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 coordinate transformation $\mathbf{Q}_k^2 = R_k\,, \quad (k = 1, 2)$

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

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 $\mathbf{P}_k = \mathbf{A}_k \, \mathbf{p}_k$

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 $\mathbf{q}_k = \frac{1}{2}\mathbf{A}_k^{\mathrm{T}}\mathbf{Q}_k$

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

Coordinates & momenta

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

Perturbed Three-Body Regularization

Regularized Hamiltonian

$$\Gamma^* = R_1 R_2 (H_3 + \mathcal{R} - E)\,, \quad E_3 = E - \mathcal{R}$$

New equations of motion

$$\frac{d\mathbf{Q}_k}{d\tau} = \frac{\partial (R_1 R_2 H_3)}{\partial \mathbf{P}_k}$$

$$\frac{d\mathbf{P}_k}{d\tau} = -(H_3 - E_3)\frac{\partial (R_1 R_2)}{\partial \mathbf{Q}_k} - R_1 R_2 \frac{\partial}{\partial \mathbf{Q}_k}(H_3 + \mathcal{R})$$

External perturbation for Plummer model

$$\frac{\partial \mathcal{R}}{\partial \mathbf{Q}_k} = \sum_{i=1}^{3} \frac{\partial \mathcal{R}}{\partial \mathbf{r}_i}\frac{\partial \mathbf{r}_i}{\partial \mathbf{q}_k}\frac{\partial \mathbf{q}_k}{\partial \mathbf{Q}_k}\,, \qquad \frac{\partial \mathcal{R}}{\partial \mathbf{r}_i} = -\frac{m_i M_{\rm p} \mathbf{r}_i}{(r_i^2 + \epsilon^2)^{3/2}}$$

Transformations and c.m. condition $\mathbf{r}_{\rm cm} = \sum m_i \mathbf{r}_i / M$

$$\mathbf{r}_1 = \mathbf{r}_{\rm cm} + (m_2 + m_3)\mathbf{q}_1/M - m_2 \mathbf{q}_2/M$$

$$\mathbf{r}_2 = \mathbf{r}_{\rm cm} - m_1 \mathbf{q}_1/M + (m_1 + m_3)\mathbf{q}_2/M$$

$$\mathbf{r}_3 = \mathbf{r}_{\rm cm} - m_1 \mathbf{q}_1/M - m_2 \mathbf{q}_2/M$$

Application of $\partial \mathbf{r}_i / \partial \mathbf{q}_k$ yields mass ratios

Motion of c.m. $$\frac{d\mathbf{v}_{\rm cm}}{d\tau} = -R_1 R_2 M_{\rm p} \sum \frac{m_i \mathbf{r}_i}{(r_i^2 + \epsilon^2)^{3/2}}$$

Basic transformation $\mathbf{q}_k = \mathbf{A}_k^{\mathrm{T}}\mathbf{Q}_k/2$ gives $\partial\mathbf{q}_k/\partial\mathbf{Q}_k = \mathbf{A}_k$

Combining terms

$$\frac{\partial\mathcal{R}}{\partial\mathbf{Q}_k} = -\frac{\mathbf{A}_k m_k}{M}[m_l(\mathbf{F}_k - \mathbf{F}_l) + m_3(\mathbf{F}_k - \mathbf{F}_3)]\,, \quad l = 3-k$$

Internal energy change

$$\frac{dE_3}{d\tau} = -\frac{d\mathcal{R}}{d\tau}$$

Conversion to known expressions

$$\frac{d\mathcal{R}}{d\tau} = \sum_{k=1}^{2}\frac{\partial\mathcal{R}}{\partial\mathbf{Q}_k}\frac{d\mathbf{Q}_k}{d\tau}$$

Substitution $\quad \dfrac{d\mathbf{Q}_k}{d\tau} = \dfrac{1}{4\mu_{k3}}R_l\mathbf{P}_k + \dfrac{1}{16m_3}\mathbf{A}_k\mathbf{A}_l^{\mathrm{T}}\mathbf{P}_l$

Orthogonality condition

$$\mathbf{A}_k\mathbf{A}_k^{\mathrm{T}} = 4R_k$$

Final energy derivative

$$\frac{d\mathcal{R}}{d\tau} = -\frac{1}{4}\sum_{k=1}^{2}R_l\mathbf{P}_k^{\mathrm{T}}\mathbf{A}_k(\mathbf{F}_k - \mathbf{F}_3)$$

