The use of Hermite scheme for the soft part of $\mathrm{P^3T}$ scheme

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Internal seminar Nov 26 2025

Summary

- We derive and test several schemes to make the soft part of $\mathrm{P^3T}$ scheme 4th order in time.
- Schemes tested include Forest and Ruth, Chin and Chen, Implicit Hermite, Hermite in PEC form.
- Hermite-Hermite pair can be regarded as a simplified form of the Ahmad-Cohen scheme, and that suggests that we do not need smooth changeover function. With approximate symmetrization the energy conservation is actually quite good.

Summary

- Splitting in 2nd and 4th order
- “Splitting” for Hermite scheme
- PEC form
- Experimental result
- Summary

Second-order splitting

Eq 1 gives a separable Hamiltonian. Here, p, q are generalized momentum and coordinate.

$$H = T(p) + V(q) \tag{1}$$

The equations of motion are

$$\begin{aligned} \frac{dq}{dt} &= \frac{\partial H}{\partial p} = \frac{\partial T}{\partial p} \\ \frac{dp}{dt} &= -\frac{\partial H}{\partial q} = -\frac{\partial V}{\partial q} \end{aligned} \tag{2}$$

In usual form

With velocity v and position x, $H = v^2/2 + V(x)$

$$\begin{aligned}
\frac{dx}{dt} &= v \\
\frac{dv}{dt} &= -\frac{\partial V}{\partial x}
\end{aligned} \tag{3}$$

Let $s = (x, v)$ be the state of the system, h step size and $D(h), K(h)$ express the operators below:

$$\begin{aligned}
K(h) : v &\leftarrow v - \frac{\partial V}{\partial x} h \\
D(h) : x &\leftarrow x + vh
\end{aligned} \tag{4}$$

Usual leapfrog scheme is given by

$$s \leftarrow K(h/2) D(h) K(h/2) s \tag{5}$$

Hamiltonian Splitting

If the potential is separated to two parts:

$$V = V_{\mathrm{slow}} + V_{\mathrm{fast}} \tag{6}$$

where V_{slow} is slowly changing and V_{fast} rapidly changing, then we can introduce

$$K'(h) : v \leftarrow v - \frac{\partial V_{\mathrm{soft}}}{\partial x} \tag{7}$$

and $D'(h)$ to be an operator which evolves $s(t)$ by $H_{\mathrm{fast}} = T + V_{\mathrm{fast}}$ to $s(t+h)$.
Then,

$$s \leftarrow K'(h/2)D'(h)K'(h/2)s \tag{8}$$

is second-order leapfrog for V_{soft} and gives accurate solution (if we use accurate integrator...) for V_{hard}.
This is the basic idea of MVS or any splitting scheme.

4th order methods

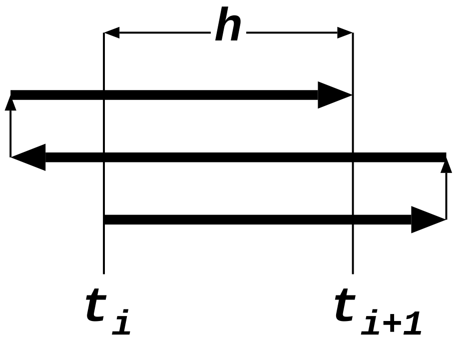
The well known Forest and Ruth scheme re-interpreted by Yoshida is the following:

$$
\begin{aligned}
S_4(h) &= L(d_1 h)L(d_2 h)L(d_1 h), \\
d_1 &= 1/(2 - 2^{1/3}), \quad d_2 = 1 - 2d_1 = -2^{1/3}/(2 - 2^{1/3})
\end{aligned} \tag{9}
$$

Here $L(h)$ is a leap frog integration with step h.

In principle, we can apply MVS like splitting to this scheme, but since this scheme includes an backward step, from time $1.35h$ to $-0.35h$, it is not convenient.

So if there is a scheme which includes only forward steps, it is much better.



