Delta t \sim \frac{r}{v}$, where v is typical speed and r is typical distance to nearest neighbour
- The system has volume of order R^3 , where R is the virial radius. Divided among N stars, each star occupies volume of order R^3/N . Hence $r \sim R/N^{1/3}$
- In N -body units (Hénon units) $v \sim 1, R = 1$, and so $\Delta t \sim N^{-1/3}$
- Each time step takes of order N operations, and there are N particles. Hence the computational effort per Hénon time unit is of order $N \times N \times N^{1/3} = N^{7/3}$

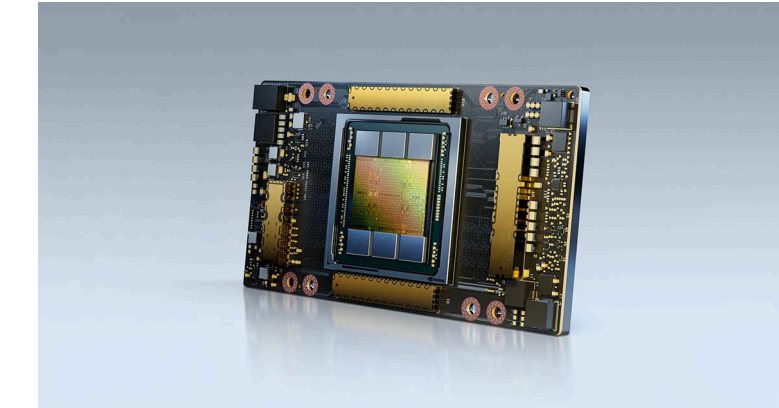
Simulating a globular cluster with NBODY6

- Includes treatment of stellar and binary evolution for various metallicities
- Based on population synthesis codes → SSE/BSE (Hurley et al. 2002) → numerous updates made to these prescriptions (Kamlah et al. 2022)
- Includes effects of external forces (the gravitational acceleration due to the Galaxy)
- Includes rudimentary treatment of collisions between stars (sticky particle approximation)
- **Main issue:**
 - Computation is slow → main bottleneck → computing new acceleration and jerk
 - Realistic globular clusters can take up to a year or more to evolve on supercomputers + GPU acceleration



Hardware acceleration of N -body codes

- Graphics Processing Units (GPUs):
 - Efficient matrix operations (used for 3D renderings)
 - **Architecture: Single instruction on multiple data threads**
 - ***Single operation: Acceleration and jerk calculation on many pairs of particles***
 - ***Each interparticle force between a pair is independent of other pairs***
 - Can be programmed with CUDA
 - Potential for scientific research/AI/Data analytics being realised (mid 2000s to present-day)
- GRAvity PipE (GRAPE): a hardware implementation of Newtonian pair-wise force calculations between particles in a self-gravitating N -body system: <https://www.ias.edu/ids/~piet/act/comp/hardware>
 - Made by researchers working on star cluster evolution in Tokyo (D. Sugimoto & Jun Mukino et al. from 1989 to 2001)
 - 2001: GRAPE-6 system at 48 TFLOP (for comparison Sony PS5 is 10.28 TFLOPS)



