The issue about accuracy!

- Simulation uses: $10^6 - 10^{10}$ steps, N force calculations per step; $N = 10^6 \sim 10^{12} - 10^{16}$ force (pairwise) calculations
- Double precision $\sim 10^{-13}$ – if all errors sum up in a „bad" way → final error 'order unity'

In our simulations it is not so serious:

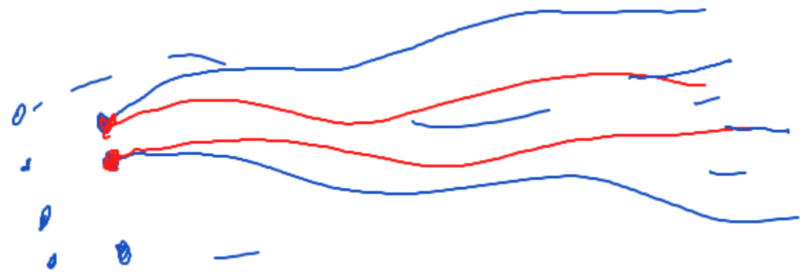
1) errors are often uncorrelated! r.m.s. error $\ll \sum |\text{error}|$!
   (depending on system symmetry) Care: for strongly asymm. systems!
2) What can we check? $\neq$ total energy (Makino 1991)
   ADJUST!!

What else? Total Angular Momentum (three vector components)
We can only look for globally conserved quantities!

3) Miller, R. 1964: exponential divergence of orbits coming from very small differences of initial pos./vel.

N-body meaningless?? See Quinlan + Tremaine (1992)

numerical N-body simulation: trajectories of particles stay always close to a real Hamiltonian solution!

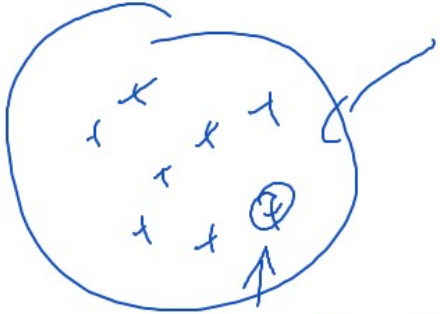


no contradiction to exponential divergence!

- star clusters, glob. cl., 1M particles

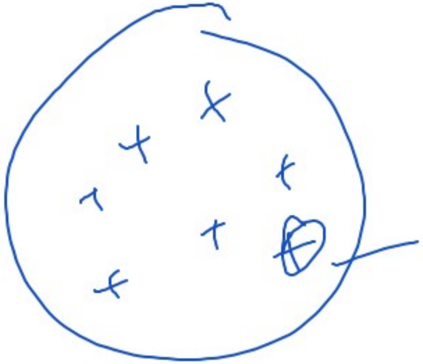
47 Tuc

Simulation



X-ray sources

BH of $10 M_\odot$



$4 M_\odot$

$25 M_\odot$

Giersz + Spurzem (1994)

General Features of the Code

- Hermite Scheme + hierarchically blocked time steps
- Ahmad - Cohen Neighbour neighbour scheme
- Regularizations: close 2, 3, few-body subsystem
  (classical, algorithmic)
- Stellar Evolution

Comparison of the code versions

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

From: Spurzem & Kamlah (2023); subm. to Living Reviews on Computational Astrophysics (LRCA)

ITS: Individual time–steps [107] Aarseth (1985)
ACS: Ahmad-Cohen neighbour scheme [109] Ahmad & Cohen (1973)
KS: KS–regularization of few-body subsystems [104] Kustaanheimo & Stiefel (1965)
HITS: Hermite scheme integration method combined with hierarchical block time-steps [111] Makino & Aarseth (1992)
PN: Post-Newtonian Kupi et al. (2006), Brem et al. (2013)
AR: Algorithmic regularization Mikkola & Tanikawa (1999ab), w/PN: Mikkola & Merritt (2008)
CC: Classical chain regularization Mikkola & Aarseth (1990, 1993, 1998), w/PN: Aarseth (2012)
MPI: Message Passing Interface, multi-node multi-CPU parallelization [139] Spurzem (1999)
GPU: use of GPU acceleration [138] (if also MPI: multi-node many GPU [144]) Nitadori & Aarseth (2012), Berczik et al. (2013)

NBODY7: Aarseth (2012), Banerjee et al. (2020)

Hermite Scheme: acceleration $\vec{a}_i$; force $\vec{F}_i = m_i \vec{a}_i$ | $\dot{} = \frac{d}{dt}$;

particle i; all other particle j

position vector $\vec{r}_i$; $\vec{v}_i = \dot{\vec{r}}_i$; Newton's Law:

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

; for Hermite:

Unit Vector $\frac{(\vec{r}_i - \vec{r}_j)}{|\quad|}$ connecting $\vec{r}_i, \vec{r}_j$

$$\dot{\vec{a}}_i = -G \sum_{\substack{j=1 \\ j \neq i}}^{N} m_j \left[\frac{\vec{v}_i - \vec{v}_j}{|\vec{r}_i - \vec{r}_j|^3} - \frac{(\vec{R}_{ij} \cdot \vec{V}_{ij})(\vec{r}_i - \vec{r}_j)}{|\vec{r}_i - \vec{r}_j|^5} \right]$$

$\vec{R}_{ij} = \vec{r}_i - \vec{r}_j$; $\vec{V}_{ij} = \vec{v}_i - \vec{v}_j$

$\vec{r}_i = (x_i, y_i, z_i)$

$$|\vec{r}_i - \vec{r}_j|^2 = (x_i - x_j)^2 + (y_i - y_j)^2 + (z_i - z_j)^2$$

Low Order Taylor series for prediction:

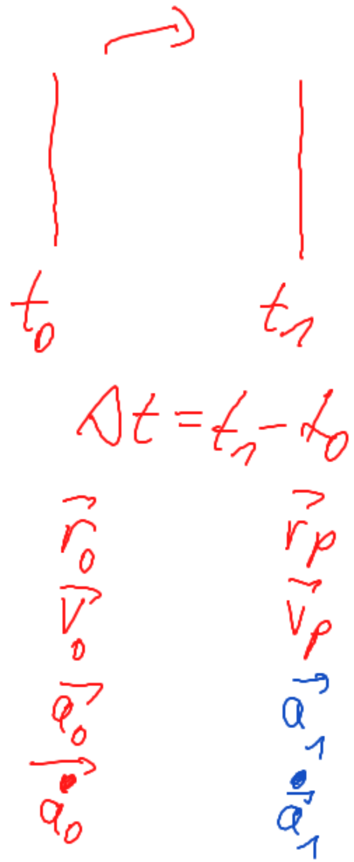
$$\vec{r}_p(t_1) = \underline{\vec{r}_0} + \underline{\vec{v}_0}\cdot\Delta t + \frac{1}{2}\underline{\vec{a}_0}\,\Delta t^2 + \frac{1}{6}\underline{\dot{\vec{a}}_0}\,\Delta t^3 + O(\Delta t^4)$$

(Assume that we sit on particle i! $\vec{r}_0 = \vec{r}_{0i}$; <u>Drop i</u>

$$\vec{v}_p(t_1) = \vec{v}_0 + \vec{a}_0\,\Delta t + \frac{1}{2}\dot{\vec{a}}_0\,\Delta t^2 + O(\Delta t^3)$$

2nd order accurate, Error $O(\Delta t^3)$

Hermite trick is to compute $\vec{a}_1, \dot{\vec{a}}_1$ in two ways!



1) Newton's law with predicted positions + velocities of all particles!

$$\vec{a}_1 = -G \sum_{\substack{j=1 \\ j \neq i}}^{N} m_j \frac{\vec{r}_p - \vec{r}_{pj}}{|\vec{r}_p - \vec{r}_{pj}|^3} \quad \text{and} \quad \dot{\vec{a}}_1 \text{ using } \vec{v}_{pj}, \dot{\vec{v}}_{pj}$$

2) Use Taylor Series to approximate $\vec{a}_1, \dot{\vec{a}}_1$:

$$\underline{\vec{a}_1} = \underline{\vec{a}_0} + \underline{\dot{\vec{a}}_0}\,\Delta t + \frac{1}{2}\underline{\vec{a}_0^{(2)}}\,\Delta t^2 + \frac{1}{6}\underline{\vec{a}_0^{(3)}}\,\Delta t^3 + O(\Delta t^4)$$

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

— Known — Unknown

Two unknowns, two equations!

$$\vec{a}_0^{(2)} = \left[-3\,(\vec{a}_0 - \vec{a}_1) - (2\,\dot{\vec{a}}_0 + \dot{\vec{a}}_1)\cdot \Delta t \right] \frac{2}{\Delta t^2} + O(\Delta t^2)$$

$O(\Delta t^4)$ $O(\Delta t^3)$ $\cdot\, O(\Delta t)$

$$\vec{a}_0^{(3)} = \left[2\,(\vec{a}_0 - \vec{a}_1) + (\dot{\vec{a}}_0 + \dot{\vec{a}}_1)\cdot \Delta t \right] \frac{6}{\Delta t^3} + O(\Delta t)$$