Chin and Chen scheme

Chin and Chen scheme (Celestial Mechanics and Dynamical Astronomy 2005, 91, 301-322), hereafter CC scheme, is given by

$$
\begin{aligned}
p_1 &= p_0 + \frac{1}{6} f(q_0) h, \quad q_1 = q_0 + \frac{1}{2} p_1 h \\
p_2 &= p_1 + \frac{2}{3} \tilde{f}(q_1) h, \quad q_2 = q_1 + \frac{1}{2} p_2 h \\
p_3 &= p_2 + \frac{1}{6} f(q_2) h
\end{aligned}
\tag{10}
$$

The p_3, q_2 pair gives the new solution at time $t+h$. Here, f is the acceleration and $\tilde{f}$ is acceleration with correction term:

$$
\begin{aligned}
\tilde{f} &= f + \frac{1}{48} g h^2 \\
g &= \mathrm{grad}(|f|^2)
\end{aligned}
\tag{11}
$$

Rewriting Chin and Chen (CC) scheme

In 10, q_1, q_2 can be rewritten as

$$
\begin{aligned}
q_1 &= q_0 + \frac{1}{2}p_0 h + \frac{1}{12}f(q_0)h^2 \\
q_2 &= q_1 + \frac{1}{2}p_3 h - \frac{1}{12}f(q_2)h^2
\end{aligned} \tag{12}
$$

And this

$$
q_2 = q_0 + \frac{1}{2}(p_0 + p_3)h + \frac{1}{12}[f(q_0) - f(q_2)]h^2 \tag{13}
$$

This is the same as 4th-order Hermite scheme.

On the other hand, p_3 is given by

$$
p_3 = p_0 + \frac{1}{6}[f(q_0) + 4\tilde{f}(q_1) + f(q_2)]h \tag{14}
$$

This is similar to the classical 4th-order RK scheme.

Hermite scheme

If the CC scheme is not too different from the Hermite scheme, can we construct splitting scheme based on Hermite scheme?
Since the Hermite scheme is not symplectic, in the exact sense the splitting is impossible. On the other hand, we can ask if

- 4th order is achievable or not
- (approximate) time symmetry is achievable or not

Hermite scheme (2)

Hermite scheme is given by

$$\begin{aligned} x_1 &= x_0 + \frac{1}{2}(v_0 + v_1)h + \frac{1}{12}[f(x_0) - f(x_1)]h^2 \\ v_1 &= v_0 + \frac{1}{2}(f(x_0) + f(x_1))h + \frac{1}{12}[j(x_0, v_0) - j(x_1, v_1)]h^2 \end{aligned} \quad (15)$$

Here j is the time derivative of f. The Hermite scheme itself is implicit. In PEC form it is 4th order but not time symmetric. With PECEC form it is practically time symmetric.

However, since the Hermite scheme does not have the form of Kick-Drift-Kick, it is unclear how we can combine Hermite soft part and hard part.

First try

In leapfrog. we first update v with

$$v_{\mathrm{softkick}} = v0 + \frac{1}{2} a_0 h \tag{16}$$

and then integrate (x_v) with H_{hard}. Finally we update v with

$$v_1 = v_{\mathrm{hard}} + \frac{1}{2} a_1 h \tag{17}$$

By analogy, we can think of applying

$$v_{\mathrm{softkick}} = v_0 + \frac{1}{2} a_0 h + \frac{1}{12} j_0 h^2 \tag{18}$$

When $H_{\mathrm{hard}} = T$, x moves with constant v_{softkick}, and integration with H_{hard} gives

$$x_{\mathrm{hard}} = x + v_0 h + \frac{1}{2} a_0 h^2 + \frac{1}{12} j_0 h^3 \tag{19}$$

First try(2)

From 15 we can rewrite x in the form without v_1, to have

$$x_1 = x_0 + v_0 h + (a_0/3 + a_1/6)h^2 + (j_0 - j_1)h^3/24 \tag{20}$$

Using x_{hard}, we have

$$x_1 = x_{\text{hard}} + (-a_0/6 + a_1/6)h^2 - (j_0 + j_1)h^3/24 \tag{21}$$

Also v_1 can be given by

$$v_1 = v_{\text{hard}} + \frac{1}{2}a_1 h - \frac{1}{12}j_1 h^2 \tag{22}$$

First try(3)

When H_{hard} contains V_{hard}, we can apply the following steps.

1. **From 18 obtain v_{softkick}**
2. **Integrate $(x, v_{\mathrm{softkick}})$ using H_{hard} to $t + h$. The result is $(x_{\mathrm{hard}}, v_{\mathrm{hard}})$**
3. **Using 21 and 22 obtain (x_1, v_1). This step is implicit.**

Even when implicit equation is solved, this scheme is not time symmetric.

