Regularization of Motion in the N-Body Problem

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Hamiltonian
$$H = T - U$$

Logarithmic Hamiltonian
$$\Lambda = \ln(T + B) - \ln(U)$$

Functional Hamiltonian
$$\Phi = f(T + B) - f(U)$$

Regularising Time Transformation(s)
$$t' = \frac{1}{\alpha U + \beta \Omega + \gamma} = \frac{1}{\alpha(T+B) + \beta\omega + \gamma}$$

1 THE PROBLEM

In N-Body systems close encounters are inevitable. Consequently the r^{-2} singularity in the relative motion equation

$$\ddot{\mathbf{r}} = -m\mathbf{r}/r^3 + \mathbf{f}(\mathbf{r}, t, ..)$$

needs to be removed by some regularization technique.

Today several ways to handle this situation are known: one may use coordinate and time transformations or Hamiltonian manipulation combined with a suitable regular algorithm. Almost always it is necessary to improve the accuracy by use of the extrapolation method in which data from a basic algorithm are used to estimate the results at zero stepsize.

2 TIME TRANSFORMATIONS

2.1 Poincare's Time Transformation

More than a century ago Poincare introduced a technique to transform the independent variable, in a Hamiltonian system.

Let $H(\mathbf{p}, \mathbf{q}, t)$ be a Hamiltonian. Take the time to be a canonical coordinate (t) by adding the momentum of time B to the Hamiltonian. Thus we have, in the extended phase space, the homogeneous Hamiltonian

$$H_h = H(\mathbf{p}, \mathbf{q}, t) + B, \tag{1}$$

If initially $B = -H$, then numerically $H_h(t) = 0$ along the entire trajectory. This is a consequence of the additional canonical equations

$$t' = \frac{\partial H_h}{\partial B} = 1, \quad B' = -\frac{\partial H_h}{\partial t}$$

and/or the fact that H_h does not depend on the independent variable.

leads to the new Hamiltonian

$$\Gamma = g\, H_h = g(\mathbf{p}, \mathbf{q})\, [H(\mathbf{p}, \mathbf{q}, t) + B]. \tag{2}$$

The time evolution of this new system is measured by the new independent variable s. Now

$$t' = \frac{\partial \Gamma}{\partial B} = g \quad \text{and} \quad \mathbf{q}' = \frac{\partial \Gamma}{\partial \mathbf{p}} = g\frac{\partial H}{\partial \mathbf{p}} + \frac{\partial g}{\partial \mathbf{p}} H_h, \tag{3}$$

and similarly

$$\mathbf{p}' = -\frac{\partial \Gamma}{\partial \mathbf{q}} = g\frac{\partial H}{\partial \mathbf{q}} + \frac{\partial g}{\partial \mathbf{q}} H_h. \tag{4}$$

Since $H_h = 0$ along the trajectory, dropping the zero terms and and forming

$$\dot{\mathbf{q}} = \mathbf{q}'/t' = \frac{\partial H}{\partial \mathbf{p}} \quad \text{and} \quad \dot{\mathbf{p}} = \mathbf{p}'/t' = -\frac{\partial H}{\partial \mathbf{q}}$$

one gets back the original Hamiltonian equations and concludes that the time transformed Hamiltonian (2) is equivalent to the original one.

2.2 KS-Transformation

The one-dimensional analogue of what is known as the KS (Kustaanheimo-Stiefel 1965) transformation is as follows: We have the Hamiltonian

$$H = p^2/2 - m/x$$

and with the transformation $x = Q^2$ the canonical point-transformation generating function is $S = px = pQ^2$, which gives

$$P = \frac{\partial S}{\partial Q} = 2pQ; \quad p = P/(2Q).$$

With the time transformation $g = |x| = Q^2$ we have

$$\Gamma = Q^2(\frac{1}{8}\frac{P^2}{Q^2} - \frac{m}{Q^2} + B) = \frac{1}{8}P^2 + BQ^2 - m,$$

i.e. a harmonic oscillator.

$$x + iy = (Q_1 + iQ_2)^2, \quad \text{or} \quad x = Q_1^2 - Q_2^2, \quad y = 2Q_1Q2$$

If the Hamiltonian is $H = \mathbf{p}^2/2 - M/r$, this transformation gives the new

$$H_h = \frac{1}{8}\mathbf{P}^2/Q^2 - M/Q^2 + B,$$

and after applying the time transformation $g = r = Q^2$, we have

$$\Gamma = \frac{1}{8}\mathbf{P}^2 + B\mathbf{Q}^2 - M.$$

which is a harmonic oscillator Hamiltonian.

2.3 KS-transformation in 3D

The KS-transformations between the 3-dimensional position and momentum $\mathbf{r}$ and $\mathbf{p}$ and the corresponding 4-dimensional KS-variables $\mathbf{Q}$ and $\mathbf{P}$ may be written

$$\mathbf{r} = \widehat{\mathbf{Q}}\mathbf{Q}; \;\; \mathbf{p} = \widehat{\mathbf{Q}}\mathbf{P}/(2Q^2). \tag{5}$$

Here $\widehat{\mathbf{Q}}$ is the KS-matrix (Stiefel & Scheifele 1971, p. 24)

$$\widehat{\mathbf{Q}} = \begin{pmatrix} Q_1 & -Q_2 & -Q_3 & Q_4 \\ Q_2 & Q_1 & -Q_4 & -Q_3 \\ Q_3 & Q_4 & Q_1 & Q_2 \\ Q_4 & -Q_3 & Q_2 & -Q_1 \end{pmatrix}. \tag{6}$$

Another way to write the transformation is

$$x = Q_1^2 - Q_2^2 - Q_3^2 + Q_4^2; \;\; y = 2(Q_1Q_2 - Q_3Q_4); \;\; z = 2(Q_1Q_3 + Q_2Q_4). \tag{7}$$

Note that the fourth components of $\mathbf{r}$ and $\mathbf{p}$ that the eq.(5) produces, are zeros due to the structure and properties of the transformation.

$$\begin{aligned} u_1 &= \sqrt{\tfrac{1}{2}(r+|x|)} \\ u_2 &= Y/(2u_1) \\ u_3 &= Z/(2u_1) \\ u_4 &= 0, \end{aligned} \tag{8}$$

and the components of $\mathbf{Q}$ are

$$\mathbf{Q} = \begin{cases} (u_1, u_2, u_3, u_4)^t & ; \quad X \geq 0 \\ (u_2, u_1, u_4, u_3)^t & ; \quad X < 0 \end{cases} . \tag{9}$$

Initial values for the KS momenta are given by

$$\mathbf{P} = 2\widehat{\mathbf{Q}}^t \mathbf{p}. \tag{10}$$

For the two-body problem $H = \frac{1}{2}\mathbf{p}^2 - M/r$ the time-transformed Hamiltonian Γ takes the form

$$\Gamma = \frac{1}{8}\mathbf{P}^2 - M + B\mathbf{Q}^2, \tag{11}$$

i.e. a harmonic oscillator, in complete analogy with the lower dimensional cases.

$$\ddot{\mathbf{r}} + M\mathbf{r}/r^3 = \mathbf{F} \tag{12}$$

take the form

$$\begin{aligned} \mathbf{Q}'' &= -\frac{1}{2}B\mathbf{Q} + \frac{1}{2}r\widehat{\mathbf{Q}}^t\mathbf{F} \\ B' &= -2\mathbf{Q}' \cdot \widehat{\mathbf{Q}}^t\mathbf{F} \\ t' &= r = \mathbf{Q} \cdot \mathbf{Q}. \end{aligned} \tag{13}$$

Here $\mathbf{F}$ is the physical perturbation exerted by other particles (or any other physical effect) and

$$B = \frac{M}{r} - \frac{\mathbf{p}^2}{2}$$

is the two-body binding (Kepler-)energy.

Since the equations are regular, they can be solved with any reasonable numerical method.

2.4 Solution algorithms

Usually the simplest algorithm to attempt a solution of the equations of motion is the leapfrog (whenever possible): If the equation can be written in the form

$$q' = G(p); \quad p' = F(q),$$

i.e. the derivatives of one set of variables q only depend on the other set of variables p and vice versa, then the leapfrog can be written

$$q_{\frac{1}{2}} = q_0 + \frac{h}{2}G(p_0); \quad p_1 = p_0 + hF(q_{\frac{1}{2}}); \quad q_1 = q_{\frac{1}{2}} + \frac{h}{2}G(p_1),$$

where h is the stepsize. Typically, however, the accuracy must be increased using an extrapolation method, such as the Bulirsch-Stoer (1966).

Especially in the methods that will be discussed from now on, the leapfrog + extrapolation is an essential part of the algorithm.

