Basic Regularization

Two-body equation $\ddot{x} = -\frac{M}{x^2}$

Smoothing function $t' \equiv \frac{dt}{d\tau} = x$

Rule of differentiation $\frac{d}{dt} = \frac{1}{x}\frac{d}{d\tau}$

Time-smoothed equation $x'' = \frac{x'^2}{x} - M$

Binding energy $h = \frac{1}{2}\dot{x}^2 - \frac{M}{x}$

Substitution $\dot{x} = \frac{x'}{x} \Rightarrow$ $x'' = 2hx + M$

Coordinate transformation $u^2 = x$

Twice diff. of u^2 and $h \Rightarrow$ $u'' = \frac{1}{2}hu$

Regular equation for $x \Rightarrow 0$

Levi-Civita Formulation

2D system: u_1, u_2

$$
\begin{aligned}
R_1 &= u_1^2 - u_2^2 \\
R_2 &= 2u_1 u_2
\end{aligned}
$$

Transformation

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

Levi-Civita [1920] matrix

$$\mathcal{L}(\mathbf{u}) = \begin{bmatrix} u_1 & -u_2 \\ u_2 & u_1 \end{bmatrix} \qquad \Rightarrow \; R = u_1^2 + u_2^2$$

Definition $\dot{\mathbf{R}}^2 = \dot{\mathbf{R}}^T \cdot \dot{\mathbf{R}}$ with $\mathbf{R}' = 2\mathcal{L}(\mathbf{u})\mathbf{u}'$ and $\dot{R} = R'/R$

$$\dot{\mathbf{R}} = 2\mathcal{L}(\mathbf{u})\mathbf{u}'/R$$

$\dot{\mathbf{R}}^T = 2\mathbf{u}'\mathcal{L}^T(\mathbf{u})/R$ and $\mathcal{L}^T(\mathbf{u})\mathcal{L}(\mathbf{u}) = R\mathbf{I}$ give

$$\dot{\mathbf{R}}^T \cdot \dot{\mathbf{R}} = 4\mathbf{u}' \cdot \mathbf{u}'/R$$

From $\mathcal{L}'(\mathbf{u}) = \mathcal{L}(\mathbf{u}')$ we have $\mathbf{R}'' = 2\mathcal{L}(\mathbf{u})\mathbf{u}'' + 2\mathcal{L}(\mathbf{u}')\mathbf{u}'$

Final equation of motion, with $\mathbf{u} \cdot \mathbf{u} = R$

$$\mathbf{u}'' = \frac{1}{2}h\mathbf{u} + \frac{1}{2}R\mathcal{L}^T(\mathbf{u})\mathbf{F}_{kl}$$

Binding energy per unit reduced mass

$$h = [(2\mathbf{u}' \cdot \mathbf{u}' - (m_k + m_l)]/R$$

Rate of change from $\dot{\mathbf{R}} \cdot \ddot{\mathbf{R}}$

$$\frac{d}{dt}\left[\frac{1}{2}\dot{\mathbf{R}}^2 - \frac{(m_k + m_l)}{R}\right] = \dot{\mathbf{R}} \cdot \mathbf{F}_{kl}$$

Conversion by $h' = \mathbf{R}' \cdot \mathbf{F}_{kl}$ and $\dot{\mathbf{R}}$

$$h' = 2\mathbf{u}' \cdot \mathcal{L}^T(\mathbf{u})\mathbf{F}_{kl}$$

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

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

DTMIN , RMIN

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

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

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

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

GMIN

Hermite KS

Standard KS

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

New notation

$$\begin{aligned}
\mathbf{F}_{\mathrm{u}} &= \mathbf{u}'' \\
\mathbf{Q} &= \mathcal{L}^T\,\mathbf{P}\,,
\end{aligned}$$

with $\mathbf{P} = \mathbf{F}_{kl}$ as the perturbing force.