First try(4)

Since the formula 21 itself is time symmetric, we can construct a new form:

$$\begin{aligned} x_{\mathrm{softkick}} &= x_0 - a_0 h^2/6 - j_0 h^3/24 \\ v_{\mathrm{softkick}} &= v_0 + \frac{1}{2} a_0 h + \frac{1}{12} j_0 h^2 \end{aligned} \tag{23}$$

we first apply O(h^2) correction to x, and then by integrating H_{hard} to $t+h$ we obtain $(x_{\mathrm{hard2}}, v_{\mathrm{hard2}})$. Then we have

$$\begin{aligned} x_1 &= x_{\mathrm{hard2}} + a_1 h^2/6 - j_1 h^3/24 \\ v_1 &= v_{\mathrm{hard2}} + \frac{1}{2} a_1 h - \frac{1}{12} j_1 h^2 \end{aligned} \tag{24}$$

We can see that this form is time symmetric.

Predictor

We need predictor. This can be obtained by the difference between the usual predictor

$$\begin{aligned} x_p &= x_0 + v_0 h + a_0 h^2/2 + j_0 h^3/6 \\ v_p &= v_0 + a_0 h + j_0 h^2/2 \end{aligned} \quad (25)$$

and $x_{\rm hard}$, and given by

$$\begin{aligned} x_p &= x_{\rm hard} + a_0 h^2/6 + j_0 h^3/12 \\ v_p &= v_{\rm hard} + a_0 h/2 + j_0 h^2/2 \end{aligned} \quad (26)$$

Problem and Possible solution

As will be seen later, This scheme is not 4th order. The reason is that we have added O(h^2) correction to x in 23.
In the case of the CC scheme, we apply the correction to v at $t + h/2$. So consider the following form:

$$
\begin{aligned}
v_{ha} &= v_0 + \frac{1}{6} f_0 h \\
x_h &= x_0 + \frac{1}{2} v_{ha} h \\
v_{hb} &= v_{ha} + \alpha \\
x_1 &= x_h + \frac{1}{2} v_{hb} h \\
v_1 &= v_{hb} + \frac{1}{6} f_1 h
\end{aligned}
\tag{27}
$$

Hermite scheme in CC-like form

Here, v_1 is expressed as

$$v_1 = v_0 + \frac{1}{6}(f_0 + f_1)h + \alpha \tag{28}$$

So, by comparing 31 and Hermite scheme 15 we have

$$\alpha = \frac{1}{3}(f_0 + f_1)h + \frac{1}{12}(j_0 - j_1)h^2 \tag{29}$$

For predictor, what we can do is to use $f_1 = f_0 + hj_0, j_1 = j_0$ and we have

$$\alpha_{\mathrm{pred}} = \frac{1}{3}(f_0 + f_0 + hj_0)h = \frac{2}{3}f_0h + \frac{1}{3}j_0h^2 \tag{30}$$

Hermite scheme in CC-like form (2)

The entire scheme is given by

$$
\begin{aligned}
v_{ha} &= v_0 + \frac{1}{6} f_0 h \\
x_h, v_{ha2} &= F(x_0, v_{ha}, H_{\mathrm{hard}}, h/2) \\
v_{hb} &= v_{ha2} + \frac{1}{3}(f_0 + f_1)h + \frac{1}{12}(j_0 - j_1)h^2 \\
x_1, v_{hb2} &= F(x_h, v_{hb}, H_{\mathrm{hard}}, h/2) \\
v_1 &= v_{hb2} + \frac{1}{6} f_1 h
\end{aligned} \tag{31}
$$

where $F(x, v, H_{\mathrm{hard}}, h)$ is the hard step.

Unlike the CC scheme, this form is implicit, since v_{hb} requires f_1 and j_1.