2.5 Functional time transformation

Mikkola and Tanikawa (1999; MT99) suggested the use of the Logarithmic Hamiltonian (logH)

$$\Lambda = \ln(T + B) - \ln(U). \tag{14}$$

This can be shown to be equivalent to the original one provided one takes initially $B = -(T - U)$. The time transformation is

$$dt/ds = \partial\Lambda/\partial B = 1/(T + B) = 1/U.$$

Preto and Tremaine (1999) suggested the more general form

$$\Lambda = f(T + B) - f(U), \tag{15}$$

where $f(z)$ is any function $(f'(z) > 0)$. In this case the time transformation is

$$\frac{dt}{ds} = f'(T + B), \tag{16}$$

which, along the correct orbit, is also $dt/ds = f'(U)$.

of motion be

$$\dot{x} = v; \quad \dot{v} = A(x),$$

introduce a time transformation function $\Omega(x)$ and an auxiliary variable ω which satisfies the differential equation

$$\dot{\omega} = \dot{\Omega} = \frac{\partial \Omega(x)}{\partial x} v,$$

so that, if $\omega(0) = \Omega(x(0))$, then along the correct trajectory $\omega = \Omega$ in numerical value.

The time-transformation is defined by $t' = 1/\omega \;\; (= 1/\Omega)$, and one can rewrite the equations of motion as

$$t' = 1/\omega; \quad x' = v/\omega; \quad v' = A(x)/\Omega(x), \quad \omega' = \frac{\partial \ln(\Omega)}{\partial x} v$$

which allows the use of an leapfrog like algorithm. (More details later.)

The one-dimensional perturbed two-body problem with the Hamiltonian

$$H = p^2/2 - 1/q + \tfrac{1}{2}\epsilon q^2.$$

can be integrated with various regularization methods:

1d-KS: Transformation $q = Q^2,\ P = p/(2Q),\ t' = Q^2$. With $B_0 = -H(0)$ the new regular Hamiltonian is

$$\Gamma = t'(H + B_0) = \frac{1}{8}P^2 + B_0 Q^2 - 1 + \tfrac{1}{2}\epsilon Q^4$$

and the equation of motion

$$\begin{aligned} P' &= -\tfrac{\partial \Gamma}{\partial Q} &&= -2BQ - 2\epsilon Q^3, \\ Q' &= \tfrac{\partial \Gamma}{\partial P} &&= P/4, \\ t' &= \tfrac{\partial \Gamma}{\partial B_0} &&= Q^2, \end{aligned}$$

can be integrated with any reasonable numerical method.

$$\Lambda = \ln(p^2/2 + B) - \ln(1/q - \tfrac{1}{2}\epsilon q^2),$$

with $B = -H(0)$. One may solve approximately the equations of motion

$$\begin{aligned} q' &= p/(p^2/2 + b_0) \\ p' &= -\frac{1}{q}\frac{1+\epsilon q^3}{1-\frac{1}{2}\epsilon q^3} \\ t' &= 1/(p^2/2 + b_0), \end{aligned} \tag{17}$$

using the leapfrog.

$$\begin{aligned} \delta t &= s/(p^2/2 + b_0) \\ q &\rightarrow q + \delta t\ p \\ t &\rightarrow t + \delta t \end{aligned}$$

and

$$\mathbf{V(s)}: \qquad p \rightarrow p - s\frac{1}{q}\frac{1+\epsilon q^3}{1-\frac{1}{2}\epsilon q^3} \tag{19}$$

one can symbolise the leapfrog by

$$\mathbf{X(h/2)V(h)X(h/2)},$$

i.e. half step X(h/2), then full step V(h), followed by a half step X(h/2).

Surprisingly, if $\epsilon = 0$, this produces the correct trajectory, having only a phase error.

```
      implicit real*8 (a-h,o-z)
      q=1  ! initialise
      p=0
      b=-(p*p/2-1/q)
      h=0.1d0
1     continue
      call qm(h/2,p,q,b,t)
      call pm(h ,p,q)
      call qm(h/2,p,q,b,t)

c      diagno
       err=log((p*p/2+b)*q) ! error of the logH
       write(6,*)t,q,err
       if(t.lt.100.)goto 1
       end

      subroutine qm(s,p,q,b,t)
      implicit real*8 (a-h,o-z)
      dt=s/(p*p/2+b)
      t=t+dt
      q=q+dt*p
      return
      end
      subroutine pm(s,p,q)
      implicit real*8 (a-h,o-z)
      p=p-s/q
      return
      end
```

equations of motion, which in our simple case read

$$\dot{p} = -1/q^2, \quad \dot{q} = p.$$

The collision ($q \to 0$) is, however, singular and the basic leapfrog does not work.

The idea of TTL is to introduce a time transformation is a such a way that a modified leapfrog can be constructed. Write

$$p' = \dot{p}/\Omega(q), \quad q' = \dot{q}/W, \quad t' = 1/W$$

where we consider W to be a 'velocity-like' variable and $\Omega(q)$ is some suitable function of q. Clearly we must have, in numerical value, $W = \Omega(q)$, but to make the construction of a leapfrog possible we obtain the value of W from the differential equation

$$\dot{W} = \dot{\Omega}(q) = \frac{\partial \Omega}{\partial q} p, \quad \text{or} \quad W' = \dot{W}/\Omega(q).$$

The equations

$$q' = p/W, \quad t' = 1/W$$

can be solved for constant p and W and

$$p' = -1/q, \quad W' = -p/q$$

are solvable for constant q, thus a leapfrog can be constructed as a composite of these two pairs.

$$\begin{aligned} \delta t &= s/W \\ q &\rightarrow q + \delta t\ p \\ t &\rightarrow t\ + \delta t \end{aligned}$$

and

$$\mathbf{V(s)}: \tag{21}$$

$$\begin{aligned} \delta p &= -s/q \\ p_a &= p + \delta p/2 \\ p &\rightarrow p + \delta p \\ W &\rightarrow W - s p_a/q \end{aligned}$$

giving the leapfrog

$$\mathbf{X(h/2)V(h)X(h/2)},$$

```
      q=1
      p=0
      b=p*p/2-1/q ! =Energy
      W=1/q       ! initial value
      h=0.1d0
      t=0

1     continue
      call qm(h/2,p,q,w,t)
      call pm(h ,p,q,w)
      call qm(h/2,p,q,w,t)

c      diagno
       err=p*p/2-1/q-b ! Energy error
       erru=q*err      !
       write(6,123)t,q,p*q,err,erru
123    format(1x,f10.4,2f10.4,1p,3g10.2)
       if(t.lt.100.)goto 1
       end

      subroutine qm(s,p,q,w,t)
      implicit real*8 (a-h,o-z)
      dt=s/w
      t=t+dt
      q=q+dt*p
      return
      end

      subroutine pm(s,p,q,w)
      implicit real*8 (a-h,o-z)
      dp=-s/q
      pa=p+dp/2
      p=p+dp
      w=w-s*pa/q
      return
      end
```

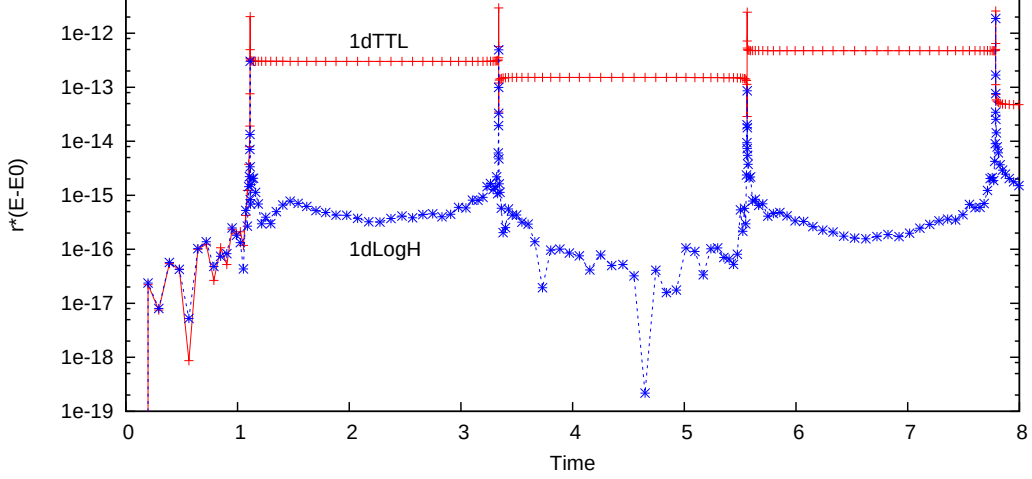
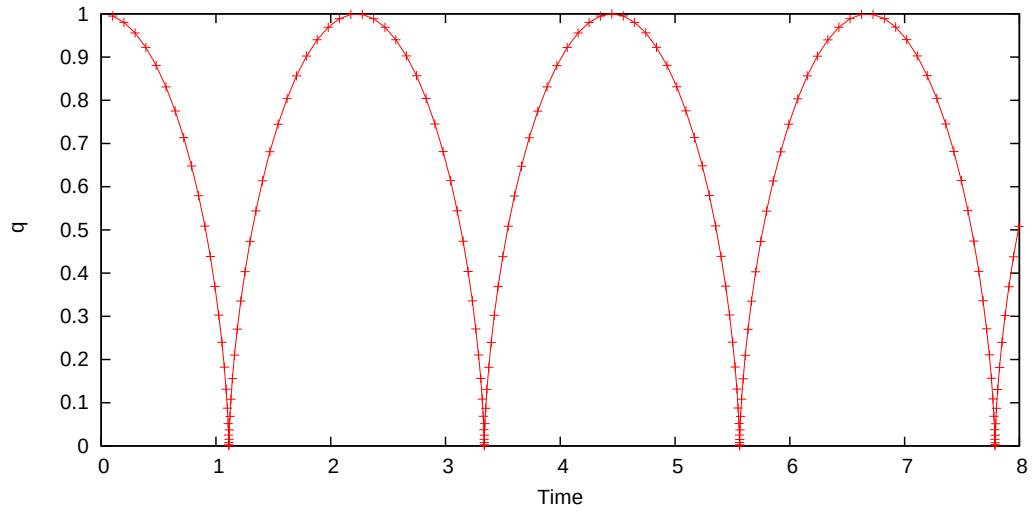


Figure 2: Motion of q



in this simple case [increment of w is equivalent to that of the kinetic energy in logH].