NVIDIA A100 GPUs



NVIDIA Titan V: 110

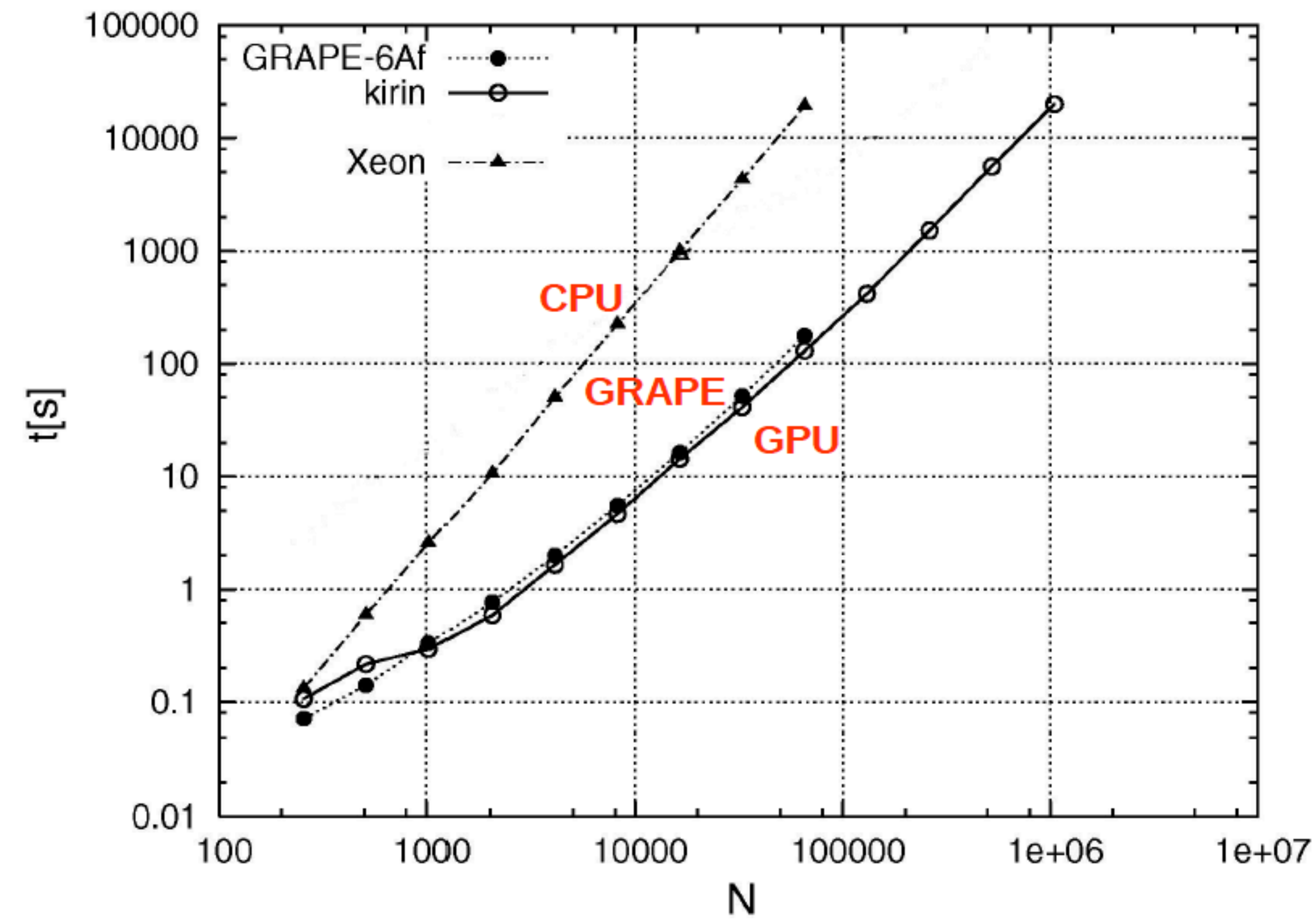


J. Makino with GRAPE-4, ca.1995

Hardware acceleration of *N*-body codes

- Graphics Processing U
- Efficient matrix operator
- **Architecture: Single ins**
 - **Single operation: Accele**
 - **Each interparticle force**
- Can be programmed with
- Potential for scientific res
- GRAVity PipE (GRAPE):
 - pair-wise force calcula
 - body system: <https://v>
- Made by researchers wor
- Jun Mukino et al. from 19
- 2001: GRAPE-6 system at

In 2004-2008, researchers found that GPUs are at least as fast as GRAPES for direct N-body codes (Portegies Zwart et al. 2007; **Belleman et al. 2008**; Gaburov et al. 2009)



NVIDIA Titan V: 110



J. MUKINO with GRAPE-4, ca.1995

NBODYX Versions

A brief comparison of the code versions:

ITS: Individual time-steps

ACS: Neighbour scheme (Ahmad-Cohen scheme) with block time-steps

KS: KS-regularization of few-body subsystems

HITS: Hermite scheme integration method combined with hierarchical block time steps

PN: Post-Newtonian terms

CC: Classical regularized chain

AR: Algorithmic regularization chain

MPI: Message Passing Interface, multi-node multi-CPU parallelization

GPU: use of GPU acceleration (if also MPI: multi-node many GPU)