Hermite scheme with PEC form

Predictor:

$$
\begin{aligned}
v_{ha} &= v_0 + \frac{1}{6} f_0 h \\
x_h, v_{ha2} &= F(x_0, v_{ha}, H_{\mathrm{hard}}, h/2) \\
v_{hb,p} &= v_{ha2} + \frac{2}{3} f_0 h + \frac{1}{3} j_0 h^2 \\
x_{1,p}, v_{hb2,p} &= F(x_h, v_{hb,p}, H_{\mathrm{hard}}, h/2) \\
v_{1,p} &= v_{hb2} + \frac{1}{6} f_{1,p} h
\end{aligned}
\tag{32}
$$

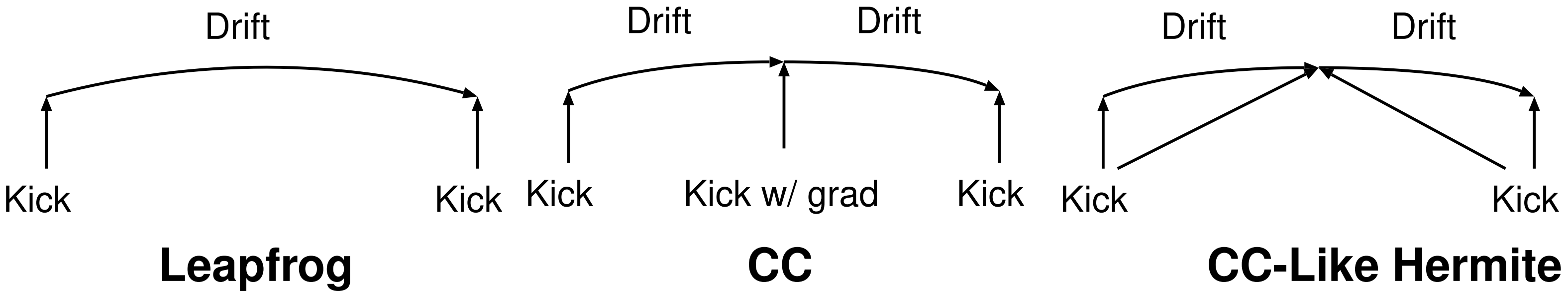
For corrector, we can of course use 31. However, that means we need to perform the hard part at each iteration. This is necessary to achieve true time symmetry, but if we do not require true time symmetry, we can store the change by H_{hard} in d_x, d_v and use it.

Corrector with single-path hard part

$$
\begin{aligned}
d_x &= x_{1,p} - x_h \\
d_v &= v_{hb2,p} - v_{hb,p} \\
v_{hb,c} &= v_{ha2} + \frac{1}{3}(f_0 + f_1)h + \frac{1}{12}(j_0 - j_1)h^2 \\
x_{1,c} &= x_h + d_x + d_v h/2 \\
v_{hb2,c} &= v_{hb,c} + d_v \\
v_{1,c} &= v_{hb2} + \frac{1}{6} f_1 h
\end{aligned} \tag{33}
$$

This scheme is not time symmetric. However, one advantage over the CC scheme is that this scheme, at least in the PEC form, requires only one soft-force calculation per timestep, and yet achieves the 4th-order accuracy.

Three schemes



- **Both CC and CC-like Hermite are 4th-order**
- **CC is symplectic/time-symmetric but requires additional force calculation**
- **CC-like Hermite is not symplectic but can be time symmetric (need corrector)**

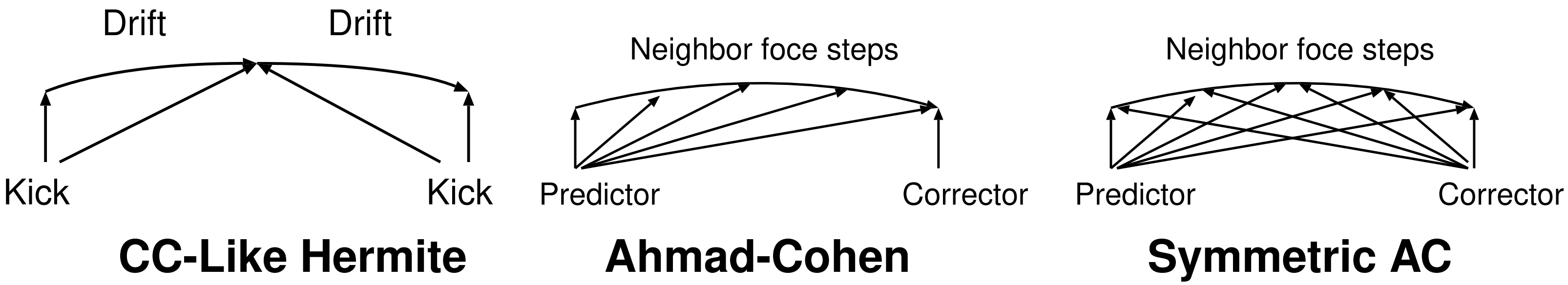
Relationship with the Ahmad-Cohen scheme