-The difference in precision is due to numerical effects: there is more round-off in updating the W-variable. One notes that in collision $W \rightarrow \infty$ and then it return back to 'normal'. All this with many increments that can be individually very large.

-Generally one may recommend the logH-method in case it is possible to use it.

4 PERTURBED 2B-PROBLEM

The very first problem that a reliable code must be able to do is simply the perturbed two-body problem.

$$\ddot{\mathbf{r}} = -m\mathbf{r}/r^3 + \mathbf{f}$$

Reliable numerical solution of a perturbed two-body problem requires some kind of regularization.

The first such method was that of Levi-Civita (1920) for two dimensions.

Later Kustaanheimo and Stiefel (1965) generalised that to three dimensions applying a transformation (KS-transformation) from four dimensional space to three dimensions.

- **Logarithmic Hamiltonian+leapfrog (logH), (Mikkola and Tanikawa 1999ab)**

  and independently (Preto and Tremaine 1999).

- **Time Transformed Leapfrog (TTL),(Mikkola and Aarseth 2002).**

- **Generalised Midpoint Method (GMM) for velocity dependent perturbations, (Mikkola and Merritt 2006). (Exploiting also logH & TTL)**

-The leapfrog is a important part of these methods.

==> Algorithmic Regularization

5 ALGORITHMIC REGULARIZATION

5.1 The logarithmic Hamiltonian

Let $\mathbf{p}$ be the momenta and $\mathbf{q}$ the coordinates
$T(\mathbf{p})$ the kinetic energy and $U(\mathbf{q}, t)$ the force function.
Then the Hamiltonian in extended phase-space is

$$H = T + B - U. \tag{22}$$

Here B the momentum of time (which is now a coordinate: $t' = \frac{\partial H}{\partial B} = 1$).

If $B(0) = -H(0)$, then the function

$$\Lambda = \log(T + B) - \log(U) \tag{23}$$

can be used as a Hamiltonian in the extended phase space.

$$\mathbf{r}_{\frac{1}{2}} = \mathbf{r}_0 + \frac{h}{2}\frac{\mathbf{v}_0}{T_0 + B} \tag{24}$$

$$\mathbf{v}_1 = \mathbf{v}_0 - \frac{h}{U_{\frac{1}{2}}}\frac{\partial U_{\frac{1}{2}}}{\partial \mathbf{r}_{\frac{1}{2}}} \tag{25}$$

$$\mathbf{r}_1 = \mathbf{r}_{\frac{1}{2}} + \frac{h}{2}\frac{\mathbf{v}_1}{T_1 + B} \tag{26}$$

$$t_1 = t_0 + \frac{h}{2}\left(\frac{1}{T_0 + B} + \frac{1}{T_1 + B}\right), \tag{27}$$

which, **for two bodies**, **produces an exact two-body trajectory for any eccentricity**.

```
        t=0
        r=sqrt(x(1)**2+x(2)**2+x(3)**2)
        vv=v(1)**2+v(2)**2+v(3)**2
        B=M/r-vv/2
c       Integration of the two-body motion
1       continue
        dt=h/(v(1)**2+v(2)**2+v(3)**2+2*B)
        do k=1,3
        x(k)=x(k)+dt*v(k)
        end do
        t=t+dt
        dtc=h/(x(1)**2+x(2)**2+x(3)**2)
        do k=1,3
        v(k)=v(k)-dtc*x(k)
        end do
        dt=h/(v(1)**2+v(2)**2+v(3)**2+2*B)
        do k=1,3
        x(k)=x(k)+dt*v(k)
        end do
        t=t+dt!-h**3/12/(M)**2  ! +O(h^5) time correction (only for small h)
c
c       diagnostics
        r=sqrt(x(1)**2+x(2)**2+x(3)**2)
        vv=v(1)**2+v(2)**2+v(3)**2
        Bt=M/r-vv/2
        Eerr=Bt-B
        write(6,123)t,x,Eerr,Eerr*r
123     format(1x,f12.4,3f10.5,1p,2g10.2)
        if(t.lt.Tmx)goto 1
        end
```

RUN toy.x & movie

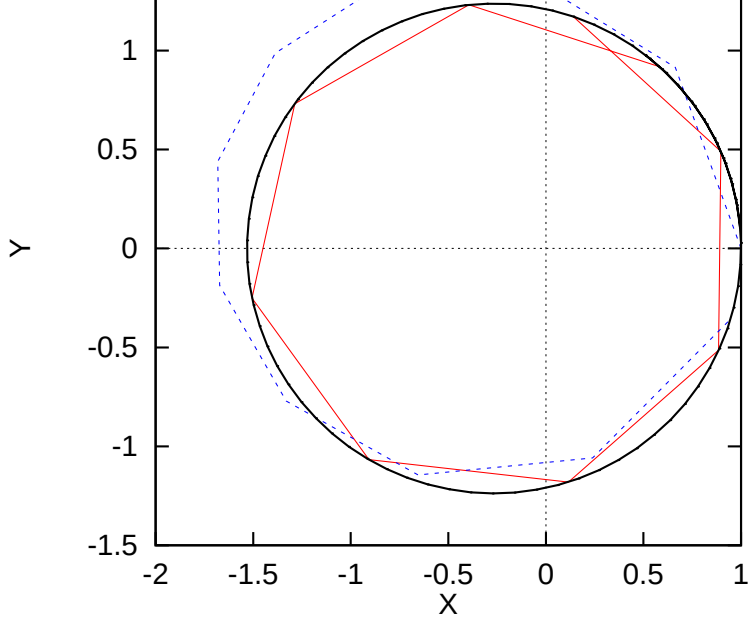


Figure 3: Lines connect the endpoints of leapfrog steps.

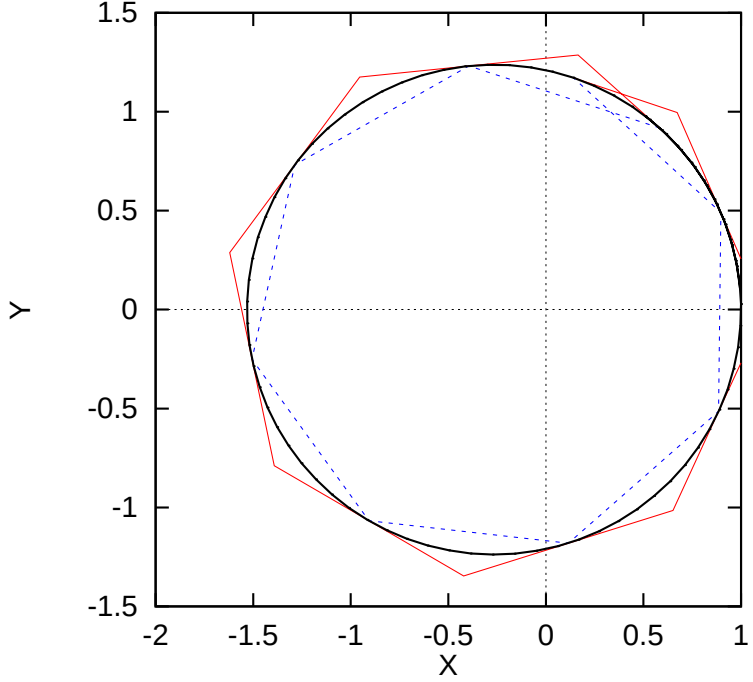


Figure 4: Lines drawn from starting- to half- to end-point....