r: restricted Post-Newtonian, only orbit-averaged energy loss by grav. radiation

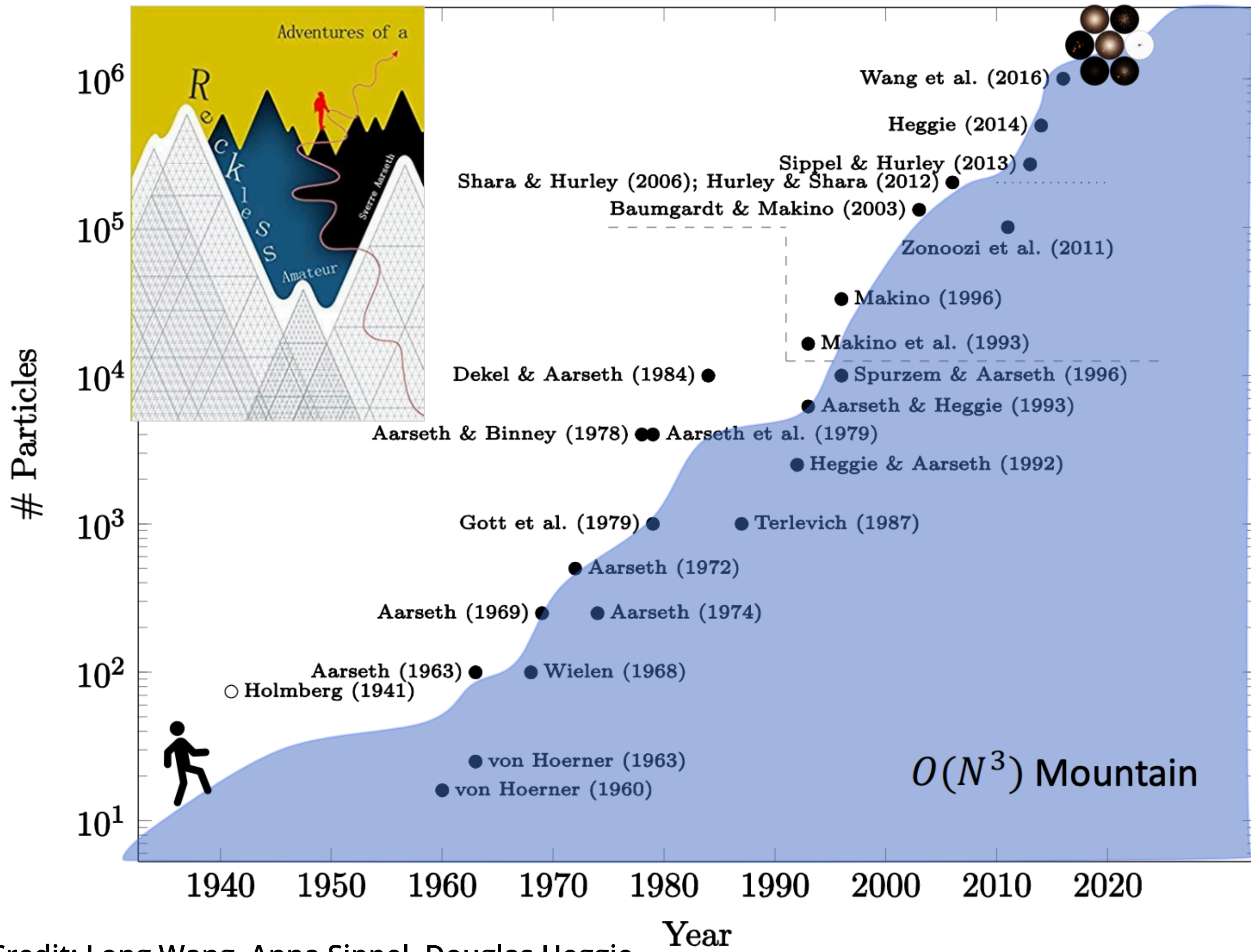
NBODY6++GPU Manual

<https://www.overleaf.com/read/hcmxcyffjkzq>

	ITS	ACS	KS	HITS	PN	CC	AR	MPI	GPU
NBODY1	✓								
NBODY2		✓		✓					
NBODY3	✓		✓						
NBODY4			✓	✓					
NBODY5	✓	✓	✓						
NBODY6		✓	✓	✓	r	✓	✓		
NBODY6GPU		✓	✓	✓	✓	✓	✓		✓
NBODY6++		✓	✓	✓		✓		✓	
NBODY6++GPU		✓	✓	✓	r	✓		✓	✓
NBODY7		✓	✓	✓	r		✓		✓

Developments in Direct N-body simulations

Direct N-body is a mountain challenge



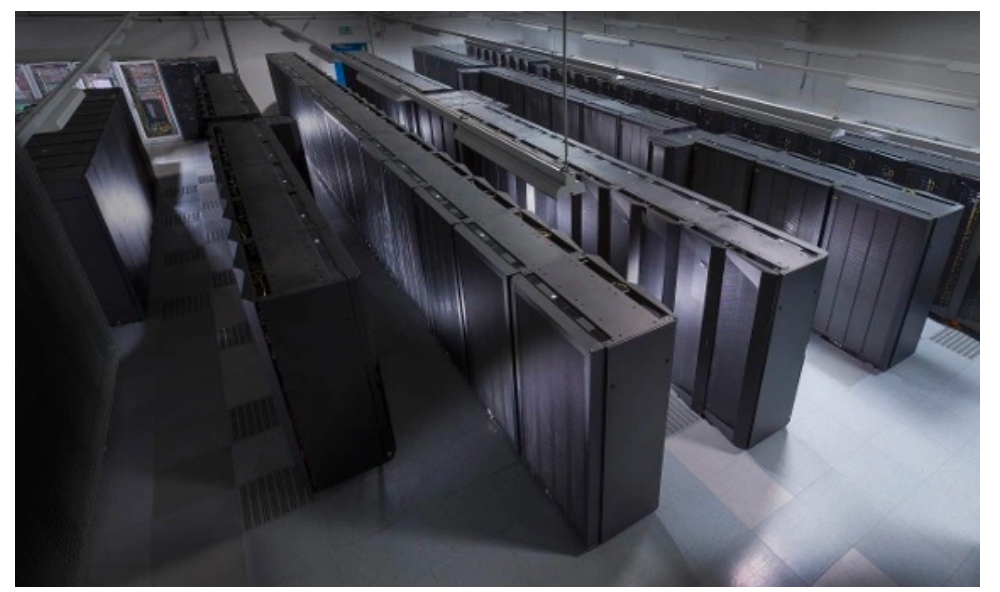
The DRAGON simulations: globular cluster evolution with a million stars

Long Wang,^{1,2*} Rainer Spurzem,^{3,4,1*} Sverre Aarseth,⁵ Mirek Giersz,⁶ Abbas Askar,⁶ Peter Berczik,^{3,4,7} Thorsten Naab,⁸ Riko Schadow⁸ and M. B. N. Kouwenhoven^{1,2}

¹Kavli Institute for Astronomy and Astrophysics, Peking University, Yiheyuan Lu 5, Haidian Qu, 100871 Beijing, China
²Department of Astronomy, School of Physics, Peking University, Yiheyuan Lu 5, Haidian Qu, 100871 Beijing, China
³National Astronomical Observatories and Key Laboratory of Computational Astrophysics, Chinese Academy of Sciences, 20A Datun Rd, Chaoyang District, 100012 Beijing, China
⁴Astronomisches Rechen-Institut, Zentrum für Astronomie, University of Heidelberg, Mönchhofstrasse 12-14, D-69120 Heidelberg, Germany
⁵Institute of Astronomy, University of Cambridge, Cambridge, CB3 0HA, UK
⁶Nicolaus Copernicus Astronomical Centre, Polish Academy of Sciences, ul. Bartycka 18, PL-00-716 Warsaw, Poland
⁷Main Astronomical Observatory, National Academy of Sciences of Ukraine, 27 Akademika Zabolotnoho St, UA-03680 Kyiv, Ukraine
⁸Max-Planck Institut für Astrophysik, Karl-Schwarzschild-Str. 1, D-85741 Garching, Germany

NBODY6++GPU (Wang 2015)