- Since we use the same Hermite scheme for both soft and hard part, in principle we can go back to the Hermite Ahmad-Cohen scheme (Makino and Aarseth 1992, PASJ, 44, 151, HACS), in which we use the predictor for the soft force and use it for hard steps.
- In that case, as in the Ahmad-Cohen scheme, it is more natural not to use the changeover function but simply change the membership of neighbor sphere in each soft timestep.
- Actually, our new form can be regarded as a simplified form of the Ahmad-Cohen scheme, where we apply the soft (distant) force only at t, $t + h/2$ and $t + h$.

(Approximate) symmetrization of non-smooth cutoff

- Simple non-smooth cutoff using neighbors at the start of the timestep results in the break of the time symmetry.
- In practice with 4th-order scheme this might be okay.
- We can restore the time symmetry to some extent by using the symmetric neighbor condition, in which we use both the current position and position at the new time (predicted time is not perfect but practically okay)

Relationship with the Ahmad-Cohen scheme



- **The AC scheme applies predicted soft force at each hard step**
- **In the AC scheme coreccted soft force is applied once. Thus, AC scheme is not time-symmetric**
- **It is possible to apply iteration of hard part, to achieve full time symmetry even with the AC scheme.**

Experimental setup

Only with 2-body problem so far. Consider

$$
\begin{aligned}
\frac{dx}{dt} &= v \\
\frac{dv}{dt} &= a \\
a &= -m\frac{x}{|x|^3}
\end{aligned}
\tag{34}
$$

with $G = 1, m = 1$. The time derivative of the acceleration is given by

$$
j = -m\frac{v}{|x|^3} + 3m\frac{x}{|x|^4}\frac{d|x|}{dt} = -m\left[\frac{v}{|x|^3} + 3\frac{(v\cdot x)x}{|x|^5}\right]
\tag{35}
$$

Velocity gradient

Velocity gradient for the CC scheme is

$$g = \mathrm{grad}(|a|^2) = 2|a|\mathrm{grad}|a| \tag{36}$$

From

$$\frac{\partial |a|}{\partial x} = -m\frac{\partial}{\partial x}\left(\frac{1}{x^2+y^2+z^2}\right) = -2m\frac{x}{|\mathrm{x}|^4} \tag{37}$$

$$g = \mathrm{grad}(|a|^2) = -4m^2\frac{\mathrm{x}}{|\mathrm{x}|^6} \tag{38}$$

With changeover function $K(r)$

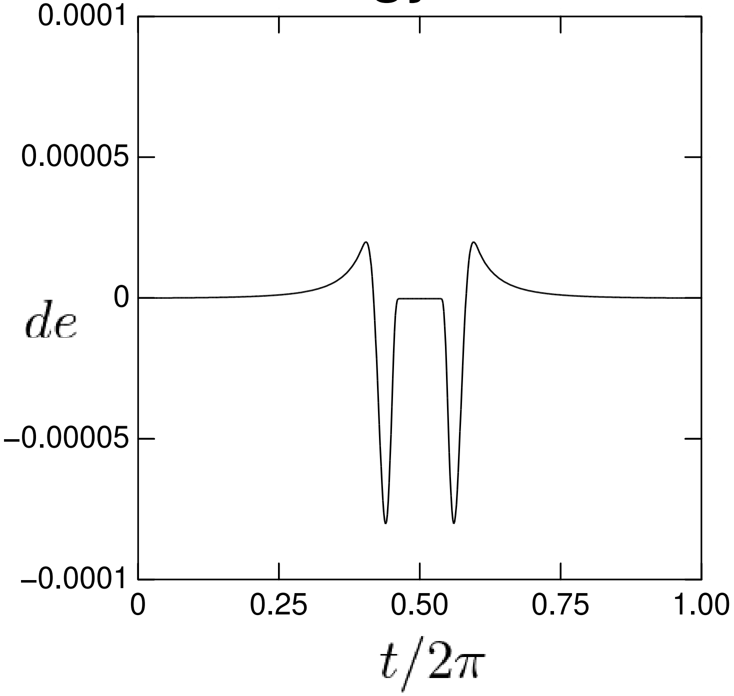
$$\begin{aligned} g &= \mathrm{grad}(|a|^2K^2) = -4m^2\frac{\mathrm{x}}{|\mathrm{x}|^6}K^2 + 2m^2\frac{1}{|\mathrm{x}|^5}K\frac{dK}{dr}\mathrm{x} \\ &= 2m^2\frac{\mathrm{x}}{|\mathrm{x}|^5}K\left(-2\frac{K}{|\mathrm{x}|} + \frac{dK}{dr}\right) \end{aligned} \tag{39}$$