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5.2 Time-Transformed Leapfrog (TTL)

Consider the system

$$\dot{\mathbf{r}} = \mathbf{v}, \quad \dot{\mathbf{v}} = \mathbf{F}(\mathbf{r}). \tag{28}$$

for which the leapfrog can be used
Let us introduce a time transformation

$$ds = \Omega(\mathbf{r})\, dt, \tag{29}$$

where $\Omega(\mathbf{r}) > 0$ is arbitrary.

Write $\omega = \Omega$, then we have

$$\mathbf{r}' = \mathbf{v}/\omega, \quad t' = 1/\omega,$$

$$\mathbf{v}' = \mathbf{F}/\Omega, \quad \omega' = \mathbf{v} \cdot \frac{\partial \Omega}{\partial \mathbf{r}}/\Omega,$$

(here prime means $\frac{d}{ds}$).

$$\frac{\partial}{\partial \mathbf{r}}\Big/\Omega,$$ (30)

instead of $\omega = \Omega$ directly, we have

$$\begin{pmatrix} \mathbf{r}' \\ t' \\ \mathbf{v}' \\ \omega' \end{pmatrix} = \begin{pmatrix} \mathbf{v}/\omega \\ 1/\omega \\ \mathbf{0} \\ 0 \end{pmatrix} + \begin{pmatrix} \mathbf{0} \\ 0 \\ \mathbf{F}(\mathbf{r})/\Omega(\mathbf{r}) \\ \mathbf{v} \cdot \partial \ln(\Omega)/\partial \mathbf{r} \end{pmatrix}. \quad (31)$$

which allows a time-transformed leapfrog:

$$\mathbf{r}_{\frac{1}{2}} = \mathbf{r}_0 + \frac{h}{2}\frac{\mathbf{v}_0}{\omega_0} \quad (32)$$

$$t_{\frac{1}{2}} = t_0 + \frac{h}{2}\frac{1}{\omega_0} \quad (33)$$

$$\mathbf{v}_1 = \mathbf{v}_0 + h\frac{\mathbf{F}(\mathbf{r}_{\frac{1}{2}})}{\Omega(\mathbf{r}_{\frac{1}{2}})} \quad (34)$$

$$\omega_1 = \omega_0 + h\frac{\mathbf{v}_0 + \mathbf{v}_1}{2\Omega(\mathbf{r}_{\frac{1}{2}})} \cdot \frac{\partial \Omega(\mathbf{r}_{\frac{1}{2}})}{\partial \mathbf{r}_{\frac{1}{2}}} \quad (35)$$

$$\mathbf{r}_1 = \mathbf{r}_{\frac{1}{2}} + \frac{h}{2}\frac{\mathbf{v}_1}{\omega_1} \quad (36)$$

$$t_1 = t_{\frac{1}{2}} + \frac{h}{2}\frac{1}{\omega_1}. \quad (37)$$

then this algorithm is mathematically equivalent with the logH-method. Numerically, however, this does not apply. The reason is that in case of a close approach W first increase, then decreases fast meaning that the increments are large numbers and there is considerable cancellation and possible round-off error.

Especially interesting is the fact that the method can be efficient for potentials that differ from the Newtonian $1/r$ behaviour at small distances. One notes that AR is useful for the soft potential

$$1/\sqrt{r^2+\epsilon^2},$$

which cannot be 'regularised' with the KS-transformation.

5.3 Generalised Midpoint Method (GMM)

The leapfrog algorithm alone is not sufficiently accurate and one must use the extrapolation method (Gragg 1964, 1965, Bulirsch & Stoer 1966) for improved precision. This requires that the basic leapfrog algorithm be time-symmetric, which is not directly possible in the case of **velocity-dependent forces**.

A new algorithm (Mikkola and Merritt 2006) is based on the realization that any general initial value problem

$$\dot{\mathbf{z}} = \mathbf{f}(\mathbf{z}), \quad \mathbf{z}(0) = \mathbf{z}_0. \tag{39}$$

can be split into two as

$$\dot{\mathbf{x}} = \mathbf{f}(\mathbf{y}), \tag{40}$$

$$\dot{\mathbf{y}} = \mathbf{f}(\mathbf{x}) \tag{41}$$

with the initial values

$$\mathbf{x}_0 = \mathbf{y}_0 = \mathbf{z}(0).$$

It is simple to see that this pair has the solution

$$\mathbf{x}(t) = \mathbf{y}(t) = \mathbf{z}(t).$$

the well-known modified midpoint method.

$$\mathbf{x}_{\frac{1}{2}} = \mathbf{x}_0 + \left(+\frac{h}{2}\mathbf{f}(\mathbf{y}_0)\right), \tag{42}$$

$$\mathbf{y}_{\frac{1}{2}} = \mathbf{y}_0 - \left(-\frac{h}{2}f(\mathbf{x}_{\frac{1}{2}})\right), \tag{43}$$

$$\mathbf{y}_1 = \mathbf{y}_{\frac{1}{2}} + \left(+\frac{h}{2}f(\mathbf{x}_{\frac{1}{2}})\right), \tag{44}$$

$$\mathbf{x}_1 = \mathbf{x}_{\frac{1}{2}} - \left(-\frac{h}{2}\mathbf{f}(\mathbf{y}_1)\right). \tag{45}$$

be any reasonable approximation to the solution of Eq. (39) over a time interval Δt. Then one step in the generalised midpoint method can now be written

$$\mathbf{x}_{\frac{1}{2}} = \mathbf{x}_0 + \mathbf{d}(\mathbf{y}_0, +\frac{h}{2}), \tag{47}$$

$$\mathbf{y}_{\frac{1}{2}} = \mathbf{y}_0 - \mathbf{d}(\mathbf{x}_{\frac{1}{2}}, -\frac{h}{2}), \tag{48}$$

$$\mathbf{y}_1 = \mathbf{y}_{\frac{1}{2}} + \mathbf{d}(\mathbf{x}_{\frac{1}{2}}, +\frac{h}{2}), \tag{49}$$

$$\mathbf{x}_1 = \mathbf{x}_{\frac{1}{2}} - \mathbf{d}(\mathbf{y}_1, -\frac{h}{2}), \tag{50}$$

$$\mathbf{A}(\mathbf{x},\mathbf{y},h): \quad \mathbf{x} \rightarrow \mathbf{x}+\mathbf{d}(\mathbf{y},+\frac{h}{2}) \tag{51}$$

$$\mathbf{y} \rightarrow \mathbf{y}-\mathbf{d}(\mathbf{x},-\frac{h}{2}), \tag{52}$$

we can write the algorithm with many (N) steps as

1. Set $\mathbf{y}=\mathbf{x}$;
2. Repeat $\mathbf{A}(\mathbf{x},\mathbf{y},h)\mathbf{A}(\mathbf{y},\mathbf{x},h)$ N times; (53)
3. Accept $\mathbf{x}$ as the final result.

Thus one simply calls the subroutine $\mathbf{A}$ alternately with arguments $(\mathbf{x},\mathbf{y})$ and $(\mathbf{y},\mathbf{x})$ such that the sequence is time-symmetric (starts and stops with $\mathbf{x}$ in Eq. 53).

This basic algorithm has the correct symmetry, and thus the Gragg-Bulirsch-Stoer **extrapolation method can be used** to obtain high accuracy.

This is true irrespective of the way one chooses the approximation $\mathbf{d}(\mathbf{x},s)$. Thus velocity dependencies can be added e.g. to algorithmic regularization.

fact that LogH is numerically much more stable. The reason is that in TTL the value of ω is obtained as a sum

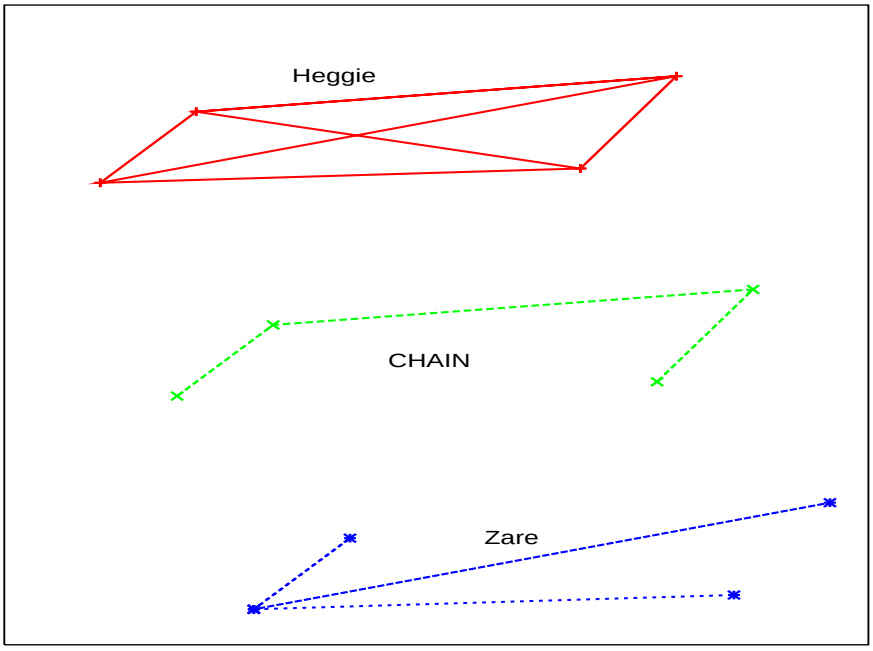
$$\omega = \omega(0) + \sum h \frac{\partial \Omega}{\partial \mathbf{r}} \cdot < \mathbf{v} > /\Omega$$

of large positive and negative increments, which causes significant round-off errors.