Note $\partial\mathcal{R}/\partial\mathbf{Q}_k$ used for $\mathbf{P}_k'$ and E_3'

Consistency check: $\quad \Delta E = H_3 - E_3$

Post-Newtonian Terms

Equation of motion
$$\frac{d^2\mathbf{r}}{dt^2} = \frac{M}{r^2}\left[(-1+A)\frac{\mathbf{r}}{r} + B\mathbf{v}\right]$$

First-order precession
$$M = m_1 + m_2, \quad \eta = \frac{m_1 m_2}{M^2}$$
$$A_1 = 2(2+\eta)\frac{M}{r} - (1+3\eta)v^2 + \frac{3}{2}\eta\dot{r}^2$$
$$B_1 = 2(2-\eta)\dot{r}$$

Higher-order precession
$$A_2 = ..., \quad B_2 = ..., \quad A_3 = ..., \quad B_3 = ...$$

Gravitational radiation
$$A_{5/2} = \frac{8}{5}\eta\frac{M}{r}\dot{r}\left(\frac{17M}{3r} + 3v^2\right)$$
$$B_{5/2} = -\frac{8}{5}\eta\frac{M}{r}\left(3\frac{M}{r} + v^2\right)$$

Total GR perturbation
$$\mathbf{P}_{GR} = \frac{M}{c^2 r^2}\left[(A_1 + \frac{A_2}{c^2} + \frac{A_{5/2}}{c^3})\frac{\mathbf{r}}{r} + (B_1 + \frac{B_2}{c^2} + \frac{B_{5/2}}{c^3})\mathbf{v}\right]$$

Radiation energy loss
$$\Delta E_{GR} = \frac{m_1 m_2}{M}\int \mathbf{P}_{GR}\cdot\mathbf{v}\,dt$$

PN splitting
$$\mathbf{P}_k = \frac{m_3}{m_k + m_3}\mathbf{P}_{GR}, \quad \mathbf{P}_3 = -\frac{m_k}{m_k + m_3}\mathbf{P}_{GR}$$

Derivatives
$$\mathbf{P}_k' = -t'\frac{\partial\mathcal{R}}{\partial\mathbf{Q}_k}, \quad E_3' = -\sum_{k=1}^{2}\mathbf{Q}_k'\cdot\frac{\partial\mathcal{R}}{\partial\mathbf{Q}_k}$$

PN Implementation

Energy $$\epsilon_b = \epsilon_0 + \frac{\epsilon_1}{c^2} + \frac{\epsilon_2}{c^4} + \frac{\epsilon_3}{c^6} \qquad a = -\frac{M}{2\epsilon_b}$$

$$\epsilon_0 = \frac{1}{2}V^2 - \frac{M}{R}, \qquad a = -\frac{M}{2\epsilon_b}$$

$$\epsilon_1 = \frac{1}{2}\frac{M}{R} + \frac{3}{8}(1-3\eta)V^4 + \frac{1}{2}\left((3+\eta)V^2 + \eta\dot{R}^2\right)\frac{M}{R}$$

