N-Body Algorithms

Sverre Aarseth

Institute of Astronomy, Cambridge

Basic Integration

Two-Body Treatments

Practical Aspects

Realistic Modelling

Three-Body Regularization

Post-Newtonian Terms

Wheel-Spoke Regularization

SSE/GPU Implementation

Hermite Integration

Taylor series for $\mathbf{F}$ and $\mathbf{F}^{(1)}$

$$\mathbf{F} = \mathbf{F}_0 + \mathbf{F}_0^{(1)}\, t + \frac{1}{2}\mathbf{F}_0^{(2)}\, t^2 + \frac{1}{6}\mathbf{F}_0^{(3)}\, t^3$$

$$\mathbf{F}^{(1)} = \mathbf{F}_0^{(1)} + \mathbf{F}_0^{(2)}\, t + \frac{1}{2}\mathbf{F}_0^{(3)}\, t^2$$

Prediction

$$\mathbf{r}_j = ((\frac{1}{6}\mathbf{F}_0^{(1)}\,\delta t'_j + \frac{1}{2}\mathbf{F}_0)\,\delta t'_j + \mathbf{v}_0)\,\delta t'_j + \mathbf{r}_0$$

$$\mathbf{v}_j = ((\frac{1}{2}\mathbf{F}_{\mathbf{0}}^{(\mathbf{1})}\,\delta t'_j + \mathbf{F}_0)\,\delta t'_j + \mathbf{v}_0\,; \qquad \delta t'_j = t - t_0$$

New forces $\quad \mathbf{F},\ \mathbf{F}^{(1)}$

Higher derivatives

$$\mathbf{F}_0^{(3)} = (2(\mathbf{F}_0 - \mathbf{F}) + (\mathbf{F}_0^{(1)} + \mathbf{F}^{(1)})\, t)\,\frac{6}{t^3}$$

$$\mathbf{F}_0^{(2)} = (-3(\mathbf{F}_0 - \mathbf{F}) - (2\mathbf{F}_0^{(1)} + \mathbf{F}^{(1)})\, t)\,\frac{2}{t^2}$$

Corrector for i

$$\Delta\mathbf{r}_i = \frac{1}{24}\mathbf{F}_0^{(2)}\Delta t^4 + \frac{1}{120}\mathbf{F}_0^{(3)}\,\Delta t^5$$

$$\Delta\mathbf{v}_i = \frac{1}{6}\mathbf{F}_0^{(2)}\Delta t^3 + \frac{1}{24}\mathbf{F}_0^{(3)}\,\Delta t^4$$

AC Neighbour Scheme

Total force $\mathbf{F}(t) = \sum_{j=1}^{n} \mathbf{F}_j + \mathbf{F}_d(t)$

Predict $\mathbf{F}(t) = \mathbf{F}_n + \dot{\mathbf{F}}_d(t - t_0) + \mathbf{F}_d(t_0)$

$$\dot{\mathbf{F}} = \dot{\mathbf{F}}_n + \dot{\mathbf{F}}_d$$

Time-scales $\Delta t_n << \Delta t_d, \quad n << N$

Time-steps $\Delta t_i = \left(\frac{\eta |\mathbf{F}|}{|\ddot{\mathbf{F}}|}\right)^{1/2}$

Sphere $R_s^{\text{new}} = R_s^{\text{old}} \left(\frac{n_p}{n}\right)^{1/3}, n_p \simeq N^{1/2}$

Strategy Constant n_p or $n_p \propto \frac{n}{R_s^3}$

Selection $|\mathbf{r}_i - \mathbf{r}_j| < R_s$, Full N loop

Membership Gain or loss of $\mathbf{F}_{ij}^{(k)}$

Corrections $\mathbf{F}_{ij}^{(2)}$, $\mathbf{F}_{ij}^{(3)}$, Explicit diff.