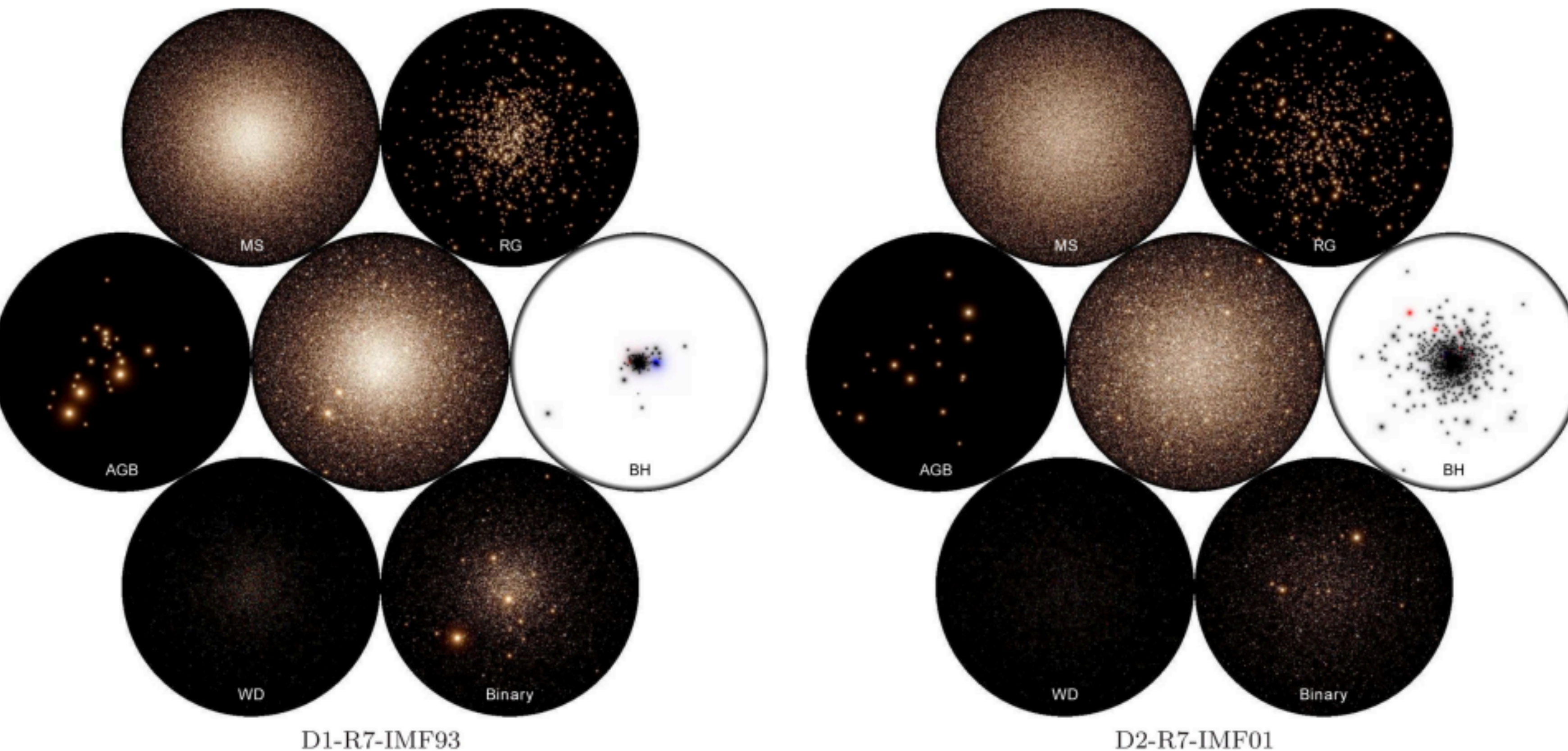
- Wang et al. (2016):
 - $N = 10^6$;
 - Initial half-mass radius: $\sim 7 pc$
 - Primordial binary 5%
 - **160** CPU cores + **16** K20x GPUs



Hydra GPU Cluster, Garching, Germany

Credit: Long Wang, Anna Sippel, Douglas Heggie

Dragon Simulations: Direct N -body with million stars



Observations of luminous stars
simulated with the COCOA code
(Askar et al. 2018)

- Wang et al. (2016):
 - $N = 10^6$;
 - Initial half-mass radius: $\sim 7 pc$
 - Primordial binary 5%
 - **160** CPU cores + **16** K20x GPUs

More black holes \rightarrow puffy cluster
with low central surface
brightness \rightarrow large core and
half-light radii

Other N -body codes for collisional N -body dynamics

- φ -GRAPE (Harfst et al. 2007) and ϕ -GPU (Berczik et al. 2011)
 - Developed by Peter Berczik: <https://github.com/berczik/phi-GPU-mole>
 - Hierarchical block time-steps
 - high (4th, 6th and 8th) order Hermite integration schemes
 - Softening
- FROST & BIFROST (Rantala et al. 2023)
 - fourth-order forward symplectic integrator
 - GPU accelerated
 - High binary fraction: secular and regularised integration for binaries, triples, multiples, few body systems
 - Small softening values
- Hybrid N -body codes: BRIDGE (Fujii et al. 2007), PeTar (Wang et al. 2020)

N-body simulations for collisionless systems

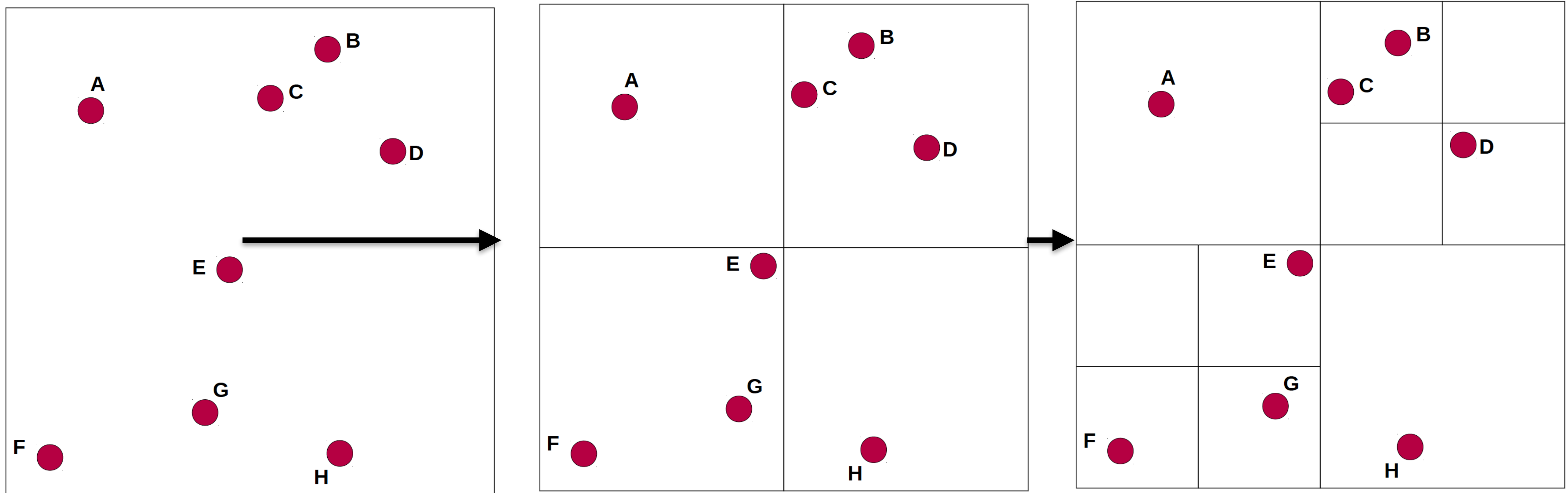
- Softening
 - What is a reasonable value of epsilon?
 - Average distance between particles or a bit less
 - Adaptive individual softening
- Time steps can be large depending on the problem at hand: lower order integrators like leapfrog can be used
 - Same time-step for all particles commonly used
- Force computation: Approximating direct summation
 - No need to estimate the force exerted by each single particle on another
 - Can estimate the cumulative force exerted by groups of particles if they are sufficiently far