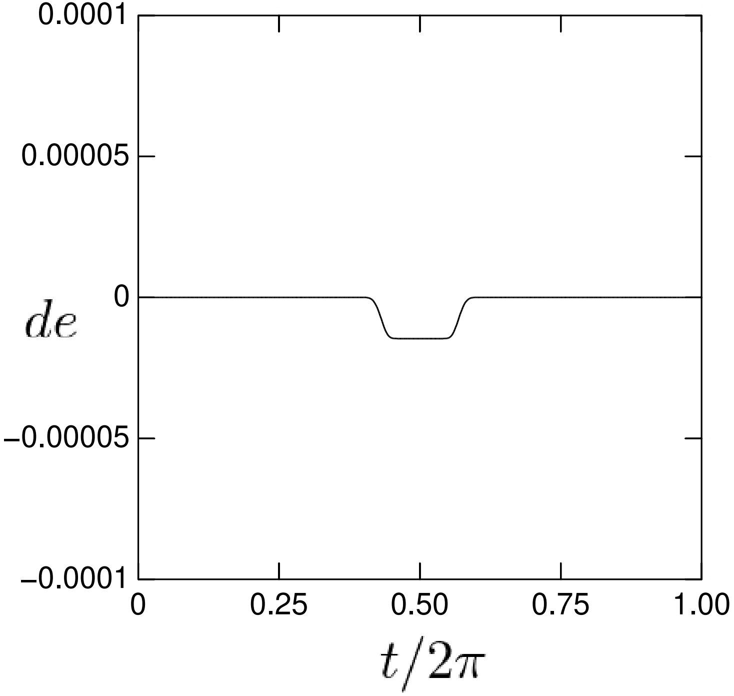
Experimental setup (2)

$e = 0.9$, $a = 1$, $K(x) = \int x^4(1-x)^4 dx$ and it is applied to $|x|$ in $(0.5, 1.0)$.
We used classical RK4 with variable timestep for hard part and various schemes derived in this note for the soft part. Unless otherwise noted $h = 0.01$.