6 N-BODY PROBLEM

Several methods have been suggested for regularisation of the N-Body problem using KS-transformations
(Aarseth & Zare 1975, Heggie 1975, Zare 1975
Mikkola 1985, Mikkola & Aarseth 1993) .

Figure 5: KS regularized interactions in the global method of Heggie, CHAIN-method and Zare's cartwheel method.



6.1 LogH in NB-Problem

The logarithmic Hamiltonian

$$\Lambda = \ln(T + B) - \ln(U)$$

gives the equations of motion

$$\begin{aligned} t' &= \frac{\partial \Lambda}{\partial B} = 1/(T + B) \\ \mathbf{r}'_k &= \frac{\partial \Lambda}{\partial \mathbf{p}_k}/(T + B) \\ B' &= \frac{1}{U}\frac{\partial U}{\partial t} \\ \mathbf{p}'_k &= \frac{1}{U}\frac{\partial U}{\partial \mathbf{r}_k}, \end{aligned}$$

which can be approximately solved using the leapfrog. The simplest way is to to use the centre-of-mass coordinates 'as usual'. Mathematically this way of using the method is as good as any, however, numerically the roundoff errors become a major problem. The way out is the use of the CHAIN.

6.2 CHAIN

The chain method [relative coordinates along a chain of particles], was originally introduced (Mikkola & Aarseth 1993) to regularise all critical interactions with the KS-transformation.

Later the importance of the chain structure in the algorithmic regularizations became clear. The reason is round-off errors. If one uses centre-of-mass coordinates, then the relative coordinates of a distant close pair are differences of large numbers and there is considerable cancellation leading to irrecoverable errors.

This section discusses a new code that uses the chain-structure and a mixture of the logH and TTL -methods.

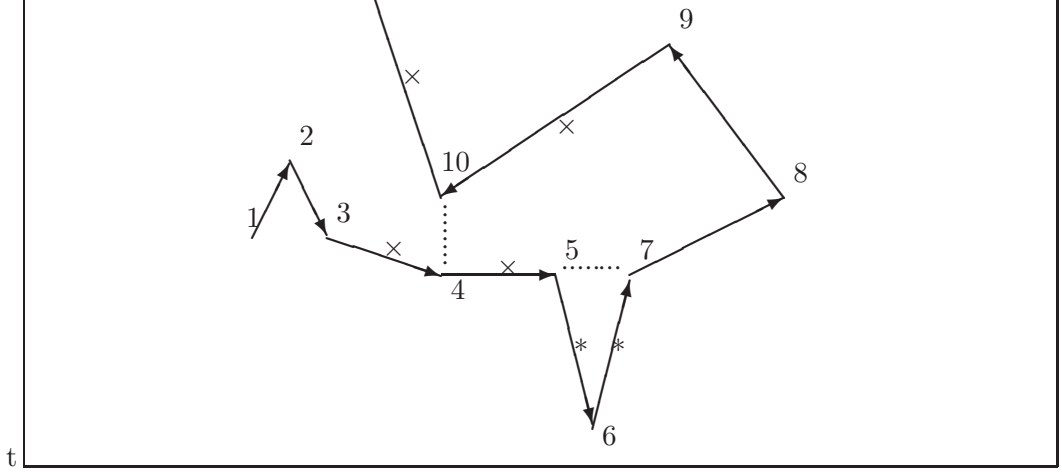


Figure 6: Illustration of the chain and the checking of switching conditions. Distances like $R_{5,7}$ are compared with the smaller of the two distances $R_{5,6}$ and $R_{6,7}$ (marked by *). Interparticle distances like $R_{4,10}$ are compared with the smallest of those in contact with the considered distance (marked by $\times$).

6.3 Finding and updating the chain

We begin by finding the shortest interparticle vector for the first part of the chain.Next we search for the particle closest to one or the other end of the presently known part of the chain. This particle is added to the closest end of the already existing chain. This is repeated until all particles are included in the chain. The particles are then re-numbered along the chain as $1, 2, ..N$ for easy of programming.

After every integration step we check for the need of updating the chain. Figure 1 illustrates the case of a 12-particle chain. To avoid round-off problems it is advantageous to carry out the transformation from the old chain vectors $\mathbf{X}_k$ to the new ones directly by expressing the new chain vectors as sums of the old ones.

tation I_k^{old} and I_k^{new} for the names in the old and new chains. Then we may write

$$\mathbf{r}_{I_k^{old}} = \sum_{\nu=1}^{k-1} \mathbf{X}_\nu^{old}, \tag{54}$$

$$\mathbf{X}_\mu^{new} = \mathbf{r}_{I_{\mu+1}^{new}} - \mathbf{r}_{I_\mu^{new}}. \tag{55}$$

Thus we need to use the correspondence between the old and new indices to express the new chain vector $\mathbf{X}$ in terms of the old ones. One finds that if k_0 and k_1 are two indices such that $I_{k_0}^{old} = I_\mu^{new}$ and $I_{k_1}^{old} = I_{\mu+1}^{new}$, then

$$\mathbf{X}_\mu^{new} = \sum_{\nu=1}^{N-1} B_{\mu\nu} \mathbf{X}_\nu^{old}, \tag{56}$$

where $B_{\mu\nu} = +1 \quad \text{if}(\ k_1 > \nu\ \&\ k_0 \leq \nu)$ and $B_{\mu\nu} = -1 \ \text{ if}(\ k_1 \leq \nu\ \&\ k_0 > \nu)$, otherwise $B_{\mu\nu} = 0$.

SHOW CHAINMOVIES

6.4 ALGORITHMIC REGULARIZATION CHAIN

Let

$$T = \sum_{k=1}^{N} \frac{m_k}{2} \mathbf{v}_k^2 i \tag{57}$$

be the kinetic energy, and

$$U = \sum_{i<j\leq N} m_i m_j / r_{ij} \tag{58}$$

the potential such that the total energy is $E = T - U$.

One forms a chain of particles such that the shortest relative vectors are in the chain (Mikkola & Aarseth 1993). [We stress that the main purpose of using the chain structure in this method is to reduce the (often significant) effect of round-off error.]

in the vector

$$\mathbf{X} = (\mathbf{X}_1, \mathbf{X}_2, .., \mathbf{X}_{N-1})$$

and let the corresponding velocities be

$$\mathbf{V} = (\mathbf{V}_1, \mathbf{V}_2, .., \mathbf{V}_{N-1})$$

. Then the Newtonian equations of motion may be formally written

$$\dot{\mathbf{X}} = \mathbf{V} \tag{60}$$

$$\dot{\mathbf{V}} = \mathbf{A}(\mathbf{X}) + \mathbf{f}, \tag{61}$$

where $\mathbf{A}$ is the N-body acceleration and $\mathbf{f}$ is some external acceleration (e.g.due to other bodies).

$$ds = [\alpha(T + B) + \beta\omega + \gamma]dt = [\alpha U + \beta\Omega + \gamma]dt, \quad (62)$$

where s is a new independent variable, B is the binding energy $B = -E$, α, β and γ are adjustable constants,Ω is an optional function of the coordinates $\Omega = \Omega(\mathbf{X})$. The initial value $\omega(0) = \Omega(0)$ and the differential equation

$$\dot{\omega} = \frac{\partial\Omega}{\partial\mathbf{X}} \cdot \mathbf{V}, \quad (63)$$

determines the value of ω (actually $\omega(t) = \Omega(t)$ along the exact solution).

variable s are denoted by a prime).

Coordinate equations:

$$t' = 1/(\alpha(T+B)+\beta\omega+\gamma) \quad (64)$$
$$\mathbf{X}' = t'\,\mathbf{V} \quad (65)$$

Velocity equations:

$$\tilde{t}' = 1/(\alpha U+\beta\Omega+\gamma) \quad (66)$$
$$\mathbf{V}' = \tilde{t}'\,(\mathbf{A}+\mathbf{f}) \quad (67)$$
$$\omega' = \tilde{t}'\,\frac{\partial\Omega}{\partial\mathbf{X}}\cdot\mathbf{V} \quad (68)$$
$$B' = -\tilde{t}'\,\frac{\partial T}{\partial\mathbf{V}}\cdot f \quad (69)$$

In these equations the right hand sides do not depend on the variables at the left hand side. Consequently it is possible to construct a regular leapfrog algorithm for obtaining the solutions (Mikkola & Tanikawa 1999ab, Mikkola & Aarseth 2003, Preto & Tremaine 1999).

as a basic integrator (results of which can, and must, be improved using an extrapolation method (e.g. Bulirsh and Stoer (1966), Press et al (1986)). [This is why the method is called Algorithmic Regularization.]