$$F_{ij} = -Gm_i m_j \frac{\mathbf{r}_i - \mathbf{r}_j}{\left(|\mathbf{r}_i - \mathbf{r}_j|^2 + \epsilon^2 \right)^{3/2}}$$

Tree code: Barnes-Hut Algorithm

- The crucial idea in speeding up the brute force n-body algorithm is to group nearby bodies and approximate them as a single body.
- Uses a hierarchical spatial tree to define localised groups of particles

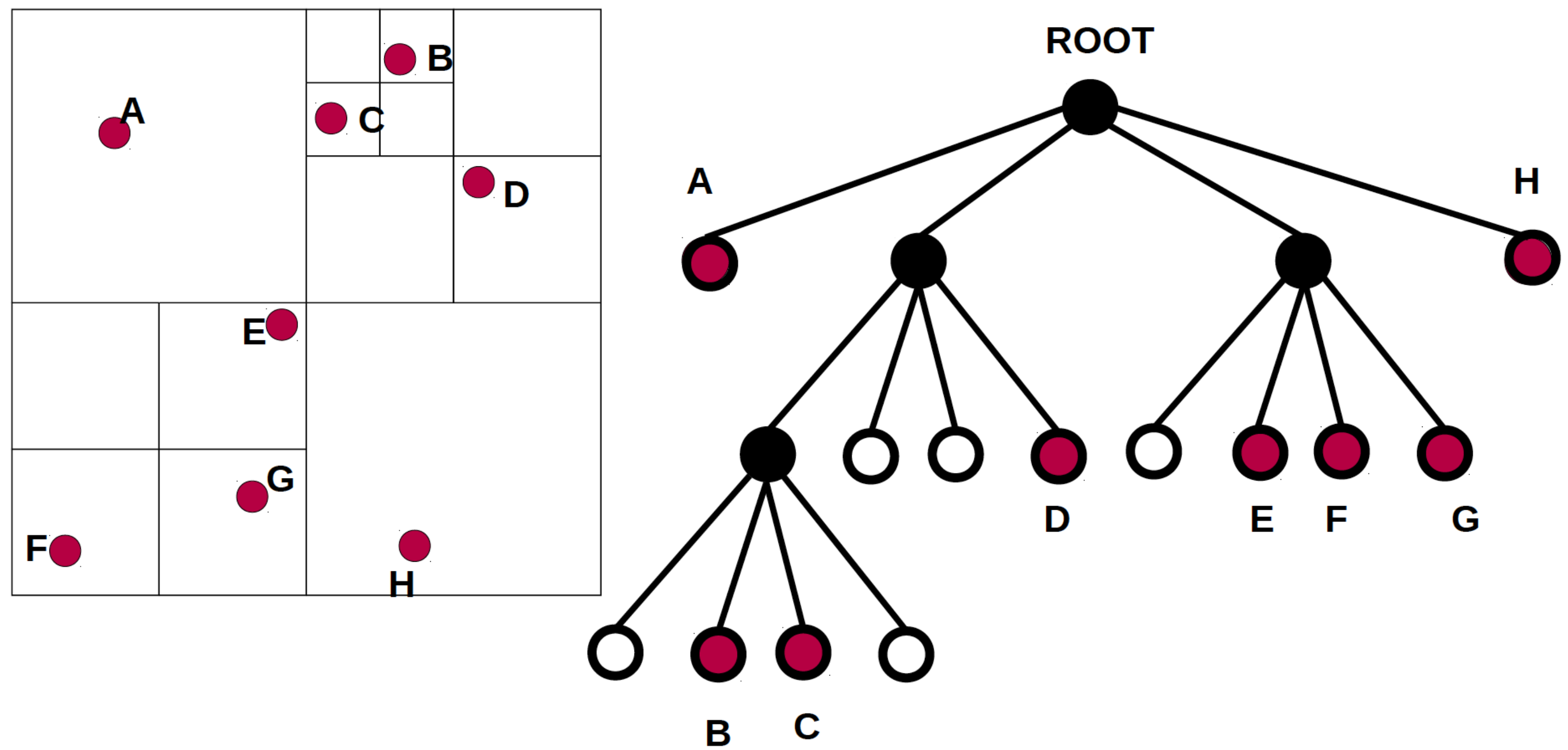
Example: quad-tree with 8 particles



Credit: Mapelli lectures on *N*-body techniques in astrophysics

Tree code: Barnes-Hut Algorithm

Example: quad-tree with 8 particles

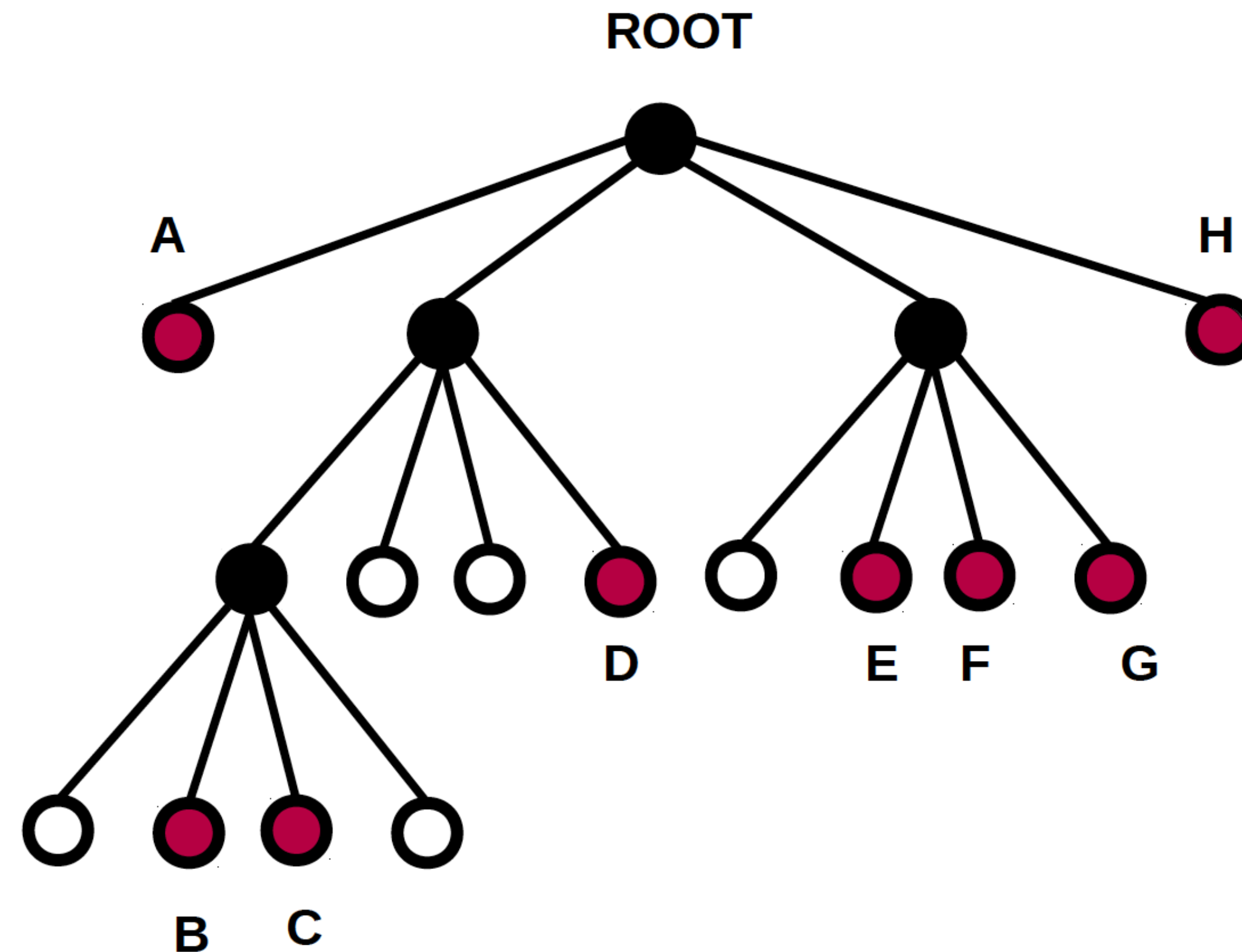


● Father node: >1 particle ○ Empty daughter node ● Daughter node with 1 particle

Credit: Mapelli lectures on *N*-body techniques in astrophysics

Tree code: Barnes-Hut Algorithm

- Force between nearby particles is calculated directly
 - e.g. the force exerted by **F** on **E**
- Force between distant particles is approximated with centre of mass
 - e.g. the force of **E, F, G** on **D** is approximated by the centre of mass of **E, F and G**
- Can significantly reduce the number of force calculations
- Need a criteria to decide when particle is far enough to avoid direct calculation
- Based on the ratio of the width of the region represented by the considered node (s) and the distance between the body and the node's center-of-mass



