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 transf. $u^2 = x, \;\; 2u'^2 + 2uu'' = x''$

Simplification $2uu'' = 2hx + M - 2u'^2 = hx$

Final equation $u'' = \frac{1}{2}hu$

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

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

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

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

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	$r_{\rm p} < \left(\dfrac{2m_{\rm p}}{m_{\rm b}\gamma_{\rm min}}\right)^{1/3} a\,(1+e)$
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	$\mathbf{F}_j,\ \dot{\mathbf{F}}_j,\ \Delta t_j,\quad j = k,\ l$

Close Encounters

Search for close companion $\Delta t_i < \Delta t_{\rm cl}$

Acceptance criterion $R < R_{\rm cl},\ \dot{R} < 0$

Define new two-body elements

$$
\begin{aligned}
P &= -\frac{2M}{R} + \frac{\mathbf{R}'^2}{R^2} \\
\mathbf{B} &= \frac{M\mathbf{R}}{R} - \frac{\mathbf{R}'^2\mathbf{R}}{R^2} + \frac{R'\mathbf{R}'}{R}
\end{aligned}
$$

Burdet–Heggie equations of motion

$$
\begin{aligned}
P' &= 2\mathbf{R}' \cdot \mathbf{F}\,, \\
\mathbf{B}' &= -2(\mathbf{R}' \cdot \mathbf{F})\mathbf{R} + (\mathbf{R} \cdot \mathbf{F})\mathbf{R}' + (\mathbf{R} \cdot \mathbf{R}')\mathbf{F}\,.
\end{aligned}
$$

Eccentricity vector $\mathbf{B} = -M\mathbf{e}$

Introduce c.m. as fictitious particle $i = N + 1$

Initialize c.m. motion $\mathbf{F}_{\rm cm},\ \dot{\mathbf{F}}_{\rm cm},\ \Delta t_{\rm cm}$

Advance regularized solution up to $t_{\rm reg} = t$

Flyby termination $R > R_0$

Collision test $R < r_1^* + r_2^*$

Treat any other particles & c.m. up to t

Escape removal or solar accretion $r_i > R_{\rm esc},\ \ e_i > 0.99$

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	$\mathbf{R} = \mathcal{L}\mathbf{u}, \quad \mathbf{r}_j = \mathbf{r}_{\rm cm} \pm \mu\mathbf{R}/m_j$
	$\dot{\mathbf{R}} = 2\mathcal{L}\mathbf{u}'/R, \quad \dot{\mathbf{r}}_j = \dot{\mathbf{r}}_{\rm cm} \pm \mu\dot{\mathbf{R}}/m_j$
Two-body elements	$a, \mathbf{J}, e$ for averaging & circularization

Three-Body Regularization

Initial conditions $\mathbf{r}_i,\ \mathbf{p}_i, \quad \mathbf{p}_3 = -(\mathbf{p}_1 + \mathbf{p}_2)$

Basic Hamiltonian $\mu_{k3} = \dfrac{m_k m_3}{m_k + m_3}$

$$H = \sum_{k=1}^{2} \frac{1}{2\mu_{k3}} \mathbf{p}_k^2 + \frac{1}{m_3} \mathbf{p}_1 \cdot \mathbf{p}_2 - \frac{m_1 m_3}{R_1} - \frac{m_2 m_3}{R_2} - \frac{m_1 m_2}{R}$$

KS transformations $\mathbf{Q}_k^2 = R_k\,, \quad \mathbf{P}_k^2 = 4 R_k \mathbf{p}_k^2, \quad (k = 1, 2)$

Time transformation $dt = R_1 R_2\, d\tau$

Regularized Hamiltonian $\Gamma^* = R_1 R_2\, (H - E_0)$

$$\Gamma^* = \sum_{k=1}^{2} \frac{1}{8\mu_{k3}} R_{3-k}\, \mathbf{P}_k^2 + \frac{1}{16 m_3} \mathbf{P}_1^T \mathbf{A}_1 \cdot \mathbf{A}_2^T \mathbf{P}_2$$

$$- m_1 m_3 R_2 - m_2 m_3 R_1 - \frac{m_1 m_2 R_1 R_2}{|\mathbf{R}_1 - \mathbf{R}_2|} - E_0 R_1 R_2$$

Equations of motion

$$\frac{d\mathbf{Q}_k}{d\tau} = \frac{\partial \Gamma^*}{\partial \mathbf{P}_k}, \qquad \frac{d\mathbf{P}_k}{d\tau} = -\frac{\partial \Gamma^*}{\partial \mathbf{Q}_k}$$

Regular solutions: $R_1 \rightarrow 0$ or $R_2 \rightarrow 0$

Singular term $<$ regular terms: $|\mathbf{R}_1 - \mathbf{R}_2| > \max(R_1, R_2)$

Three-Body Transformations

Coordinates & momenta $\quad \mathbf{q}_k = \tilde{\mathbf{q}}_k - \tilde{\mathbf{q}}_3, \quad \mathbf{p}_k = \tilde{\mathbf{p}}_k$

Regularized coordinates ($q_1 \geq 0$)

$$\begin{aligned} Q_1 &= [\tfrac{1}{2}(|\mathbf{q}_1| + q_1)]^{1/2} \\ Q_2 &= \tfrac{1}{2} q_2 / Q_1 \\ Q_3 &= \tfrac{1}{2} q_3 / Q_1 \\ Q_4 &= 0 \end{aligned}$$