Performance Break-even $N \simeq 50$

Micro-Grape vs NBODY6

. Factor of 11, $N = 25,000$

Time-Steps

Basic time-step $\Delta t = \frac{\alpha |\mathbf{r}|}{|\mathbf{v}|}, \quad \Delta t = \frac{\beta |\mathbf{F}|}{|\mathbf{F}^{(1)}|}$

Taylor series $\mathbf{F} = \mathbf{F}_0 + \mathbf{F}_0^{(1)} \Delta t + \frac{1}{2} \mathbf{F}_0^{(2)} \Delta t^2 + \ldots$

Natural time-step $\Delta t = \left(\frac{\eta |\mathbf{F}|}{|\mathbf{F}^{(2)}|} \right)^{1/2}, \quad \eta = 0.02$

General expression $\Delta t = \left(\frac{\eta (|\mathbf{F}||\mathbf{F}^{(2)}| + |\mathbf{F}^{(1)}|^2)}{|\mathbf{F}^{(1)}||\mathbf{F}^{(3)}| + |\mathbf{F}^{(2)}|^2} \right)^{1/2}$

Relative criterion Δt independent of mass

Block-steps $\Delta t_n = \frac{\Delta t_1}{2^{n-1}}, \quad \Delta t_1 = 1$

Hierarchical levels $\mathcal{N}_k$ particles with steps Δt_k

Scheduling $i = \min\ (t_j + \Delta t_j)$

KS Decision-Making

Close encounter	$R_{\rm cl} \; = \; \dfrac{4\, r_{\rm h}}{N\, C^{1/3}}, \quad \Delta t_{\rm cl} \; = \; \beta \left(\dfrac{R_{\rm cl}^3}{\bar{m}} \right)^{1/2}$
Time-step criterion	$\Delta t_k \; < \; \Delta t_{\rm cl}$
Neighbour list search	list all $r_{kj}^2, \quad \Delta t_j \; < \; 2\, \Delta t_{\rm cl}$
Two-body selection	$R_{kl} \; < \; R_{\rm cl}, \quad \dot{R}_{kl} \; < \; 0$
Dominant motion	$\dfrac{m_k \, + \, m_l}{R_{kl}^2} \; > \; \dfrac{m_k \, + \, m_j}{R_{kj}^2}$
KS initialization	$\mathbf{F}_U, \, \mathbf{F}'_U, \, \Delta\tau \; \& \; t^{(n)} \;\; \Rightarrow \;\; \Delta t$
Initialization of c.m.	$\mathbf{r}_{\rm cm} \; = \; \dfrac{m_k\, \mathbf{r}_k \, + \, m_l\, \mathbf{r}_l}{m_k \, + \, m_l}$
Perturber search	$r_{\rm p} \; < \; \left(\dfrac{2 m_{\rm p}}{m_{\rm b} \gamma_{\rm min}} \right)^{1/3} \; a\,(1+e)$
Slow-down adjustment	$\gamma \; < \; \gamma_0, \quad \Delta\tau \; \Rightarrow \; \kappa\, \Delta t$
Termination test	$R \; > \; R_0, \quad \gamma \; > \; \gamma^*$
Delayed termination	$T_{\rm block} \; - \; t \; > \; \Delta t_i$
Final iteration	$\Delta\tau$ from $\dot{\tau}, \, \ddot{\tau}, \ldots$ and δt
Polynomial initialization	$\mathbf{F}_j, \, \dot{\mathbf{F}}_j, \, \Delta t_j, \quad j = k, \, l$

N-Body Interface

Centre of mass acceleration

$$\ddot{\mathbf{r}}_{cm} = (m_k \mathbf{F}_k + m_l \mathbf{F}_l)/(m_k + m_l)$$

Global coordinates

$$\begin{aligned} \mathbf{r}_k &= \mathbf{r}_{cm} + \mu \mathbf{R}/m_k \\ \mathbf{r}_l &= \mathbf{r}_{cm} - \mu \mathbf{R}/m_l \end{aligned}$$

Relative perturbation

$$\gamma = |\mathbf{F}_k - \mathbf{F}_l| R^2/(m_k + m_l)$$

Tidal approximation

$$r_\gamma = R[2m_p/(m_k + m_l)\gamma_{\rm min}]^{1/3}, \qquad \gamma_{min} \simeq 10^{-6}$$

Perturber selection

$$r_{ij} < r_\gamma, \qquad R = a(1+e)$$

Regularized time-step

$$\Delta\tau = \eta_u (1/2|h|)^{1/2} 1/(1 + 1000\gamma)^{1/3}$$

Physical time-step

$$\Delta t = \sum_{k=1}^{n} \frac{1}{k!} t_0^{(k)} \Delta\tau^k, \qquad n = 6$$

Time derivatives

$$\begin{aligned} t_0'' &= 2\mathbf{u}' \cdot \mathbf{u} \\ t_0^{(3)} &= 2\mathbf{u}'' \cdot \mathbf{u} + 2\mathbf{u}' \cdot \mathbf{u} \end{aligned}$$