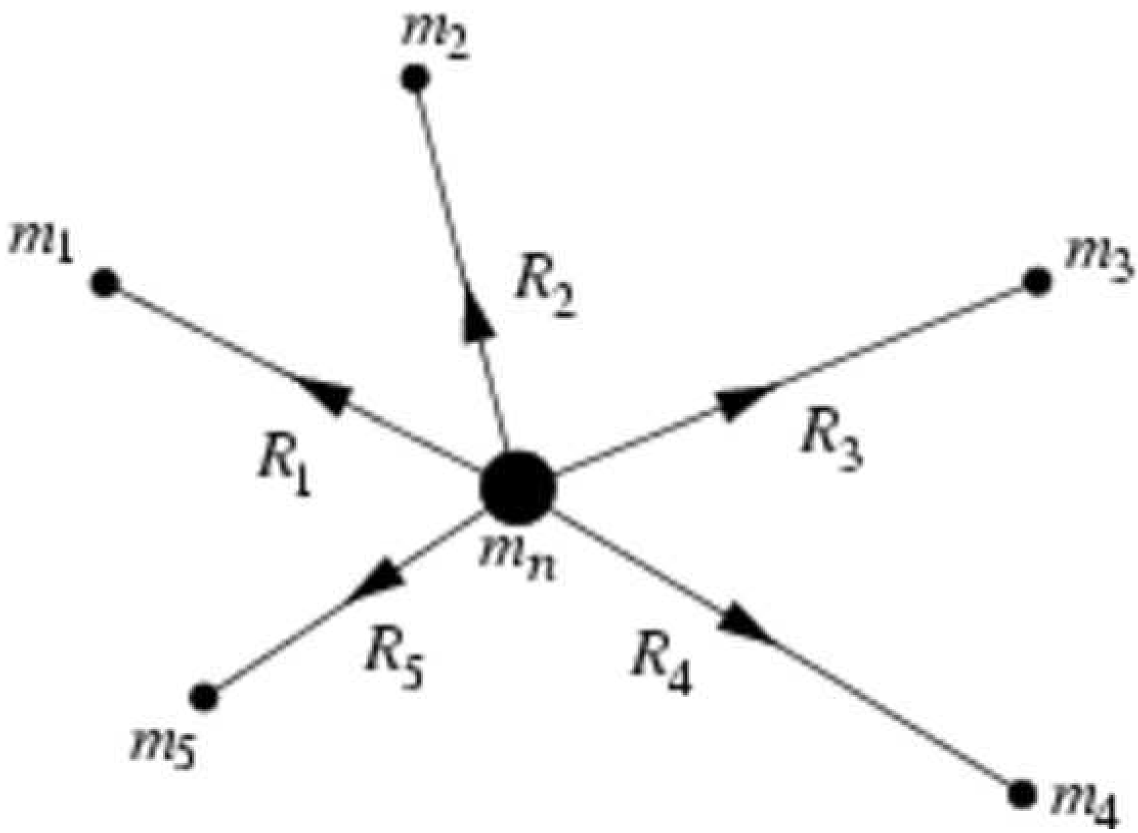
$$\eta = \frac{m_1 m_2}{M^2}$$

Lenz vector $$\mathbf{e} = \mathbf{V} \times \mathbf{R} \times \mathbf{V}/M - \mathbf{R}/R$$

Periapse advance $$\Delta\omega = \frac{6\pi M}{c^2 a(1-e^2)}$$

PN2.5 $$\tau_{GR} = \frac{5g(e)}{64}\frac{a^4 c^5}{X(1+X)m_3^3}, \qquad X = \frac{m_k}{m_3}$$

$$g(e) \simeq \frac{(1-e^2)^{7/2}}{4.5}$$



m_2
m_1
R_2
m_3
R_1
R_3
m_n
R_5
R_4
m_5
m_4

Wheel-Spoke Regularization   Zare 1972

Initial conditions $\quad m_i,\ \tilde{\mathbf{q}}_i,\ \tilde{\mathbf{p}}_i,\quad i = 0, \ldots, n, \qquad \sum_{i=0}^{n} \tilde{\mathbf{p}}_i = 0$

Coordinates and momenta $\quad \mathbf{q}_i = \tilde{\mathbf{q}}_i - \tilde{\mathbf{q}}_0, \qquad \mathbf{p}_i = \tilde{\mathbf{p}}_i - \tilde{\mathbf{p}}_0$

Hamiltonian $\quad H = \sum_{i=1}^{n} \frac{\mathbf{p}_i^2}{2\mu_i} + \frac{1}{m_0} \sum_{i<j}^{n} \mathbf{p}_i^{\mathrm{T}} \cdot \mathbf{p}_j - m_0 \sum_{i=1}^{n} \frac{m_i}{R_i} - \sum_{i<j}^{n} \frac{m_i m_j}{R_{ij}}$

Separable W function $\quad W(\mathbf{p}_i, \mathbf{Q}_i) = \sum_{i=1}^{n} \mathbf{p}_i^{\mathrm{T}} \cdot \mathbf{f}_i(\mathbf{Q}_i)$

Canonical relations $\quad \mathbf{q}_k = \partial W / \partial \mathbf{p}_k\,, \quad \mathbf{P}_k = \partial W / \partial \mathbf{Q}_k$

Regularized momenta $\quad \mathbf{P}_i = \mathbf{A}_i \mathbf{p}_i,$ Levi-Civita matrix

Inverse transformations $\quad \mathbf{q}_i = \frac{1}{2} \mathbf{A}_i^{\mathrm{T}} \mathbf{Q}_i, \qquad \mathbf{p}_i = \frac{1}{4} \mathbf{A}_i^{\mathrm{T}} \mathbf{P}_i / R_i$