Corrected: Hermite Formula for $a_0^{(2)}, a_0^{(3)}$

$$\vec{r}_c(t) = \vec{r}_p(t) + \frac{1}{24}\, a_0^{(2)} \Delta t^4 + \frac{1}{120}\, a_0^{(3)} \Delta t^5 + O(\Delta t^6)$$

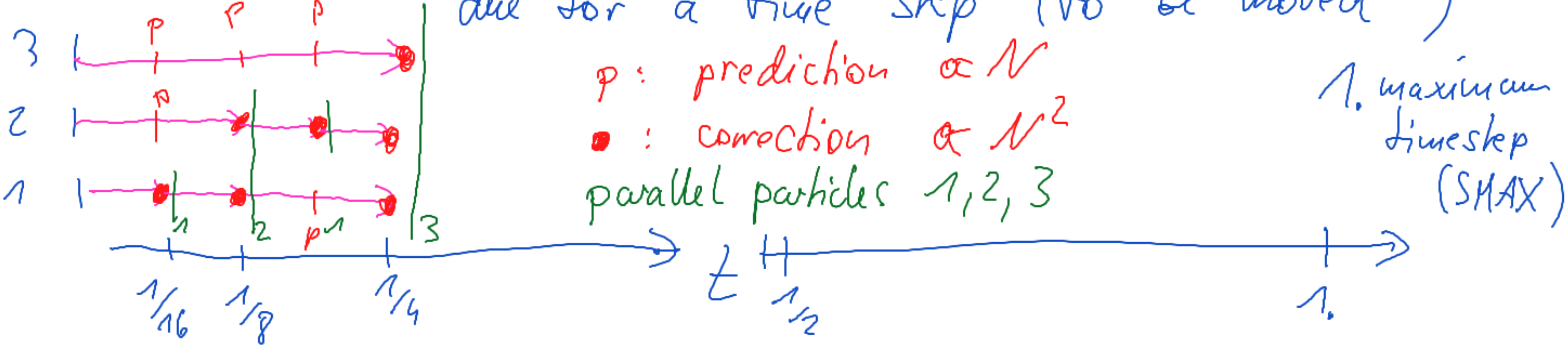
$$\vec{v}_c(t) = \vec{v}_p(t) + \frac{1}{6}\, a_0^{(2)} \Delta t^3 + \frac{1}{24}\, a_0^{(3)} \Delta t^4 + O(\Delta t^5)$$

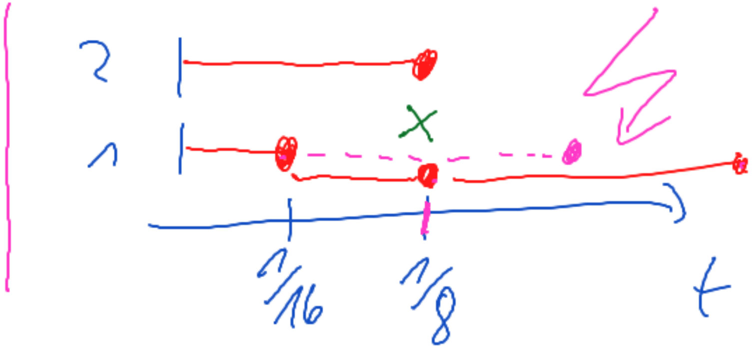
Global Error is $O(\Delta t^5)$!

t_0		t_1
$\vec{r}_0$		$\vec{r}_p$
$\vec{v}_0$		$\vec{v}_p$
$\vec{a}_0$	—	$\vec{a}_1$
$\dot{\vec{a}}_0$	—	$\dot{\vec{a}}_1$
$a_0^{(2)}$		
$a_0^{(3)}$		

- Hermite Scheme: 2nd order Predictor $O(\Delta t^3)$ – 4th order Corrector $O(\Delta t^5)$

- Hierarchically Blocked Time Step Scheme:
  - Predictor is always done for all particles
  - Corrector is only done for particles which are due for a time step (to be moved)





X: particle one would miss the parallel correction at $t = 1/8$!