Leapfrog and simple symmetrized Hermite

We show energy error in one orbit

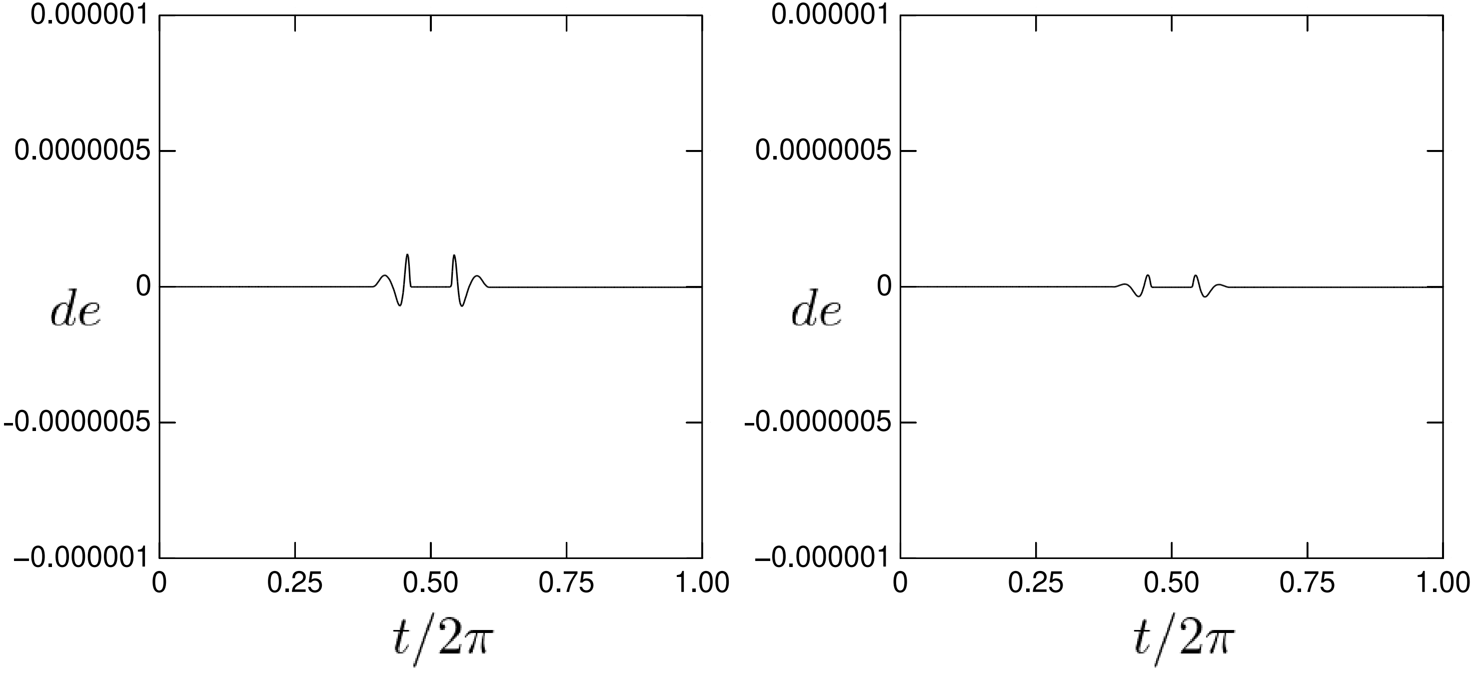




Leapfrog **Equations 23、 24**

We can see the jump in the energy is still there.

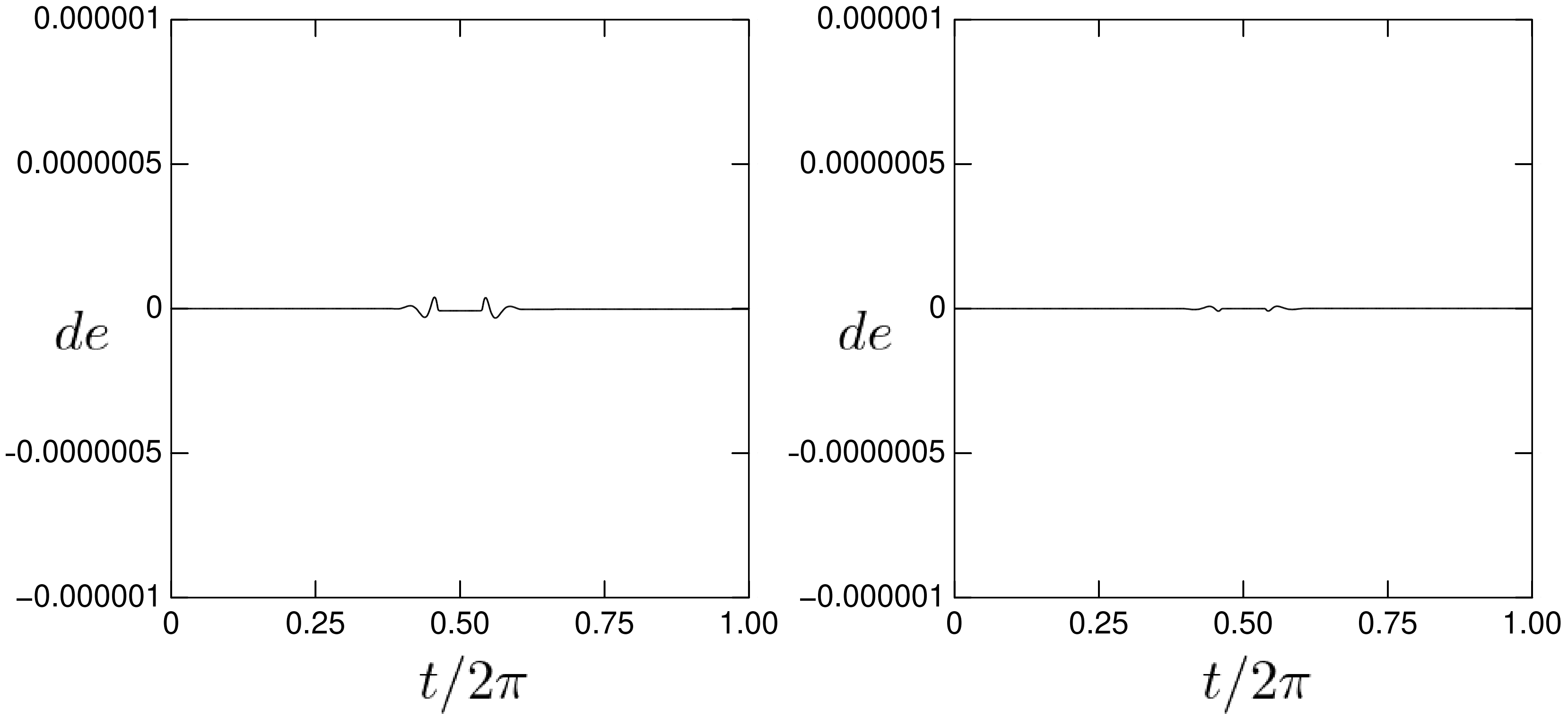
True 4th schemes (1)