Time transformation $\quad t' = 1/L, \quad L = T + U$

Regularized Hamiltonian $\quad \Gamma^* = t'(H - E)$

Local coordinates & momenta

$$
\begin{aligned}
\tilde{\mathbf{q}}_0 &= -\sum_{i=1}^{n} m_i \mathbf{q}_i \Big/ \sum_{i=0}^{n} m_i \\
\tilde{\mathbf{q}}_i &= \tilde{\mathbf{q}}_0 + \mathbf{q}_i \\
\tilde{\mathbf{p}}_i &= \mathbf{p}_i\,, \qquad\qquad (i = 1, \ldots, n) \\
\tilde{\mathbf{p}}_0 &= -\sum_{i=1}^{n} \mathbf{p}_i
\end{aligned}
$$

Wheel-Spoke Implementation

Select members	$\Delta t_{\rm cm} < \Delta t_{\rm cl}, \quad R < R_{\rm cl}$
Initialize in local c.m.	$\sum m_i \mathbf{r}_i, = 0, \quad \sum m_i \dot{\mathbf{r}}_i = 0$
Chain indices & vectors	$\mathbf{Q}, \mathbf{P}, \quad N_{\rm eq} = 8\,(N-1)$
Define useful quantities	$T_{\rm cr} = \left(\frac{r_1^3}{M}\right)^{1/2}, \quad R_{\rm grav} = \sum_{i<j} \frac{m_i m_j}{\vert E\vert}$
Softening of singularities	$\epsilon = f\,R_{\rm grav}, \quad \Rightarrow E = {\rm const}$
Form perturber list	$r_{\rm p} < \left(\frac{2m_{\rm p}}{M\gamma_0}\right)^{1/3} R_{\rm grav}$
Check time-step	$\Delta\tau = \int L\,dt, \quad L = T - \Phi$
Perturber prediction	$\mathbf{r}_i = ((\frac{1}{6}\dot{\mathbf{F}}_i\delta t_i + \frac{1}{2}\mathbf{F}_i)\delta t_i + \dot{\mathbf{r}}_i)\delta t_i$
Physical variables	$\mathbf{R}_k = \frac{1}{2}\mathbf{A}_k\,\mathbf{Q}_k, \quad \mathbf{p}_k = \frac{1}{4}\frac{\mathbf{A}_k\,\mathbf{P}_k}{\mathbf{Q}_k^2}$
Overall perturbation	$\gamma = \frac{2m_{\rm p}}{M}\left(\frac{R_{\rm grav}}{r_{\rm p}}\right)^3$
Addition of member	$\gamma > 0.05 m_{\rm p}/m_0, \quad r_{\rm p} \leq \sum R_k$
Removal of member	$\dot{r}^2 > 2M/r, \quad r > R_{\rm cl}, \quad \dot{r} > 0$
Continue N-body integration	$t > t_{\rm max} = t_{\rm blk}$

Decision-Making

Perturber selection $d < \left[\frac{2m_j}{m_0\gamma_0}\right]^{1/3} R_{\rm grav}\,, \quad \gamma_0 = 10^{-6}$

Membership $d < 2R_{\rm cl}\,, \quad \dot{d} < 0\,, \quad N_{\rm ch} < 7, \quad N_{\rm pert} \simeq 10$

Progressive time-scales

2.5PN for $\tau_{\rm GR} < 1000$

1PN for $\tau_{\rm GR} < 100$

2PN for $\tau_{\rm GR} < 50$

3PN for $\tau_{\rm GR} < 10$

Kozai cycle $T_{\rm Kozai} = \frac{T_1^2}{T_0}\left(\frac{1+q}{q}\right)(1-e_1^2)^{3/2}\, g(e_0,\omega_0,\psi)$