For the case of velocity dependent perturbation $\mathbf{f} = \mathbf{f}(\mathbf{X}, \mathbf{V})$, which occurs e.g if one introduces relativistic Post-Newtonian terms, related algorithms were discussed by (Mikkola & Merritt 2006).

In the presence of external perturbations the binding energy evolves according to

$$\dot{B} = -\frac{\partial T}{\partial \mathbf{V}} \cdot \mathbf{f} \tag{70}$$

$\mathbf{X}(s)$:

$$\begin{aligned}
\delta t &= s/(\alpha(T+B)+\beta\omega+\gamma) && (71)\\
t &= t+\delta t && (72)\\
\mathbf{X} &\rightarrow \mathbf{X}+\delta t\mathbf{V} && (73)\\
& && (74)
\end{aligned}$$

$\mathbf{V}(s)$:

$$\begin{aligned}
\widetilde{\delta t} &= s/(\alpha U+\beta\Omega+\gamma) && (75)\\
\mathbf{V} &\rightarrow \mathbf{V}+\widetilde{\delta t}(\mathbf{A}+\mathbf{f}) && (76)\\
B &\rightarrow B+\widetilde{\delta t}<\frac{\partial T}{\partial \mathbf{V}}>\cdot\mathbf{f} && (77)\\
\omega &\rightarrow \omega+\widetilde{\delta t}\frac{\partial\Omega}{\partial\mathbf{X}}\cdot<\mathbf{V}>, && (78)
\end{aligned}$$

where $<\frac{\partial T}{\partial \mathbf{V}}>$ and $<\mathbf{V}>$ are the averages over the advancement of $\mathbf{V}$.

NOTE: If the GMM method is used then then one can use for $\mathbf{V}$ simply the most recent value available.

The leapfrog with the above maps reads

$$\mathbf{X}(h/2)\left(\mathbf{V}(h)\mathbf{X}(h)\right)^{n-1}\mathbf{V}(h)\mathbf{X}(h/2), \qquad (79)$$

for a macro-step of length $= nh$.

The leapfrog results then can easily be improved with the extrapolation method. If one uses for Ω a form

$$\Omega=\sum_{i<j\leq N}\Omega_{ij}/r_{ij}, \qquad (80)$$

where the constants Ω_{ij} are suitably chosen [to make the effect significant even when two small bodies approach each other], the algorithm successfully regularises the motions in any N-body system independent of mass ratios. Also, as is clear from the structure of the equations of motion, there is no any

chain (Mikkola & Aarseth (1993), Aarseth (2003)), in which there are divisions by masses and the total energy appear in equations of motion in a such a way that any particle included must have a significant effect into the energy in order to be regularised.

SHOW MOVIE.30

After selecting the chain, and renaming the particles as $1, 2, \ldots, N$ along the chain, one can evaluate the initial values for the chain vectors and velocities as

$$\mathbf{X}_k = \mathbf{r}_{k+1} - \mathbf{r}_k \tag{81}$$

$$\mathbf{V}_k = \mathbf{v}_{k+1} - \mathbf{v}_k. \tag{82}$$

where $\mathbf{v}_k = \dot{\mathbf{r}}_k$. At the same time one may evaluate the centre-of-mass quantities

$$M = \sum_k m_k \tag{83}$$

$$\mathbf{r}_{cm} = \sum_k m_k \mathbf{r}_k / M \tag{84}$$

$$\mathbf{v}_{cm} = \sum_k m_k \mathbf{v}_k / M, \tag{85}$$

$$\tilde{\mathbf{r}}_1 = \mathbf{0} \tag{86}$$

$$\tilde{\mathbf{v}}_1 = \mathbf{0} \tag{87}$$

$$\tilde{\mathbf{r}}_{k+1} = \tilde{\mathbf{r}}_k + \mathbf{X}_k \tag{88}$$

$$\tilde{\mathbf{v}}_{k+1} = \tilde{\mathbf{v}}_k + \mathbf{V}_k, \tag{89}$$

followed by reduction to the centre of mass

$$\tilde{\mathbf{r}}_{cm} = \sum_k m_k \tilde{\mathbf{r}}_k / M \tag{90}$$

$$\tilde{\mathbf{v}}_{cm} = \sum_k m_k \tilde{\mathbf{v}}_k / M \tag{91}$$

$$\mathbf{r}_k = \tilde{\mathbf{r}}_k - \tilde{\mathbf{r}}_{cm} \tag{92}$$

$$\mathbf{v}_k = \tilde{\mathbf{v}}_k - \tilde{\mathbf{v}}_{cm}. \tag{93}$$

However, it is not always necessary to reduce the coordinates to the centre-of-system since accelerations only depend on the differences.

The equations of motion read

$$\dot{\mathbf{X}}_k = \mathbf{V}_k \tag{94}$$
$$\dot{\mathbf{V}}_k = \mathbf{A}_{k+1} - \mathbf{A}_k, \tag{95}$$

where the accelerations $\mathbf{A}_k$, with possible external effects $\mathbf{f}_k$, are

$$\mathbf{A}_k = -\sum_{j\neq k} \frac{\mathbf{r}_{jk}}{|\mathbf{r}_{jk}|^3} + \mathbf{f}_k, \tag{96}$$

and, for $j < k$

$$\mathbf{r}_{jk} = \begin{cases} \mathbf{r}_k - \mathbf{r}_j; & \text{if } k > j+2 \\ \mathbf{X}_j; & \text{if } k = j+1 \\ \mathbf{X}_j + \mathbf{X}_{j+1}; & \text{if } k = j+2 \end{cases}, \tag{97}$$

and for $k > j$ one uses the fact that $\mathbf{r}_{jk} = -\mathbf{r}_{kj}$. The use of $\mathbf{X}_j$ and $\mathbf{X}_j + \mathbf{X}_{j+1}$ reduces the round-off effect significantly. More generally one could also use

$$\mathbf{r}_{kj} = \sum_{\nu=j}^{k-1} \mathbf{X}_\nu, \tag{98}$$

but, for many bodies it is faster to use the above recipe (97) and the latter alternative seems not to improve the results.

$$T = \frac{1}{2}\sum_k m_k \mathbf{v}_k \tag{99}$$

and the potential energy

$$U = \sum_{i<j} \frac{m_i m_j}{|\mathbf{r}_{ij}|}, \tag{100}$$

which is evaluated along with the accelerations according to (97). We introduce further a time transformation function

$$\Omega = \sum_{i<j} \frac{\Omega_{ij}}{|\mathbf{r}_{ij}|}, \tag{101}$$

where Ω_{ij} are some selected coefficients.

where $\alpha,\ \beta$ and γ are adjustable constants.

Since $T = U + E$, we have

$$B = -\alpha E + \beta\Omega + \gamma, \tag{103}$$

which expression is used only for the initial value of B and later this quantity must be obtained by solving the differential equation

$$\dot{B} = -\alpha \sum_k \mathbf{v}_k \cdot \mathbf{f}_k + \beta \sum_k \frac{\partial \Omega}{\partial \mathbf{r}_k} \cdot \mathbf{v}_k. \tag{104}$$

and coordinates respectively,

$$t' = 1/(\alpha T + B), \tag{105}$$
$$\mathbf{r}'_k = t'\mathbf{v}_k \tag{106}$$

and for velocities and B

$$\tau' = 1/(\alpha U + \beta\Omega + \gamma), \tag{107}$$
$$\mathbf{v}'_k = \tau'(\frac{\partial U}{\partial \mathbf{r}_k} + \mathbf{f}_k)/m_k, \tag{108}$$
$$B' = \tau' \sum_k \left(-\alpha \mathbf{f}_k + \beta \frac{\partial \Omega}{\partial \mathbf{r}_k}\right) \cdot \mathbf{v}_k. \tag{109}$$

Here the (possible) velocity dependence of the additional forces $\mathbf{f}_k$ can be handled as in the two-body example earlier. However, to account for the (explicitly written) $\mathbf{v}$-dependence of B' one must follow Mikkola & Aarseth 2002, i.e. first the $\mathbf{v}_k$ are advanced and then the average $< \mathbf{v}_k >= (\mathbf{v}_k(0) + \mathbf{v}_k(h))/2$ is used to evaluate B'. Thus the leapfrog can be constructed in obvious analogy with the perturbed two-body case.

