



Wheel-Spoke Regularization

Initial conditions $m_i, \tilde{\mathbf{q}}_i, \tilde{\mathbf{p}}_i, \quad i = 0, \dots, N$

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

Variables
$$W(\mathbf{p}_i, \mathbf{Q}_i) = \sum_{i=1}^N \mathbf{p}_i^T \cdot \mathbf{f}_i(\mathbf{Q}_i)$$

Momenta $\mathbf{P}_i = \mathbf{A}_i \mathbf{p}_i, \quad (i = 1, \dots, N)$

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

Wheel-Spoke Implementation

Select members $\Delta t_{\text{cm}} < \Delta t_{\text{cl}}, \quad R = a(1+e)$

Initialize $\sum m_i \mathbf{r}_i = 0, \quad \sum m_i \dot{\mathbf{r}}_i = 0$

Create spokes $\mathbf{Q}, \mathbf{P}, \quad N_{\text{eq}} = 8N$

Perturber list $d < \left(\frac{2m}{M_{\text{ch}} \gamma_0} \right)^{1/3} R_{\text{grav}}$

Prediction $\mathbf{r}_i = \left(\left(\frac{1}{6} \dot{\mathbf{F}}_i \delta t_i + \frac{1}{2} \mathbf{F}_i \right) \delta t_i + \dot{\mathbf{r}}_i \right) \delta t_i$

Add member $\gamma > 0.01, \quad r_p \leq \sum R_k$

Escape $\dot{R}^2 > 2M/R, \quad R > R_{\text{cl}}$

Decision-Making

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

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

Progressive time-scales

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

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

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

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

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

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

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

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

Profiling with GRAPE-6

Wheel-spoke: 6.5% of CPU

N-body part: 14% of CPU

Chain Regularization

Chain vectors $\mathbf{R}_k = \mathbf{r}_{k+1} - \mathbf{r}_k; \quad k = 1, \dots, N - 1$

Physical momenta $\mathbf{p}_k = m_k \mathbf{v}_k; \quad k = 1, \dots, N$

Relative momenta $\mathbf{W}_k = \mathbf{W}_{k-1} - \mathbf{p}_k; \quad k = 2, \dots, N - 2$

Hamiltonian

$$H = \frac{1}{2} \sum_{k=1}^{N-1} \left(\frac{1}{m_k} + \frac{1}{m_{k+1}} \right) \mathbf{W}_k^2 - \sum_{k=2}^{N-1} \frac{1}{m_k} \mathbf{W}_{k-1} \cdot \mathbf{W}_k - \sum_{k=1}^{N-1} \frac{m_k m_{k+1}}{R_k} - \sum_{1 \leq i \leq j-2}^N \frac{m_i m_j}{R_{ij}}$$

Equations of motion

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

KS relations $\mathbf{R}_k = \mathcal{L}_k \mathbf{Q}_k; \quad \mathbf{W}_k = \mathcal{L}_k \mathbf{P}_k / 2\mathbf{Q}_k^2$