Time-scale $T_{\rm Kozai} < 10, \qquad \Rightarrow 2PN$ if less

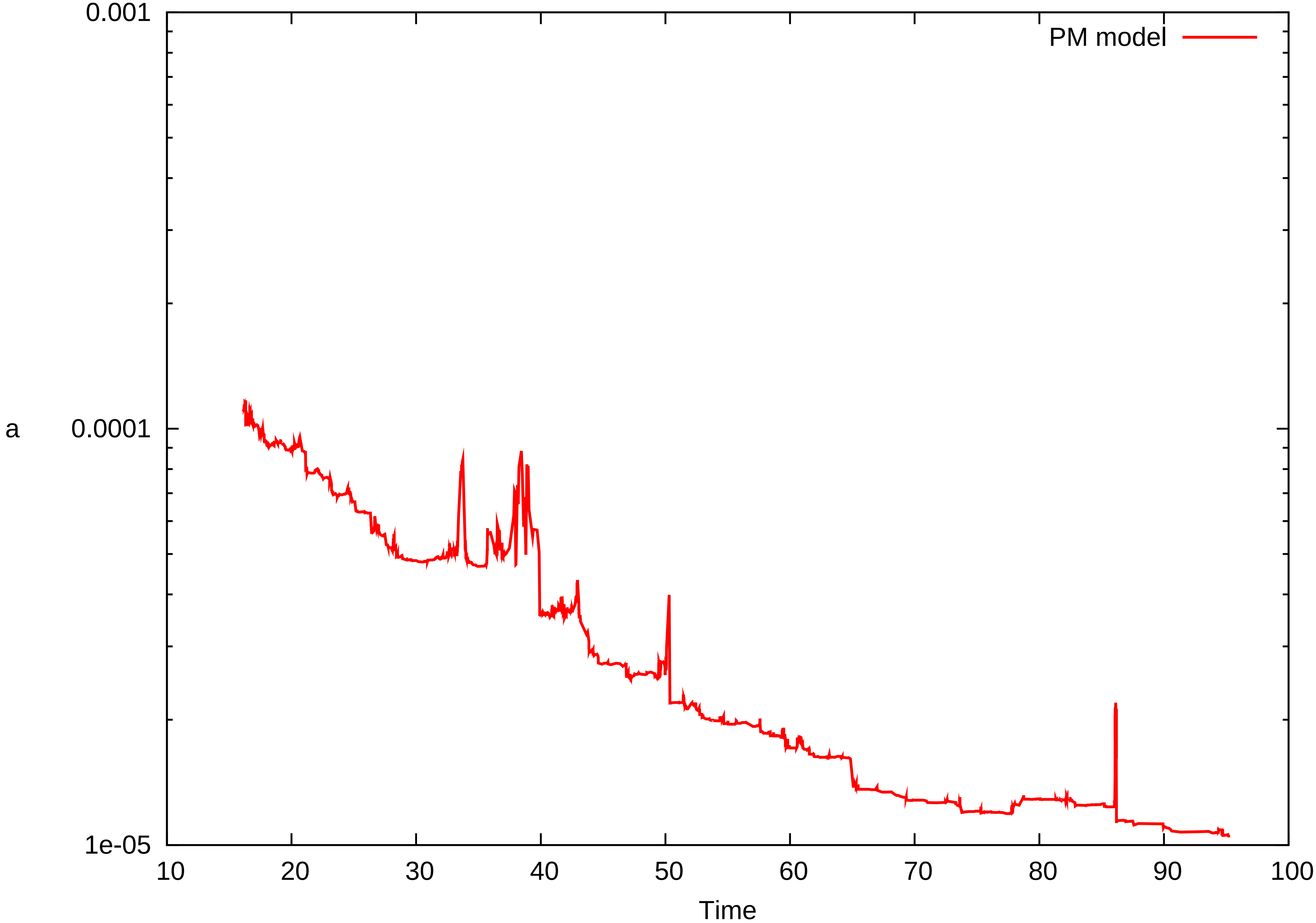
IMBH modelling $N = 10^5, \quad m_0 = 300\, M_\odot$