Basic equations

$$\begin{aligned}
\mathbf{F}_{\mathrm{u}} &= \frac{1}{2} h\,\mathbf{u} + \frac{1}{2} R\,\mathbf{Q} \\
h' &= 2\,\mathbf{u}' \cdot \mathbf{Q} \\
t' &= \mathbf{u} \cdot \mathbf{u}
\end{aligned}$$

Hermite $\mathbf{F}$, $\mathbf{F}'$ formulation

$$\begin{aligned}
\mathbf{F}_{\mathrm{u}} &= \frac{1}{2} h\,\mathbf{u} + \frac{1}{2} R\,\mathbf{Q} \\
\mathbf{F}'_{\mathrm{u}} &= \frac{1}{2}(h'\mathbf{u} + h\mathbf{u}' + R'\mathbf{Q} + R\mathbf{Q}') \\
h' &= 2\,\mathbf{u}' \cdot \mathbf{Q} \\
h'' &= 2\mathbf{F}_{\mathrm{u}} \cdot \mathbf{Q} + 2\mathbf{u}' \cdot \mathbf{Q}' \\
t' &= \mathbf{u} \cdot \mathbf{u}
\end{aligned}$$

The derivatives of $\mathbf{P}$, $\mathbf{Q}$ and t' are readily available. Note that $\mathbf{P}' = R\dot{\mathbf{P}}$ and that $\mathcal{L}^T(\mathbf{u}')$ can be obtained by substituting $\mathbf{u}'$ for $\mathbf{u}$. For implementation, significant accuracy can be gained by high-order prediction (not used in standard Hermite).