Regularized momenta $\quad \mathbf{P}_k = \mathbf{A}_k \, \mathbf{p}_k$

Basic matrix

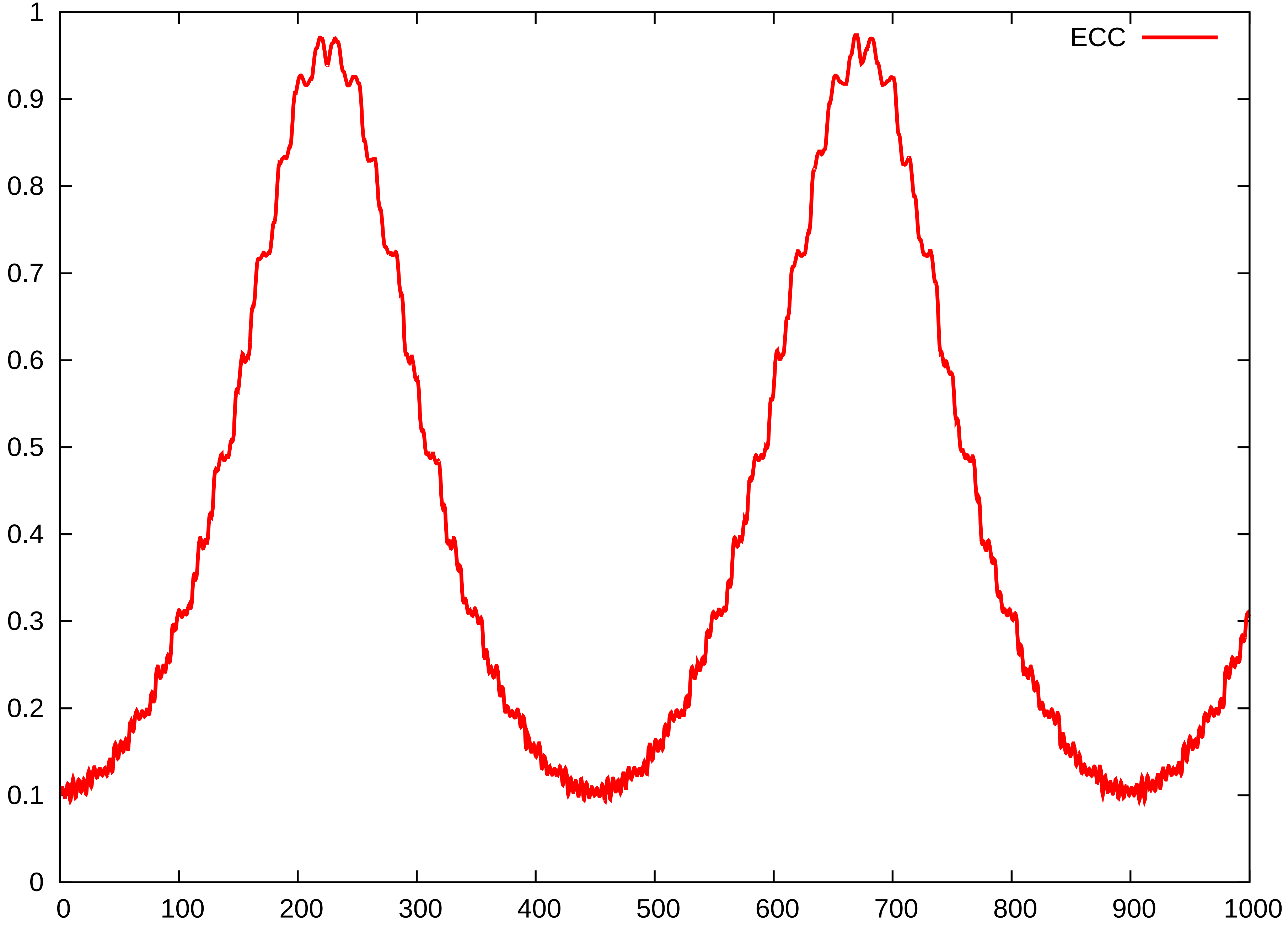
$$\mathbf{A}_1 = 2 \begin{bmatrix} Q_1 & Q_2 & Q_3 & Q_4 \\ -Q_2 & Q_1 & Q_4 & -Q_3 \\ -Q_3 & -Q_4 & Q_1 & Q_2 \\ Q_4 & -Q_3 & Q_2 & -Q_1 \end{bmatrix}$$

KS transformations $\quad \mathbf{q}_k = \tfrac{1}{2} \mathbf{A}_k^{\mathrm{T}} \mathbf{Q}_k$

Physical momenta $\quad \mathbf{p}_k = \tfrac{1}{4} \mathbf{A}_k^{\mathrm{T}} \mathbf{P}_k / R_k$

Coordinates & momenta

$$\begin{aligned} \tilde{\mathbf{q}}_3 &= -\sum_{k=1}^{2} m_k \mathbf{q}_k / M \\ \tilde{\mathbf{q}}_k &= \tilde{\mathbf{q}}_3 + \mathbf{q}_k \\ \tilde{\mathbf{p}}_k &= \mathbf{p}_k \\ \tilde{\mathbf{p}}_3 &= -(\mathbf{p}_1 + \mathbf{p}_2) \qquad (k = 1, 2) \end{aligned}$$



ECC
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