Forest and Ruth **Symmetric (iterated) Hermite**

Max energy error is around 1/1000 of that of leapfrog (with 600 steps/orbit)

True 4th schemes (2)

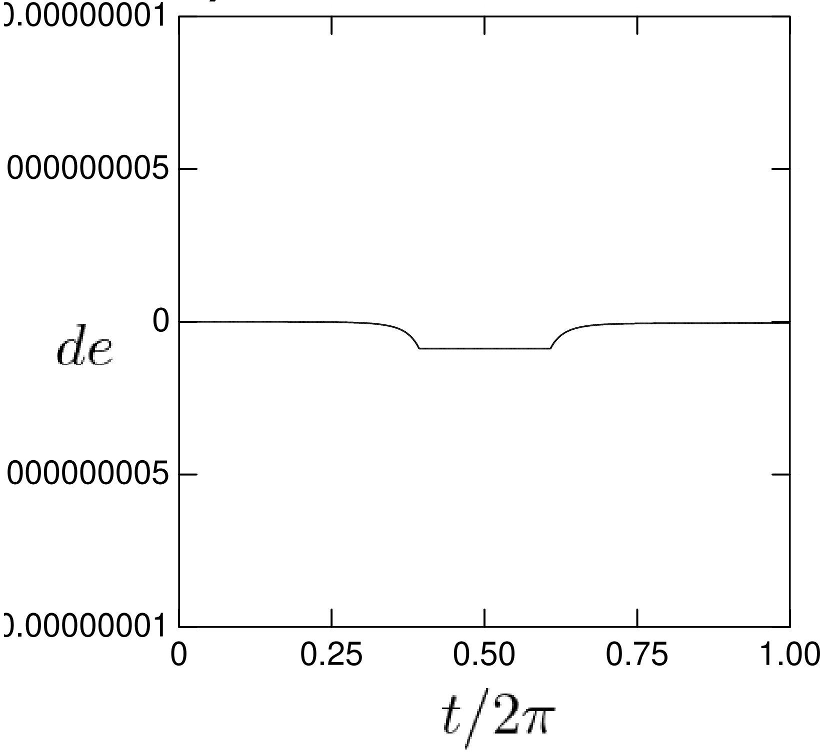


PEC Hermite **CC scheme**

PEC hermite requires one force calculation per step and CC

True 4th schemes (3)

Non-smooth switching with approximate symmetrization (switch at $\mathrm{r} = 1$)



Max energy error is around 1/100 of that of 4th-order schemes with smooth changeover function.
Since the time derivatives of the changeover functions do not appear in the error, the max error is small.

Summary

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- Schemes tested include Forest and Ruth, Chin and Chen, Implicit Hermite, Hermite in PEC form.
- Hermite-Hermite pair can be regarded as a simplified form of the Ahmad-Cohen scheme, and that suggests that we do not need smooth changeover function. With approximate symmetrization the energy conservation is actually quite good.