Demand: Time and Step are commensurate

$$\mathrm{TIME}/\Delta t \;\hat{=}\; \text{integer}$$

Step: $\frac{2}{16} = \frac{1}{8}$

Time: $\frac{3}{16}$

$$\left.\begin{array}{l} \text{Step: } \frac{2}{16} = \frac{1}{8} \\ \text{Time: } \frac{3}{16} \end{array}\right\} \frac{\mathrm{TIME}}{\mathrm{Step}} \neq \text{integer}$$

Hierarchically Blocked ITS (HITS)

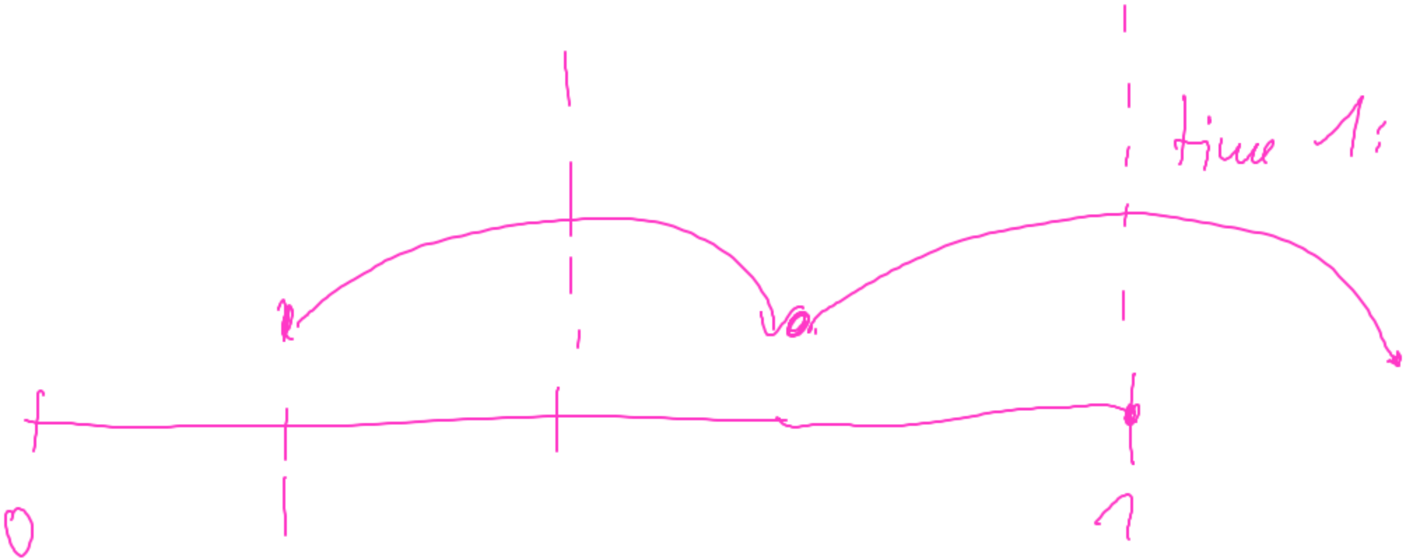
- 1: $\Delta t = \frac{1}{2^n}$, $n = 0, \ldots 32, \ldots$
- 2: $\mathrm{DMOD}(\mathrm{TIME}, \mathrm{STEPI}_R) = 0.D0$

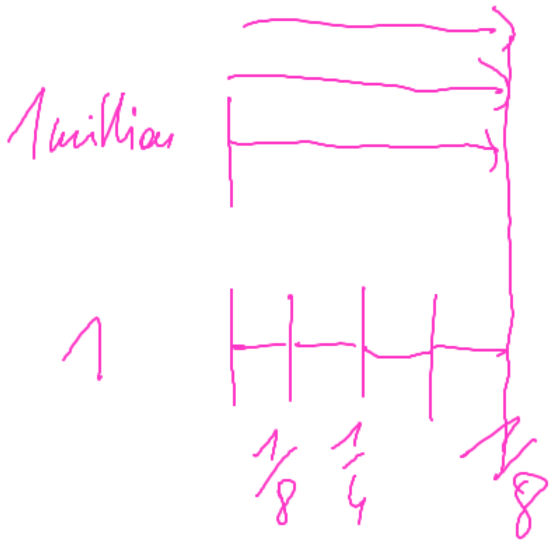
(We do not allow TIME to grow too large!
TIME < DTOFF ~ 100.

Physical Time: TTOT = TIME + TOFF

In that way: we get maximum number of parallel connections! SMAX = 1.0

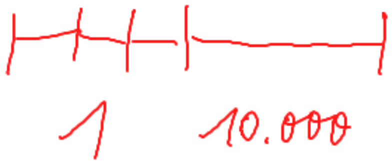
time 1: all particles





Sequential:

To reach 1/8: 1 million + 3



10.000 + 3

Speedup ~ 100