Scaling $V^* = \frac{3\times 10^5}{c}, \qquad V^* = 12\ km\ s^{-1}$

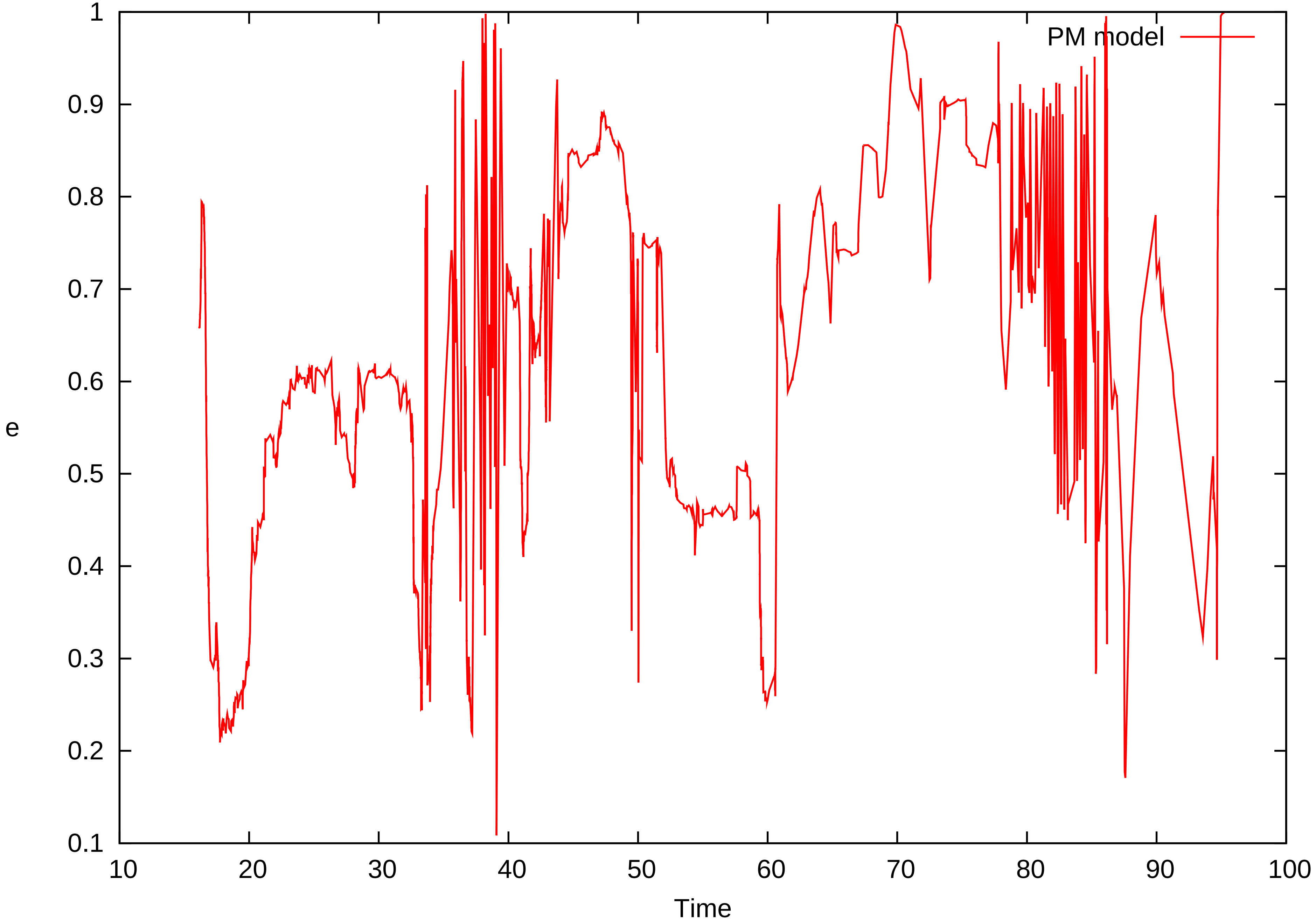
Profiling with GRAPE-6

Wheel-spoke: 6.5 % of CPU

N-body part: 14 % of CPU



0.001
0.0001
1e-05
a
10
20
30
40
50
60
70
80
90
100
Time
PM model



PM model
e
Time
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
10
20
30
40
50
60
70
80
90
100

GPU/SSE with NBODY6

Version	Regular force	Irregular force
Standard	1 cpu	1 cpu
OpenMP	4 cpu	4 cpu
OpenMP + SSE	4 cpu + SIMD	4 cpu ***
GPU	1 cpu + GPU	4 cpu ***

***: irregular force in parallel & REAL*8

GPU: regular force accumulated in REAL*8

GPU: neighbour lists and fast potential

Extra Routines

gpunb.xxx: main routine for GPU & SSE

intgrt.omp.f: predictions and flow control

gpcorr.f: regular force corrector & time-step

nbintp.f: parallel irregular force & corrector

cnbint.f: used by nbintp.f (C++)

gpupot.xx: fast potential for GPU or SSE

phicor.f: differential corrections of potentials

energy2.f: total energy from potentials

$$\frac{\Delta\Phi}{\Phi} \simeq 1 \times 10^{-8}, \quad N = 5 \times 10^{4}$$

GPU/SSE Comparison

N	GPU	SSE
16000	37 s	51 s
32000	120 s	186 s
64000	467 s	810 s
100000	1600 s	

$T = 2.0 \rightarrow 4.0$, $f(m)$, Plummer model

GRAPE6: $N = 64\,K$, $CPU = 480\,\mathrm{s}$

NBODY6: $N = 64\,K$, $CPU = 13600\,\mathrm{s}$