Hermite Integration

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

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

Prediction

$$\begin{aligned}
\mathbf{r}_j &= ((\frac{1}{6}\mathbf{F}_0^{(1)}\, \delta t_j' + \frac{1}{2}\mathbf{F}_0)\, \delta t_j' + \mathbf{v}_0)\, \delta t_j' + \mathbf{r}_0 \\
\mathbf{v}_j &= ((\frac{1}{2}\mathbf{F}_{\mathbf{0}}^{(\mathbf{1})}\, \delta t_j' + \mathbf{F}_0)\, \delta t_j' + \mathbf{v}_0\,; \qquad \delta t_j' = t - t_j
\end{aligned}$$

Higher derivatives

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

Corrector

$$\begin{aligned}
\Delta\mathbf{r}_i &= \frac{1}{24}\mathbf{F}_0^{(2)}\Delta t^4 + \frac{1}{120}\mathbf{F}_0^{(3)}\, \Delta t^5 \\
\Delta\mathbf{v}_i &= \frac{1}{6}\mathbf{F}_0^{(2)}\Delta t^3 + \frac{1}{24}\mathbf{F}_0^{(3)}\, \Delta t^4
\end{aligned}$$

Quantized time-steps

$$\Delta t_n = \left(\frac{1}{2}\right)^{n-1}$$

AC Neighbour Scheme

Total force	$\mathbf{F}(t) = \sum_{j=1}^{n} \mathbf{F}_j + \mathbf{F}_d(t)$
Prediction scheme	$\mathbf{F}(t) = \mathbf{F}_n + \dot{\mathbf{F}}_d(t - t_0) + \mathbf{F}_d(t_0)$ $\dot{\mathbf{F}} = \dot{\mathbf{F}}_n + \dot{\mathbf{F}}_d$
Time-scales	$\Delta t_n << \Delta t_d, \quad n << N$
Individual time-steps	$\Delta t_i = \left(\frac{\eta \lvert\mathbf{F}\rvert}{\lvert\ddot{\mathbf{F}}\rvert}\right)^{1/2}, \quad \eta \simeq 0.02 - 0.03$
Neighbour sphere	$R_s^{\text{new}} = R_s^{\text{old}} \left(\frac{n_p}{n}\right)^{1/3}, \quad n_p \simeq N^{1/2}$
Neighbour selection	$\lvert\mathbf{r}_i - \mathbf{r}_j\rvert < R_s,$ Full N loop
Derivative corrections	$\ddot{\mathbf{F}}_{ij}, \mathbf{F}_{ij}^{(3)},$ Explicit differentiation
Performance	Break-even for $N \simeq 50$
micro-Grape vs NBODY6	Factor of 11 for $N = 25,000$
Integration scheme	Divided differences or Hermite

Time-Step Criteria

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

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

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

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

Planetesimals $$\Delta t \;=\; \frac{\beta R^2}{|\mathbf{R}\cdot\mathbf{V}|}, \quad \beta = 0.1$$

KS regularization $$\mathbf{F}_{\mathrm{U}} \;=\; \frac{1}{2} h \mathbf{U}$$

Substitution $$\Delta\tau \;=\; \frac{\eta_{\mathrm{U}}}{(2|h|)^{1/2}}, \quad \eta_{\mathrm{U}} = 0.2$$

Implications Δt independent of mass

Bulirsch–Stoer absolute tolerance

KS Regularization

New coordinates $$R = u_1^2 + u_2^2 + u_3^2 + u_4^2$$

Time transformation $$dt = R\, d\tau$$

Coordinate transformation $$\mathbf{R} = \mathcal{L}(\mathbf{u})\, \mathbf{u}$$

Levi-Civita matrix

$$\mathcal{L}(\mathbf{u}) = \begin{bmatrix} u_1 & -u_2 & -u_3 & u_4 \\ u_2 & u_1 & -u_4 & -u_3 \\ u_3 & u_4 & u_1 & u_2 \end{bmatrix}$$

Equations of motion

$$\begin{aligned} \mathbf{u}'' &= \frac{1}{2} h\, \mathbf{u} + \frac{1}{2} R\, \mathcal{L}^{\mathcal{T}}\, \mathbf{P} \\ h' &= 2\, \mathbf{u}' \cdot \mathcal{L}^{\mathcal{T}}\, \mathbf{P} \\ t' &= \mathbf{u} \cdot \mathbf{u} \end{aligned}$$