Time transformation $dt = g d\tau; \quad g = 1/L$

Regularized Hamiltonian $\Gamma^* = g(H - E)$

Regular solutions $R_k \rightarrow 0; \quad k = 1, \dots, N - 1$

Chain Decision-Making

Perturber search	$R = a(1 + e), \quad \Delta t_{\text{cm}} < \Delta t_{\text{cl}}$
Selection criterion	$d_j < R_{\text{cl}}, \quad \dot{d}_j < 0, \quad j \leq N \text{ or } j > N$
Binary termination	$\text{KS} \Rightarrow \text{S} + \text{S}, \quad t = t_{\text{block}}$
Chain initialization	\mathbf{Q}, \mathbf{P} from $m_i, \mathbf{r}_i, \dot{\mathbf{r}}_i$
Time inversion	$\Delta\tau = \int L dt, \quad \Delta t = t_{\text{max}} - t$
Slow-down procedure	$\gamma = \frac{8a^3}{m_b} \sum \frac{m_j}{r_{ij}^3}, \quad \kappa = \left(\frac{\gamma_0}{\gamma}\right)^{1/2}$
Collision test	$\min \{R_k\} < f \max(r_k^*, r_{k+1}^*)$
Addition of member	$\sum R_k + d_j < R_{\text{cl}}, \quad \dot{d}_j < 0$
Escape	$\frac{1}{2}\dot{d}^2 - M/d > 0, \quad d > R_{\text{cl}}, \quad \dot{d} > 0$
Termination	$\max \{R_j\} > R_{\text{cl}}, \quad \dot{R}_k > 0$
Stability check	$\text{B} + \text{B} \Rightarrow \text{T} + \text{S}, \quad a_{\text{out}}(1 - e_{\text{out}}) > \Psi a_{\text{in}}$
Time quantization	$t_{\text{new}} = t_{\text{prev}} + [(t - t_{\text{block}})/\delta t] \delta t$
Re-initialization	$R_{ij}^2 \Rightarrow \text{KS} + \text{S} + \text{S}, \text{ or } \text{KS} + \text{KS} + \text{S}$

Chain Procedures

Initialize in c.m. frame	$\sum m_i \mathbf{r}_i = 0, \quad \sum m_i \dot{\mathbf{r}}_i = 0$
Total energy of subsystem	$E = \frac{1}{2} \sum m_i \mathbf{v}_i^2 - \sum \frac{m_i m_j}{r_{ij}}$
Select chain indices & vectors	$\mathbf{Q}, \mathbf{P}, \quad N_{\text{eq}} = 8(N - 1)$
Define useful quantities	$T_{\text{cr}}, R_{\text{grav}}, \Delta\tau_0$
Form perturber list	$d < \left(\frac{2m}{M_{\text{ch}} \gamma_0} \right)^{1/3} R_{\text{grav}}$
Check time-step	$\Delta\tau = \int L dt, \quad L = T - \Phi$
B-S integration step	Tolerance 10^{-12}
Perturber prediction	$\mathbf{r}_i = \left(\left(\frac{1}{6} \dot{\mathbf{F}}_i \delta t_i + \frac{1}{2} \mathbf{F}_i \right) \delta t_i + \dot{\mathbf{r}}_i \right) \delta t_i + \mathbf{r}_0$
Transform to physical variables	$\mathbf{R}_k = \mathcal{L} \mathbf{Q}_k, \quad \mathbf{W}_k = \frac{\mathcal{L} \mathbf{P}_k}{2 \mathbf{Q}_k^2}$
Check slow-down & switching	$\gamma < \gamma_0, \quad R_{12} < \max(R_1, R_2)$
Termination test	$\dot{R}^2 > 2M/R, \quad R > R_{\text{cl}}$
Chain as decision tool	$a \dots b \dots c \dots d$
Continue N -body integration	$t > t_{\text{max}} = t_{\text{blk}}$

A Dynamical Zoo

(a) Concepts

Single stars	S
Binaries	B
Long-lived triples	$T = [B,S]$
Quadruples	$Q = [B,B]$
Higher-order systems	$H = [T,T]$
Ghosts	G

(b) Treatments

- S: Basic integration
- B: Relative two-body motion and c.m. integration
- T: Outer orbit around inner c.m. and c.m. integration
- Q: Two binaries in relative orbit, etc.
- G: Skip integration

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	1 CPU *
GPU2	1 CPU + 2GPU	1 CPU *

*: irregular force in parallel C++ & Real*4/8

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 Optimization

Simplified neighbour definition

Stabilization of neighbour number

Parallel neighbour force on host

Parallel perturbing force

Enforced KS regularization

Neighbour change and corrections

KS candidates from small blocks

Potential energy on GPU

Randomized particle swapping

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: $N = 64 K$, $CPU = 480 s$

NBODY6: $N = 64 K$, $CPU = 13600 s$