$\mathbf{X}(s)$:

$$\begin{aligned} \delta t &= s/(\alpha T + B) && (110)\\ t &= t + \delta t && (111)\\ \mathbf{X}_k &\rightarrow \mathbf{X}_k + \delta t \mathbf{V}_k && (112)\\ & && (113) \end{aligned}$$

$\mathbf{V}(s)$:

$$\begin{aligned} \widetilde{\delta t} &= s/(\alpha U + \beta\Omega + \gamma) && (114)\\ \mathbf{V}_k &\rightarrow \mathbf{V}_k + \delta t(\mathbf{A}_{k+1} - \mathbf{A}_k) && (115)\\ B &\rightarrow B + \widetilde{\delta t}\sum_k \left(-\alpha \mathbf{f}_k + \beta \frac{\partial \Omega}{\partial \mathbf{r}_k}\right) \cdot < \mathbf{v}_k > && (116) \end{aligned}$$

where $< \mathbf{v}_k >$ is the average of the initial and final $\mathbf{v}$'s in this routine.

One leapfrog step can then be written simply as

$$\mathbf{X}(h/2)\mathbf{V}(h)\mathbf{X}(h/2)$$

and a longer sequence of n steps (that is needed when the extrapolation method is used) reads

$$\mathbf{X}(h/2)\left[\Pi_{\nu=1}^{n-1}(\mathbf{V}(h)\mathbf{X}(h))\right]\mathbf{V}(h)\mathbf{X}(h/2)$$

tained is the logarithmic Hamiltonian method (Mikkola & Tanikawa 1999a).

(ii) If $(\alpha, \beta, \gamma) = (0, 1, 0)$ then we have the time transformed leapfrog (TTL) (Mikkola & Aarseth 2002).

(iii) If $(\alpha, \beta, \gamma) = (0, 0, 1)$ then the method is just the normal basic leapfrog.

(iv) The question of which combination of the numbers (α, β, γ) is best cannot be answered in general, but experimentation is necessary. For N-body systems with very large mass ratios, however, it seems that one must have $\beta \neq 0$, which means a form of the TTL method. This is because low mass bodies do not contribute significantly to the energies (kinetic and/or potential) and consequently, if $\beta = 0$, there is no significant reduction in stepsize during a close encounter.

6.7 Alternative time-transformation

If one takes

$$\Omega_j = m_i m_j, \tag{117}$$

then $\alpha = 0,\ \beta = 1,\ \gamma = 0$ is mathematically equivalent to $\alpha = 1,\ \beta = \gamma = 0$ as was shown in Mikkola & Aarseth 2002. However, numerically these are not equivalent, but the logH alternative is much more stable. On the other hand, as noted above, it is desirable to get stepsize shortening (and thus regularization) also for encounters of small bodies and thus some function Ω should be used.

The increase the numerical stability for strong interactions of big bodies and also smooth the encounters of small bodies one may use $\alpha = 1,\ \beta \neq 0$ and

$$\Omega_{ij} = \begin{cases} = 1; & \text{if } m_i * m_j < \epsilon mm \\ = 0; & \text{otherwise} \end{cases}, \tag{118}$$

where $mm = \sum_{i<j} m_i m_j / (N(N-1)/2)$ is the mean mass product and β and ϵ adjustable parameters.

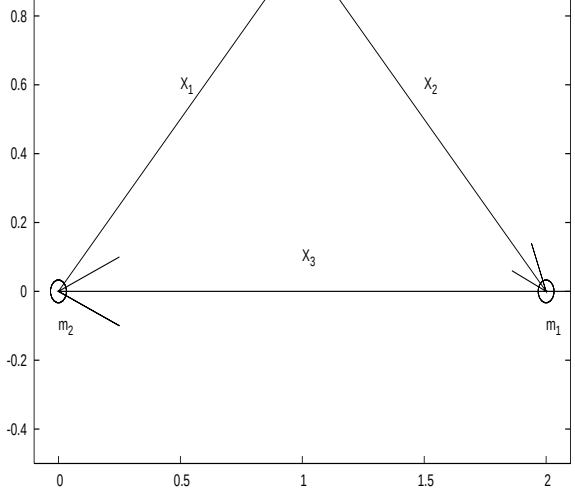


Figure 7: Labelling of vectors in the three-body regularization.

7 A simple logH algorithm for the three-body problem

The three-body problem is still one of the most studied problems in few-body dynamics. Therefore it may be of interest to consider in more detail a simple regular three-body algorithm. This also serves as further illustration of the use of the algorithmic regularization.

Following Heggie (1974) we use the three interparticle vectors (see Figure 7)

$$\mathbf{X}_1 = \mathbf{r}_3 - \mathbf{r}_2; \quad \mathbf{X}_2 = \mathbf{r}_1 - \mathbf{r}_3; \quad \mathbf{X}_3 = \mathbf{r}_2 - \mathbf{r}_1. \qquad (119)$$

as new coordinates. Let the corresponding velocities be $\mathbf{V}_k =$

$$T = \frac{1}{2M}\sum_{i<j} m_i m_j \mathbf{V}_{k_{ij}}; \quad U = \sum_{i<j}\frac{1}{|X_{k_{ij}}|}, \qquad (120)$$

where $M = \sum_k m_k$ is the total mass and $k_{ij} = 6 - i - j$.

The equations of motion are

$$\dot{\mathbf{X}}_k = \mathbf{V}_k; \quad \dot{\mathbf{V}}_k = -M\frac{\mathbf{X}_k}{|\mathbf{X}_k|^3} + m_k\sum_\nu \frac{\mathbf{X}_\nu}{|\mathbf{X}_\nu|^3}, \qquad (121)$$

and after the application of the logarithmic Hamiltonian modification they read

$$t' = 1/(T+B); \quad \mathbf{X}'_k = \dot{\mathbf{X}}_k/(T+B); \quad \mathbf{V}'_k = \dot{\mathbf{V}}_k/U, \ (122)$$

which are suitable for the leapfrog algorithm, as well as for Yoshida's higher order leapfrogs.

The usage of the relative vectors, instead of some inertial coordinates, is advantageous in attempting to avoid large round-off effects. One could also integrate only two of the triangle sides, obtaining the remaining one from the conditions

$$\sum_k \mathbf{X}_k = \mathbf{0}; \quad \sum_k \mathbf{V}_k = \mathbf{0}.$$

However this hardly reduces the computational effort required by the method. Instead one may, occasionally, compute the longest side, and the corresponding velocity, from the above triangle conditions. Note, however, that the sums of the sides are not only integrals of the exact solution, but they are also exactly conserved by the leapfrog mapping.

The transformation from the variables $\mathbf{X}$ to centre-of-mass coordinates $\mathbf{r}$ can be done as

$$\mathbf{r}_1 = \frac{(m_3\mathbf{X}_2 - m_2\mathbf{X}_3)}{M}; \ \mathbf{r}_2 = \frac{(m_1\mathbf{X}_3 - m_3\mathbf{X}_1)}{M}; \ \mathbf{r}_3 = \frac{(m_2\mathbf{X}_1 - m_1\mathbf{X}_2)}{M}, \qquad (123)$$

and the velocities obey the same rule.

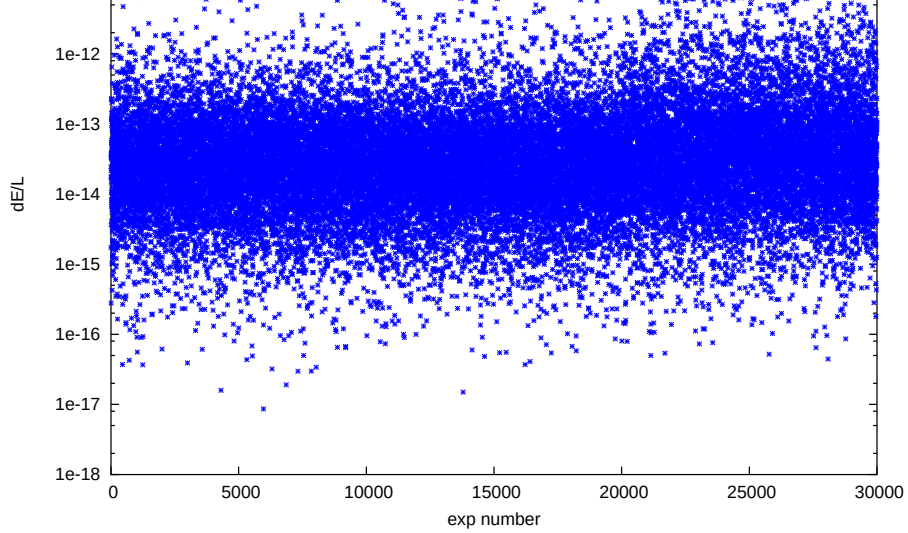


Figure 8: Energy errors in 30,000 triple experiments.