Close encounter $$\Delta t_i < \Delta t_{cl}\,; \quad R < r_{cl}$$

Termination $$\gamma \equiv \frac{|\mathbf{P}|\, R^2}{m_i + m_j} > 0.5$$

Centre of mass motion $$\ddot{\mathbf{r}} = \frac{m_i\, \mathbf{P}_i + m_j\, \mathbf{P}_j}{m_i + m_j}$$

Perturber selection $$r_k < \lambda\, R\,, \quad \gamma > 1 \times 10^{-6}$$

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	$\mathbf{F}_j,\, \dot{\mathbf{F}}_j,\, \Delta t_j, \quad j = k,\, l$

Practical Aspects of KS

Regular equations	Perturbed harmonic oscillator, $\gamma < 1$
Constant time-step	$\Delta\tau = \eta \left(\frac{1}{2\lvert h\rvert}\right)^{1/2}$ vs $\Delta t \propto R^{3/2}$
Linearized equations	Higher accuracy per step
Faster force calculation	Tidal perturbation, $P \propto 1/r^3$
Unperturbed motion	$\gamma < 10^{-6}, \quad \Delta t > t_{\rm K}$
Slow-down procedure	Adiabatic invariance, $\tilde{P} = \kappa P$
Energy rectification	Improve $\mathbf{u}, \mathbf{u}'$ from integration of h'
C.m. approximation	$d > 100\, a\, (1 + e)$
Transformations	$\mathbf{R} = \mathcal{L}\mathbf{u}, \qquad \mathbf{r}_j = \mathbf{r}_{\rm cm} \pm \mu\mathbf{R}/m_j$
	$\dot{\mathbf{R}} = 2\mathcal{L}\mathbf{u}'/R, \quad \dot{\mathbf{r}}_j = \dot{\mathbf{r}}_{\rm cm} \pm \mu\dot{\mathbf{R}}/m_j$
Two-body elements	$a, \mathbf{J}, e$ for averaging & circularization

Hierarchical Systems

Hierarchical formation	$\mathrm{B} + \mathrm{B} \Rightarrow \mathrm{T} + \mathrm{S}$ or $\mathrm{B} + \tilde{\mathrm{B}}$, $e_{\rm out} < 1$
Dynamical molecules	[B,S], [B,B], [[B,S],S], [[B,B],S]
Formation rate	binary fraction
Stability	$a_{\rm out}(1 - e_{\rm out}) > \Psi(m, e_{\rm in}, i)\, a_{\rm in}$
Chaos boundary	fuzzy region & holes
Inclination effect	prograde vs retrograde stability
Kozai cycles	$\cos^2 i\,(1 - e_{\rm in}^2) = $ const
Eccentricity modulation	orbit averaging
Instability	$\dot{e}_{\rm out} > 0 \;\Rightarrow$ slingshot
Superfast particles	time-step reduction

Initialization of Hierarchy

1. Increase merger index `IM` for `IPAIR` and `JCOMP`
2. Save m_k, m_l in merger table `CM(K,IM)`, `K`$\longrightarrow 4$ if `JCOMP > N`
3. Copy c.m. neighbour list for later corrections
4. Terminate KS solution and update `NPAIRS` and arrays
5. Evaluate potential energy of components and old neighbours
6. Record $\mathbf{R} = \mathbf{r}_k - \mathbf{r}_l$, $\mathbf{V} = \mathbf{v}_k - \mathbf{v}_l$ and h in merger table
7. Form binary c.m. in primary location `ICOMP = 2*NPAIRS + 1`
8. Define ghost $(m = 0,\ X = 10^6)$ and initialize prediction variables
9. Obtain potential energy of inner c.m. body and neighbours
10. Remove ghost from neighbour lists
11. Initialize new KS for outer component in `JCOMP = ICOMP + 1`
12. Define c.m. and ghost names: $\mathcal{N}_{\rm cm} = -\mathcal{N}_{\tt ICOMP}$, $\mathcal{N}_{\rm ghost} = \mathcal{N}_{\tt JCOMP}$
13. Set pericentre stability limit in R_0(`IP`) for termination test
14. Update merger energy $\Delta E = \mu h_0 + \Delta\Phi$