$$s/d < \theta \quad \theta = \text{threshold value}$$

$\theta = 0.5$ commonly used in practice

Credit: Mapelli lectures on N -body techniques in astrophysics

Tree code: Barnes-Hut Algorithm

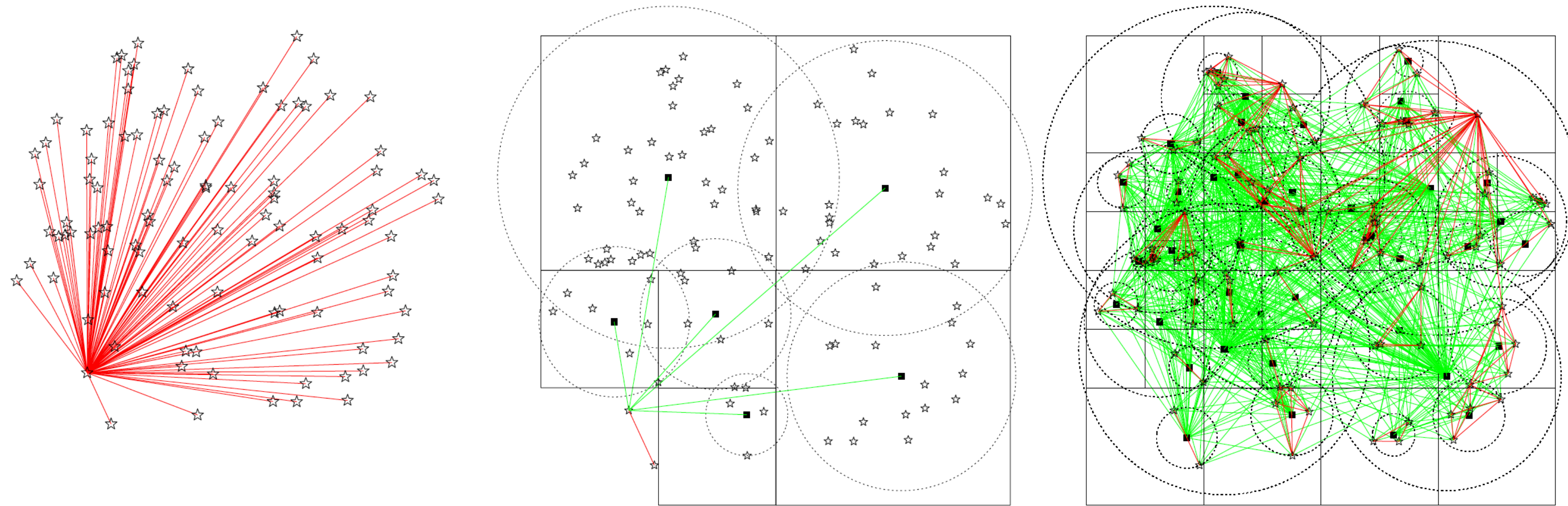


Fig. 5. Left: computation of the force for one of 100 particles (asterisks) in two dimensions (for graphical simplicity) using direct summation: every line corresponds to a single particle-particle force calculation. Middle: approximate calculation of the force for the same particle using the tree code. Cells opened are shown as black squares with their centres z indicated by solid squares and their sizes w by dotted circles. Every green line corresponds to a cell-particle interaction. Right: approximate calculation of the force for all 100 particles using the tree code, requiring 902 cell-particle and 306 particle-particle interactions ($\theta = 1$ and $n_{\max} = 1$), instead of 4950 particle-particle interactions with direct summation.

From Dehnen & Read (2011)

See Dehnen & Read (2011) for
Fast multipole method (FMM)
and Grid-based methods

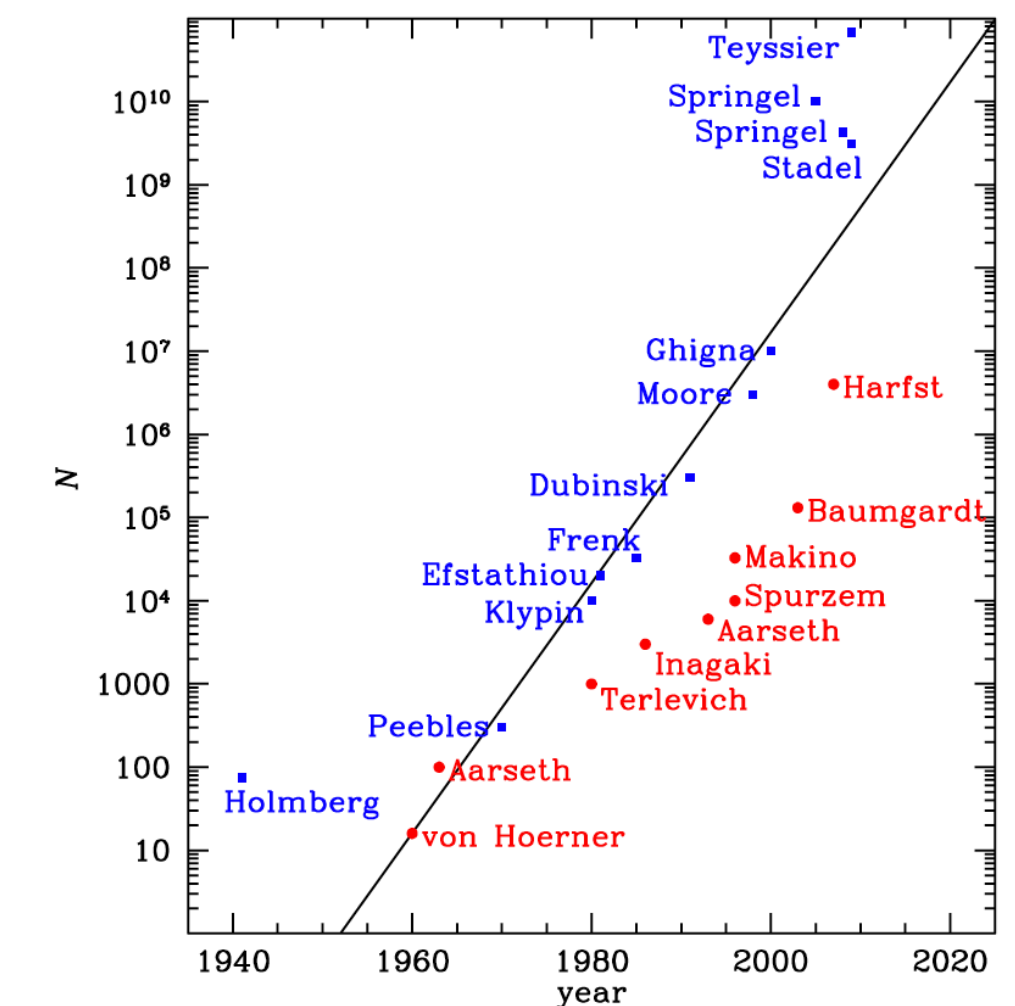
In direct summation for
acceleration calculation:

$$N(N - 1)/2$$

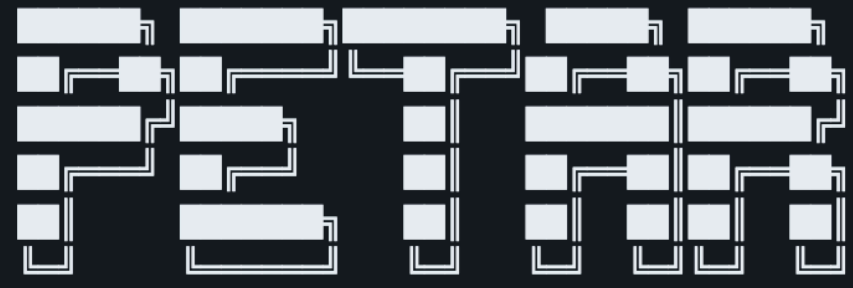
For $N=100$, 4950 particle-
particle interactions