Hierarchical Stability

Requirement	a_0 secularly constant
Kozai cycles	$e_{\rm max} = \left(1 - 5cos^2 i/3\right)^{1/2}$
Candidates	$\Delta t_{\rm cm} < \Delta t_{\rm cl},\ a_1(1 - e_1) > 3a_0$
Restrictions	$\mu_1 M_{123}/2a_1 > E_{\rm hard},\ \gamma_1 < 0.01$
Stability test	$f(a_0, a_1, e_0, e_1, \phi, m_1, m_2, m_3)$
Data structure	New KS, m_3 + inner c.m.
Merger table	$m_1, m_2, \mathbf{R}, \mathbf{V}, h, \mathbf{u}, \mathbf{u}', \mathcal{N}_g, \mathcal{N}_{cm}$
Initialization	New polynomials for KS and c.m.
Assessment	New check $R_{\rm apo} < P_{\rm crit}$
Mass loss	Update $h, \mathbf{u}, \mathbf{u}'$, stability check
Termination	$\gamma > 0.1$, $R > R_{\rm cl}$ or $\gamma > 0.25$
Re-initialize	Triple $\Rightarrow$ KS + m_3

Program Control

Scheduling	Sorted list with $N^{1/2}$ members
Current time	$t = t_i + \Delta t_i, \quad i = NEXT(1)$
Next time	$T_{\rm min} = \min\,(t + \Delta t_j)$
Next block	All $t_j + \Delta t_j = T_{\rm min}$
Prediction	Full N or joint neighbour list
Irregular force	$\mathbf{F}_i, \mathbf{F}_i^{(1)}$ for n members
Regular force	$t_{\rm reg} + \Delta t_{\rm reg} = t_{\rm new}$
Continuity	Identical $\mathbf{F}_{\rm n}$, $\mathbf{F}_{\rm n}^{(1)}$ if no change
Strategy	Predicted coordinates for $\mathbf{F}_{\rm reg}$

Data Structure

Singles $2\,N_{\rm p} < i \leq N, \; \mathcal{N}_i = i$

KS $1 \leq i \leq 2\,N_{\rm p}\,, \quad i_p = i_{\rm icm} - N$

C.m. $i > N, \; \mathcal{N} = N_0 + \mathcal{N}_k$

Triple KS + ghost, $\mathcal{N}_{\rm cm} = -\mathcal{N}_k$

Ghost $\mathcal{N}_{\rm g} = \mathcal{N}_{2i_{\rm p}-1}, \; m_{\rm g} = 0$

Quad KS + KS ghost, $\mathcal{N}_{\rm cm} = -\mathcal{N}_k$

Quint T + KS, $\mathcal{N}_{\rm cm} = -(2N_0 + \mathcal{N}_k)$

Chain $2\,N_{\rm p} < i_{\rm cm} \leq N, \; \mathcal{N}_{\rm cm} = 0$

Escape $2N_{\rm p} < i \leq N, \; r_i > 2r_{\rm tide}$

Binary $i > N, \; r_i > 2r_{\rm tide}, 2i_p - 1, \; 2i_p$

Hierarchy $i > N\,, \; r_i > 2r_{\rm tide},$
. $2i_p - 1, \; 2i_p\,, \; i_{\rm ghost}$

Units

(a) Scaling relations

Length scale R_{V} in pc and M_S in $M_\odot$

Fiducial velocity $\quad V^2 = GNM_S/R_V$

$$\tilde{V}^* = 1 \times 10^{-5} (GM_\odot/L^*)^{1/2} \text{ km/s}$$
$$L^* = 3 \times 10^{18} \text{ cm}$$

Velocity unit $\quad V^* = 6.5 \times 10^{-2} \left(\frac{NM_{\mathsf{S}}}{R_{\mathsf{V}}}\right)^{1/2}$ km/s