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

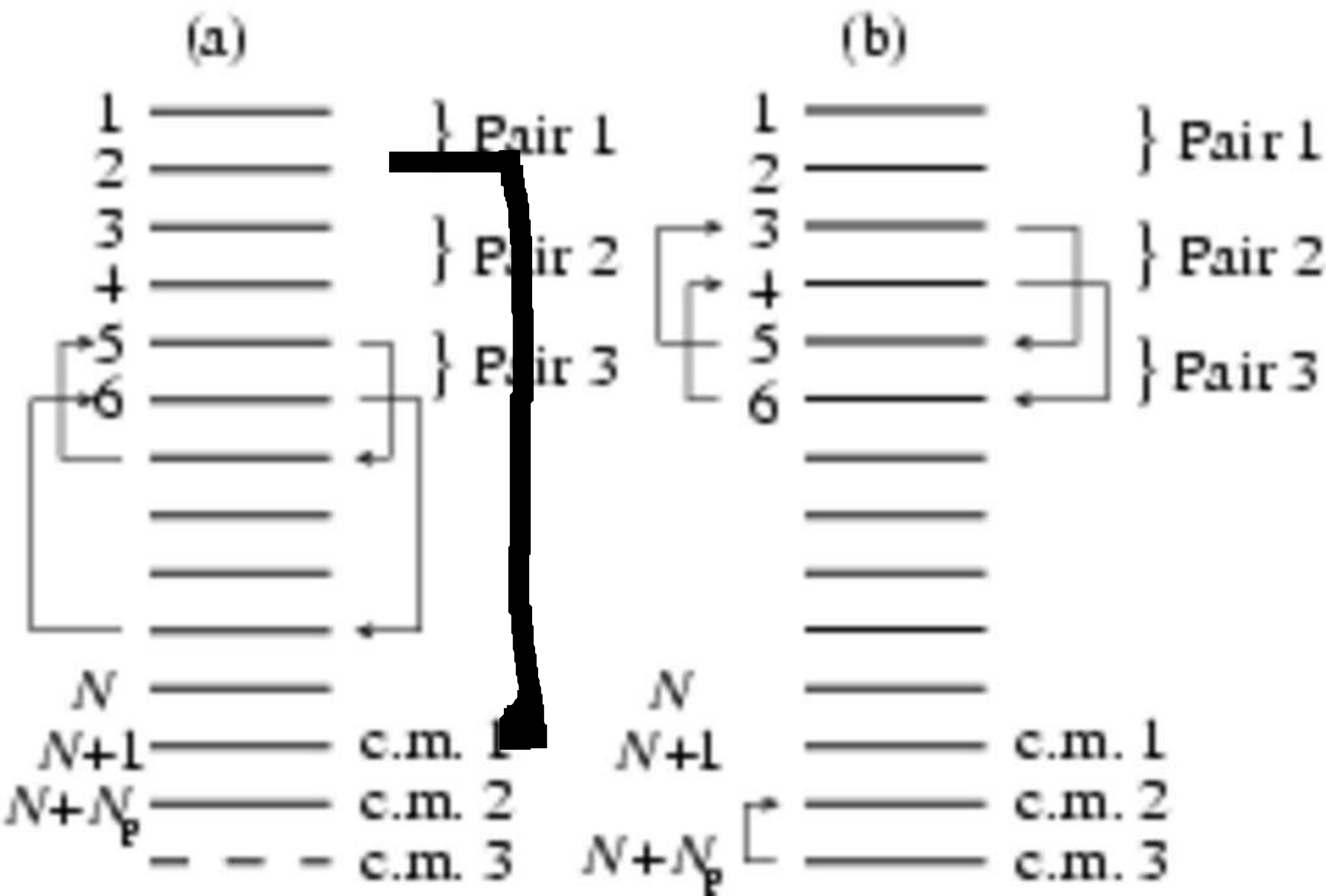
Practical Aspects of KS

Regular equations	Perturbed harmonic oscillator, $\gamma < 1$
Constant time-step	$\Delta\tau = \eta \left(\frac{1}{2\vert h\vert}\right)^{1/2}$ 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 Stability

Requirement	a_0 secularly constant
Kozai cycles	$e_{\text{max}} = \left(1 - 5cos^2 i/3\right)^{1/2}$
Candidates	$\Delta t_{\text{cm}} < \Delta t_{\text{cl}},\ a_1(1 - e_1) > 3a_0$
Restrictions	$\mu_1 M_{123}/2a_1 > E_{\text{hard}},\ \gamma_1 < 0.01$
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 $R_{\text{apo}} < P_{\text{crit}}$
Mass loss	Update h, $\mathbf{u}$, $\mathbf{u}'$, stability check
Termination	$\gamma > 0.1$, $R > R_{\text{cl}}$ or $\gamma > 0.25$
Re-initialize	Triple $\Rightarrow$ KS + m_3

Particles 1....N NPAIRS = 3; first single: 7=IF



Unperturbed Two-Body Motion

Maximum force:

$$j = \mathrm{max}_i \, (m_i / |\mathbf{r}_i - \mathbf{r}_{cm}|^2), \qquad i = 1, n$$

Smallest inverse travel time

$$\beta_s = \mathbf{r}_s \cdot \dot{\mathbf{r}}_s / r_s^2, \qquad \mathbf{r}_s - \mathbf{r}_{cm} \Rightarrow \mathbf{r}_s$$

Perturber boundary $\quad r_\gamma = R[2\tilde{m}/(m_b \gamma_{\mathrm{min}})]^{1/3}$

Travel time: $\qquad \dot{r}_s < 0, \quad \Delta t_{\mathrm{in}} = (r_s - r_\gamma)/|\dot{r}_s|$

Free-fall time $\quad \Delta t_a = [2\Delta t_{\mathrm{in}} \dot{r}_s r_s^2 / (m_b + m_s)]^{1/2}$

Return time of dominant body

$$\Delta t_j = [2(r_j - r_\gamma) r_j^2 / (m_b + m_j)]^{1/2}$$

Unperturbed time interval

$$\Delta t_\gamma = \mathrm{min} \, (\Delta t_{\mathrm{in}}, \Delta t_a, \Delta t_j, \Delta t_{cm})$$

Unperturbed periods $\quad K = 1 + \frac{1}{2} \Delta t_\gamma / t_K$

Final time interval $\qquad \Delta t = K \, \mathrm{min} \, (t_K, \Delta t_{\mathrm{cm}})$

Program Flow

New time	Determine block-step members
New procedures	Check output, new KS or HI
Regularization	Advance KS/chain up to t_{new}
Data structure	Repeat #1 on major change
Prediction	Neighbours or all particles
Integration	Advance block-step members
Stellar evolution	Mass loss or updating r^*
CPU time	Repeat cycle

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

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

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

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