With tree code: 902 cell-particle
and 306 particle-particle
interactions

Evaluation of force scales as $O(N \log N)$



Hybrid N -body code: PeTar



PeTar is an N -body code specifically designed for modeling collisional stellar systems, where factors such as multiplicity (binaries, triples, etc.) and close encounters play a crucial role in dynamical evolution. PeTar offers several key advantages:

- **Precise gravitational force modeling:** PeTar does not employ any softening of gravitational force, enabling accurate tracking of the orbital evolution of binaries, triples, and close encounters.

<https://github.com/lwang-astro/PeTar>

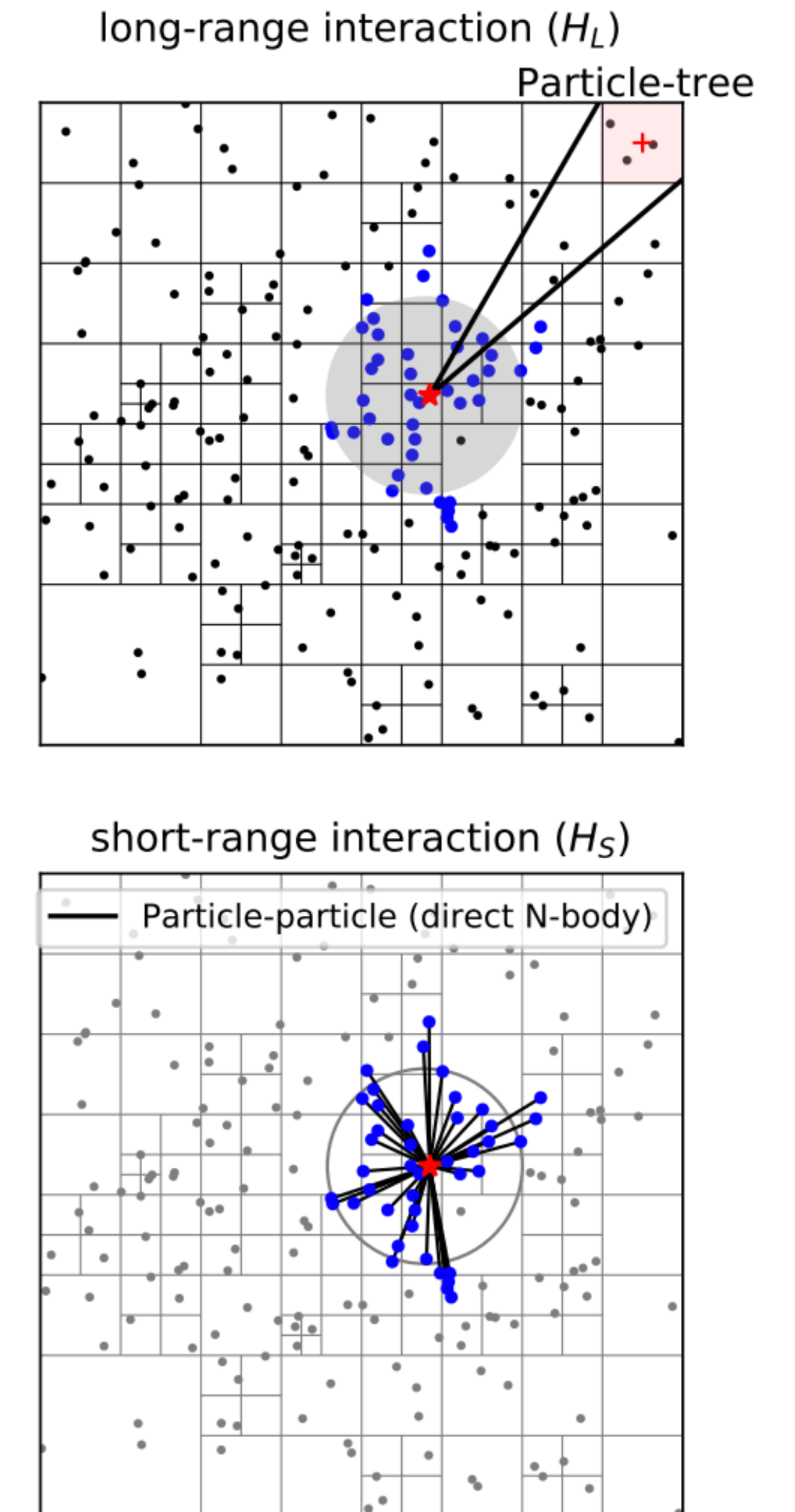


Fig. 1 from Wang et al. (2020)

- PeTar (Wang et al. 2020): Barnes-Hut Tree Algorithm + Hermite Integrator + slow-down algorithmic regularization
- Leverages multi-CPU processors/threads and GPU acceleration to accelerate simulations
- Up to 11 times faster than NBODY6++GPU
- Can treat high multiplicity fraction (binaries and triples)
- No Softening

Key takeaways

- Direct summation N -body codes for collisional systems are slow but accurate!
- Solving equation of motions seems straightforward but computationally challenging $\sim O(N^2)$
- Several techniques to speed up calculations:
 - Neighbour scheme
 - Hierarchical block time steps
 - Regularization
 - Parallelization
- Hardware acceleration has enabled long-term simulations of realistic globular clusters models
 - GPUs (game changer)
- Collisionless N -body systems are relatively less tedious
 - Softening and lower order integrators
 - Direct summation can be avoided: Tree Methods
- Up next: Monte Carlo modelling is a realistic practical alternative to simulating large globular clusters