Fiducial time $\quad \tilde{T}^* = (L^{*3}/GM_\odot)^{1/2} = 14.9$ Myr

Time unit $\quad T^* = \tilde{T}^* \left(\frac{R_{\mathsf{V}}^3}{NM_{\mathsf{S}}}\right)^{1/2}$ Myr

(b) Conversion from N-body units

$\tilde{r} = R_{\mathsf{V}}\, r$ pc, $\quad \tilde{v} = V^*\, v \ km/s$
$\tilde{t} = T^*\, t$ Myr, $\quad \tilde{m} = M_{\mathsf{S}}\, m/ < m > \ M_\odot$

Crossing time $\quad T_{\mathsf{cr}} = 2\sqrt{2}\, T^*$ Myr

Initial Scaling

Main input $N,\ N_{\mathsf{b}},\ M_S,\ R_{\mathsf{V}}$

Initial data $m_i, \tilde{\mathbf{r}}_i, \tilde{\mathbf{v}}_i, \ldots, i = 1, N$

Total energy $E = T - U$

Virial theorem $\mathbf{v}_i = q\tilde{\mathbf{v}}_i,\ q = \left[\frac{Q_{\mathsf{V}}U}{T}\right]^{1/2}$

Units $G = 1, \sum m_i = 1, E_0 = -0.25$

Scaling $\hat{\mathbf{r}}_i = \frac{\mathbf{r}_i}{S^{1/2}},\ \hat{\mathbf{v}}_i = \mathbf{v}_i S^{1/2},$

$$S = \frac{E_0}{q^2 T - U}$$

Initial Conditions

Coordinates: Plummer density or King model

Velocities: Isotropic or $f(E, \mathbf{J})$

Masses: Salpeter or Kroupa IMF

Primordial binaries: Observational evidence

Clumped subsystems: Hierarchical star formation

Initial segregation: Heavy stars near the centre

Gas expulsion: Imposed mass loss or SN

Intermediate mass BH: GC or Galactic centre

Stellar Evolution

Stellar HR types	$K^* = 0, ..., 15$
Fast look-up	$r^*(t),\ m_c(t),\ L^*(t),\ K^*(t)$
Wind mass loss	$\dot{m} = -2\times10^{-13}\, r^*\, L^*/m$
Single stars	Small $\Delta\, m/\, m$, new r^*
Updating times	$T_{\rm ev} = t + \min\,(\Delta t_{\rm ev},\, \Delta t_{\rm rem})$
Stellar rotation	$\Delta J_{\rm spin} = \frac{2}{3} \Delta m r^2 \Omega_{\rm rot}$
White dwarfs	Cooling curves
Supernovae	$m_{\rm c} > 1.44 \Rightarrow$ SN, $v >> v_\infty$
Binary mass loss	$m\, a =$ const
Spin–orbit coupling	$J_{\rm tot} = J_{\rm orb} + J_{\rm spin}$
Tides	Circularization and breaking
Roche-lobe overflow	$r^* > \dfrac{0.49 q^{2/3}}{0.6 q^{2/3} + ln(1 + q^{1/3})}\, a$

Physical Collisions

Simple definition	$R_{\rm coll} = \frac{3}{4}(r_1^* + r_2^*)$
Two-body encounter	KS regularization
Pericentre condition	$R_0' \, R' < 0, \quad R < a$
Pericentre determination	$\Delta t_{\rm peri}$ from Kepler's equation
Predict $\mathbf{R}_{peri}$ or iterate	$d\tau_0 = \frac{\Delta t_{peri}}{R}, \quad$ Newton-Raphson
Implement collision	$m_{\rm cm} = m_1 + m_2, \quad r_{\rm cm} = \frac{m_1\mathbf{r}_1 + m_2\mathbf{r}_2}{m_1 + m_2}$
Mass loss	$\Delta m = f(K_1^*, K_2^*)$
Initialize single body	$\mathbf{F}_1, \dot{\mathbf{F}}_1, \Delta t_1$
Compact subsystem	$\dot{R} \simeq 0$ by iteration
Transformation	$\mathbf{Q}, \mathbf{P} \Rightarrow \mathbf{r}, \dot{\mathbf{r}}$
New chain construction	$N_{\rm ch} \Rightarrow N_{\rm ch} - 1, \quad E_{\rm coll} = E_{\rm ch} - \mathcal{V}$