Termination of Hierarchy

1. Locate current position in merger table: $\mathcal{N}_{\mathtt{IM}} = \mathcal{N}_{\rm cm}$
2. Save c.m. neighbours for correction procedure
3. Terminate outer KS solution and update `NPAIRS`
4. Evaluate potential energy of c.m. and neighbours +`JCOMP`
5. Determine location of ghost: $\mathcal{N}_j = \mathcal{N}_{\rm ghost}\,, \quad j = 1, \mathtt{N} + \mathtt{NPAIRS}$
6. Restore inner binary components from $\mathtt{CM}(\mathtt{K}, \mathtt{IM})$, $\mathbf{R}$, $\mathbf{V}$
7. Add `JCOMP` to neighbour lists containing `ICOMP`
8. Initialize force polynomials for outer component
9. Copy basic KS variables h, $\mathbf{u}$, $\mathbf{u}'$
10. Re-activate inner binary as new KS solution
11. Include copy and KS procedure for $\mathcal{N}_{\mathtt{JCOMP}} > N$
12. Obtain potential energy of inner components and perturbers
13. Update merger energy for conservation $\Delta E = \Delta\Phi - \mu h$
14. Reduce merger index and compress tables (including escapers)

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	$m_{\rm cm} = m_1 + m_2, \quad r_{\rm cm} = \frac{m_1 \mathbf{r}_1 + m_2 \mathbf{r}_2}{m_1 + m_2}$
Initialize single body	$\mathbf{F}_i, \, \dot{\mathbf{F}}_i, \, \Delta t_i$
Compact subsystem	$\dot{R} \simeq 0$ by iteration
Transformation	$\mathbf{Q}, \, \mathbf{P} \Rightarrow \mathbf{r}, \, \dot{\mathbf{r}}$
New chain construction	$N_{\rm ch} \Rightarrow N_{\rm ch} - 1, \quad E_{\rm coll} = E_{\rm ch} - \mathcal{V}$

Quantization of Time

Hierarchical block-steps $\Delta t_n = \dfrac{\Delta t_1}{2^{n-1}}, \quad n = 1, 40$

Initialization $t_{\rm next} = t_0 + \Delta t_i$

Truncation $\Delta \tilde{t}_i, \quad \Rightarrow n$ by fast iteration

Commensurability $mod\,(t,\, \Delta t_i) = 0$

New time $t = \min\,(t_0 + \Delta t_i)$

Scheduling algorithm ....

Multiple regularizations - termination or collision

Define quantized interval $\delta \tilde{t} = (t_{\rm ch} - t_{\rm prev})/8$

New time for initialization $t_{\rm new} = t_{\rm prev} + [(t_{\rm ch} - t_{\rm prev})/\delta \tilde{t}]\, \delta \tilde{t}$

Decision-Making

Condition for special treatment	$\Delta t_i < \Delta t_{\rm cl}$
1. Two-body encounter	$i \leq N, \quad R < R_{\rm cl}, \quad \dot{R} < 0$
2. Chain regularization	$i > N, \quad a_{\rm out}\,(1 - e_{\rm out}) < 2\,a_{\rm in}$
3. Stable triple formation	$a_{\rm out}\,(1 - e_{\rm out}) > 3\,a_{\rm in}$
Apocentre test (#2 & #3)	$\dot{R}_0\,\dot{R} < 0, \quad R > a$
Case #1 algorithm	$\dfrac{P\,R^2}{m_1 + m_2} < 0.25, \ldots.$
Case #2 algorithm	$R + d < R_{\rm cl}, \ldots.$
Case #3 algorithm	$\dfrac{M_{\rm b} m_3}{2\,a_{\rm out}} > \dfrac{1}{2}\bar{m}\,V^2, \ldots.$

Control and Size Parameters

`IPHASE` indicator	0	Standard value
	1	New KS regularization
	2	KS Termination
	3	Output and energy check
	4	Three-body regularization
	5	Four-body regularization
	6	New hierarchical system
	7	Termination of hierarchy
	8	Chain regularization
	9	Physical collision
	-1	Enforce time-step list

`COMMON` blocks	`NMAX`	Number of objects, $N_0 = N_{\rm s} + N_{\rm b}$
	`KMAX`	KS solutions
	`LMAX`	Size of neighbour lists
	`MMAX`	Hierarchical systems
	`NCMAX`	Chain membership