8 Remarks

The authors impressions, based on experience, can be summarised as:

1. The importance of the chain structure is due to several things: In KS-regularised chain, it takes care that all the strong interactions are properly regularised. However, equally important is that the round-off problems are significantly reduced. This is why chain is useful even with the algorithmic regularization.
2. KS-CHAIN is the most efficient KS-regularised code, but restricted to comparable masses. However, 'comparable' means here a maximum mass ratio of 10^3 (maybe even 10^4).
3. A drawback of the KS-regularization is that a soft potential makes is singular (thus cannot be used).
4. LogH is a good alternative, but still restricted to comparable masses(?).
5. TTL can handle large mass ratios, but sometimes suffers from serious round-off errors.
6. AR-CHAIN is probably one of the best,since it can handle **large mass ratios** and **soft potential** with no problem.
7. For the chain algorithms, use of a high order numerical integrator, such as the extrapolation method (Press et al. 1986), is necessary. Similarly the TTL, LogH and AR-CHAIN requires extrapolation to improve the leapfrog results. These can also be improved alternatively by using a higher order leapfrog (Yoshida, 1990).

Suppose the Hamiltonian can be written

$$H = T(\mathbf{p}) + R(\mathbf{r}) - m/r,$$

and suppose further that $T + R$ is integrable (easily) if considered alone. Then a possibility is to use the logarithmic Hamiltonian

$$\Lambda = \ln(T + R + B) - \ln(m/r),$$

which regularises the $1/r$ interaction even here. There are also other possibilities:

The perturbed two-body problem

$$H = \tfrac{1}{2}\mathbf{p}^2 - \mathbf{n}\cdot\mathbf{r}\times\mathbf{p} - M/r - R(\mathbf{r})$$

can be integrated using the LogH-method:

$$\Lambda = \ln(\underbrace{\tfrac{1}{2}\mathbf{p}^2 - \mathbf{n}\cdot\mathbf{r}\times\mathbf{p} + B}_{T_B}) - \ln(M/r + R(\mathbf{r}))$$

In this case

$$t' = \frac{\partial\Lambda}{\partial B} = 1/T_B,$$

and the Hamiltonian T_B is integrable since it represents free particle in a rotating coordinate system ($\mathbf{n}$=angular velocity vector). $(\{\mathbf{p}^2, \mathbf{n}\cdot\mathbf{r}\times\mathbf{p}\} = \mathbf{0})$.

$$\mathbf{p} \to \mathbf{p} + c_1(\epsilon^2)\vec{\epsilon} \times \mathbf{p} + c_2(\epsilon^2)\vec{\epsilon} \times (\vec{\epsilon} \times \mathbf{p})$$
$$\mathbf{r} \to \mathbf{r} + c_1(\epsilon^2)\vec{\epsilon} \times \mathbf{r} + c_2(\epsilon^2)\vec{\epsilon} \times (\vec{\epsilon} \times \mathbf{r}).$$

The second part $-\ln(M/r)$ generates the velocity jump:

$$\mathbf{V}(s): \quad \widetilde{\delta t} = \frac{s}{M/r + R}; \quad \mathbf{F} = -M\mathbf{r}/r^3 + \frac{\partial R}{\partial \mathbf{r}}$$

$$\mathbf{p} \to \mathbf{p} + \widetilde{\delta t}\mathbf{F}.$$

Remark:

-If $R = 0$, then this algorithm conserves energy and angular momentum exactly. Thus the errors will be proportional to the perturbation.

-Possible applications: Restricted 3-B, (especially the Copenhagen problem).

If the perturbing function R is a (small) rotating quadratic expression $= \frac{1}{2}\mathbf{r}^t\widehat{\mathbf{G}}\mathbf{r}$, like the galactic tidal field, then one may move R to T_B as

$$\Lambda = \ln(\underbrace{\tfrac{1}{2}\mathbf{p}^2 - \mathbf{n}\cdot\mathbf{r}\times\mathbf{p} + \tfrac{1}{2}\mathbf{r}^t\widehat{\mathbf{G}}\mathbf{r} + B}_{T_B}) - \ln(M/r),$$

where we can assume that $\frac{1}{2}\mathbf{r}^t\widehat{\mathbf{G}}\mathbf{r}$ is independent of time (arranged by $\mathbf{n}$).

Here again

$$t' = 1/T_B \quad (\approx r/M)$$

and one must construct solution for the problem defined by the Hamiltonian $= \ln(T_B)$.

Since the Hamiltonian

$$T_B = \tfrac{1}{2}\mathbf{p}^2 - \mathbf{n}\cdot\mathbf{r}\times\mathbf{p} + \tfrac{1}{2}\mathbf{r}^t\widehat{\mathbf{G}}\mathbf{r} + B,$$

is quadratic in all the (canonical) variables, it is integrable.

$$\dot{\mathbf{p}} = -\mathbf{n} \times \mathbf{p} - \widehat{\mathbf{G}}\mathbf{r}; \quad \dot{\mathbf{r}} = \mathbf{p} - \mathbf{n} \times \mathbf{r}.$$

define the motion generated by T_B, while the velocity jump is simply

$$\mathbf{V}(s): \quad \mathbf{p} \to \mathbf{p} - s\mathbf{r}/r^2.$$

This algorithm is not any more energy preserving, but high accuracy can be used for any eccentricity.

9.3 $1/r^2$-perturbation

If

$$H = \tfrac{1}{2}\mathbf{p}^2 - m/r - \epsilon/r^2,$$

then

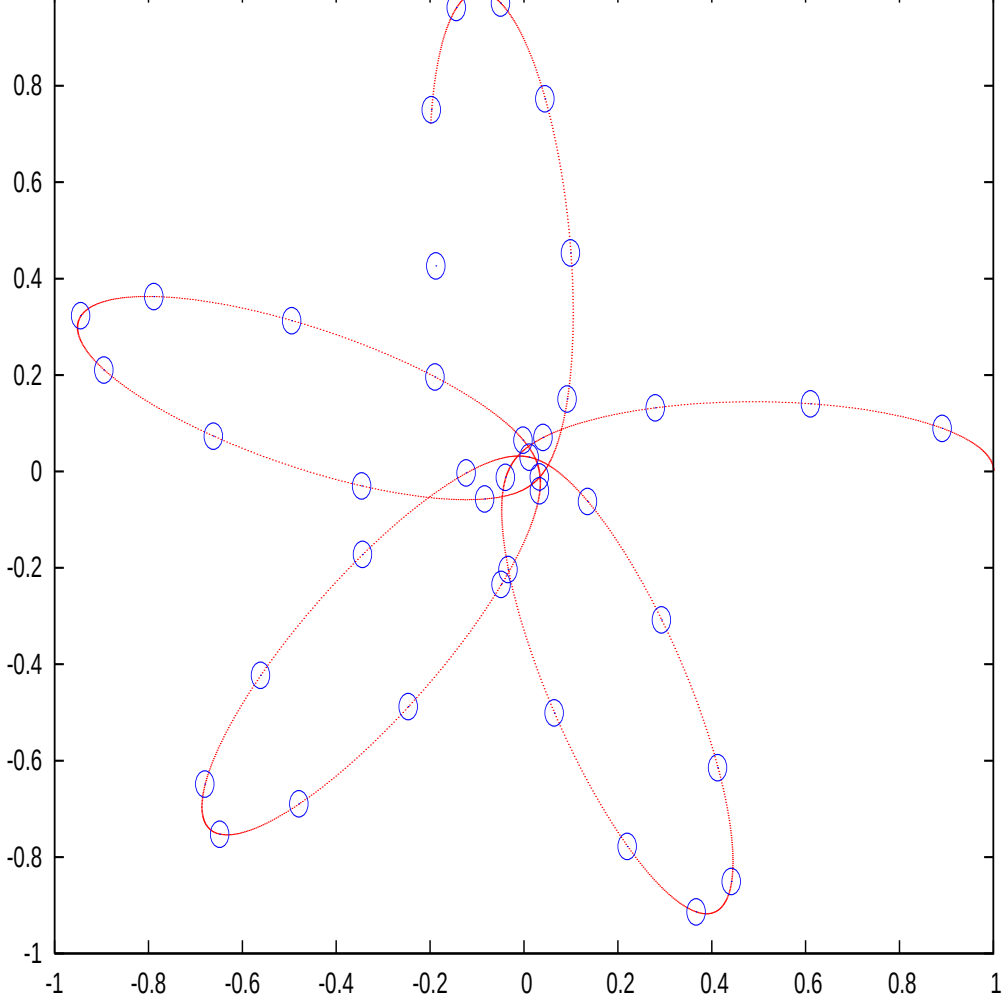
$$\Lambda = \ln(\tfrac{1}{2}\mathbf{p}^2 - \epsilon/r^2 + B) - \ln(m/r)$$

is useful since the first part

$$H_0 = \tfrac{1}{2}\mathbf{p}^2 - \epsilon/r^2 = \tfrac{1}{2}p_r^2 + \tfrac{1}{2}\frac{p_\theta^2 - 2\epsilon}{r^2}$$

is easily integrable in polar coordinates $r,\ \theta$ (momenta $p_r,\ p_\theta$).

A surprising fact is that the resulting generalised leapfrog produces a correct trajectory with only a time error. Also the time correction formulae are the same as for the logH-twobody case. Proved thus far only numerically!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1

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