Geometric Integrators for N-Body Systems

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Overview

Application of Geometric Integrators to N-Body systems, methods that exactly conserve some qualitative properties associated with the system being studied.

Higher Order methods derived from low order methods by composition.

Application of Sundman type time transformations to N-Body systems.

Higher order methods with time transformations.

Motivation

The Adaptive Verlet method is an explicit variation of the Verlet method with the application of a Sundman time transformation.

It has been observed that when applying composition methods to this method that orders above the 4^{th} are not obtained.

We look at an analasis of the problem and provide two schemes to allow higher orders to be obtained.

Consider a system of N bodies with masses $m_1, m_2, \cdots, m_N$ with:
body coordinates $q := (q_1, q_2, \cdots, q_N)^T$
body momenta $p := (p_1, p_2, \cdots, p_N)^T$
given a potential energy function $V(q)$ and kinetic energy function $T(p)$ we have a Hamiltonian or energy function

$$H(q,p) = T(p) + V(q)$$

The differential equations for a Hamiltonian system are

$$\dot{q} = \nabla_p T(p), \quad \dot{p} = -\nabla_q V(q)$$

This can be re-written, with $z = (q,p)$, as

$$\dot{z} = J\nabla_z H(z)$$

where J is a skew symmetric matrix i.e. $J^T = -J$.

The Solar system is an N-body system and N=10 if only the main planets are included, with the Sun, in the model. The Hamiltonian equation, where m_i is the mass of the i^{th} planet and G is the gravitational constant is

$$H(q,p) = \frac{1}{2}\sum_{i=1}^{10}\frac{||p_i||^2}{m_i} - \sum_{i=1}^{10}\sum_{j=i+1}^{10}\frac{Gm_im_j}{||q_i - q_j||}$$

Then the differential equations are

$$\dot{q}_i = \frac{p_i}{m_i}, \quad \dot{p}_i = \sum_{j=1,j\neq i}^{10}\frac{Gm_im_j(q_i - q_j)}{||q_i - q_j||^3}, \quad i = 1, 2, \cdots, N$$

This model treats the Sun as one of the bodies and the entire system orbits around the centre of mass of the system.

The Arenstorf orbit is a 3-body model which consists of two larger bodies which rotate about their centre of mass, and a third body which moves in the same plane. If system units are such that sum of masses, G and angular velocity are one then

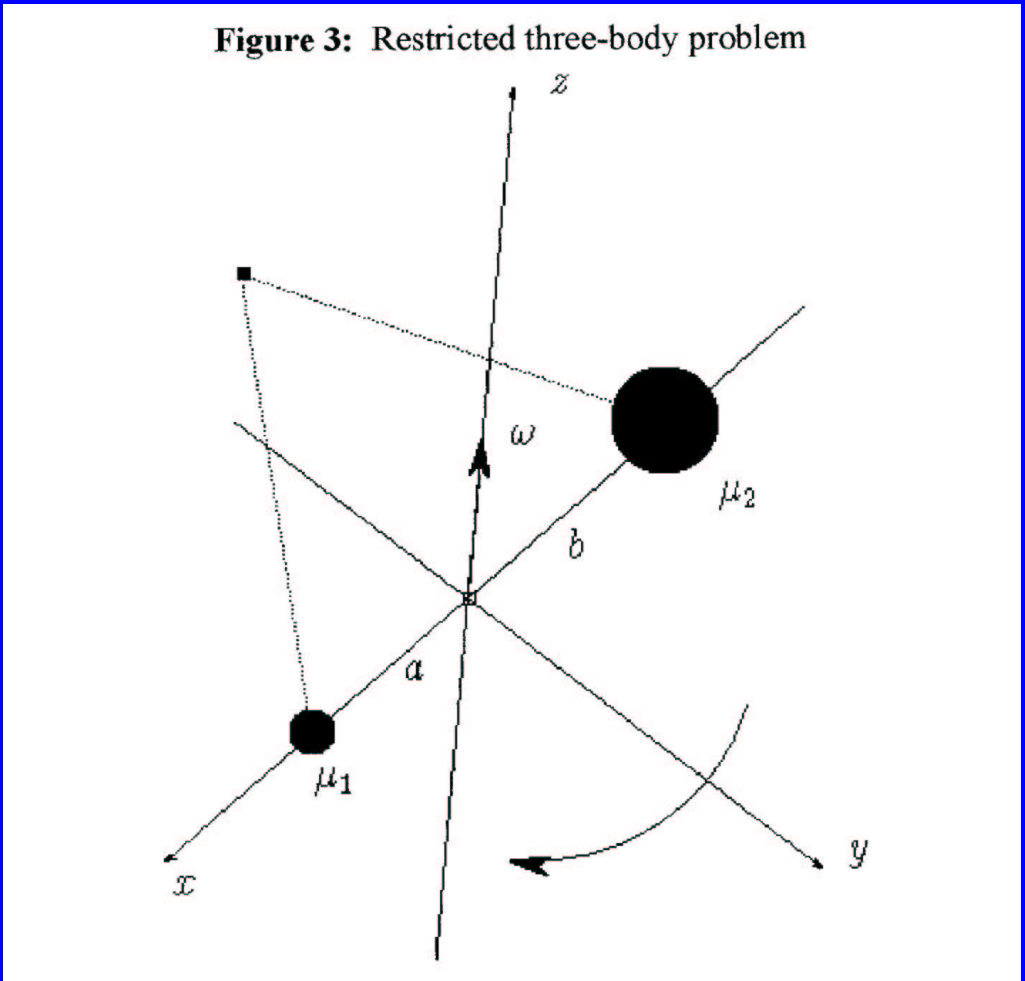
$$\ddot{x} = 2\dot{y} - V_x(x,y), \quad \ddot{y} = 2\dot{x} - V_y(x,y)$$

where

$$V(x,y) = -\frac{x^2+y^2}{2} - \frac{M_2}{r_1} - \frac{M_1}{r_2},\ r_i = \sqrt{(x+M_i)^2+y^2},\ i = 1,2$$

Let $q = (x, y, 0)^T,\ p = (\dot{x}, \dot{y}, 0)^T$ then we get a Hamiltonian $H = \frac{||p||^2}{2} + V(q),\ V(q) = v(x,y)$
The equations of motion are equivalent to
$\dot{q} = p, \quad \dot{p} = B \times p - \nabla_q V(q)$, where $B = (0, 0, -2)^T$

Arenstorf Orbit diagram



If $N \geq 3$ then the N-body problem has no general analytic solution, so we need to simulate it using a time-stepping scheme such as a Geometric Integrator.

Geometric Integrators will approximate the actual solution of the system, but will also have charictoristics which will be usefull in qualitativly improving the simulation.

Two charictoristics which are improtant in the simulation of Hamiltonian systems are Symplectic and being Time-reversible.

Hamiltonian systems have a symplectic structure which gives it geometric implications on the way the flow map acts on initial conditions. For example, the volume of a set of points in phase space is conserved by a Hamiltonian flow.

Given a Hamiltonian $\dot{z} = J\nabla_z H(z)$ and a smooth symplectic mapping $\Psi = \Psi(z)$ this is characterised by the algebraic condition

$$\frac{\delta}{\delta z}\psi^T J^{-1}\frac{\delta}{\delta z}\psi = J^{-1}$$

Geometric Integrators which are symplectic include Implicit Midpoint and Verlet method.

Time-reversibity is an important geometric property of Newton's equations of motion. A Hamiltonian

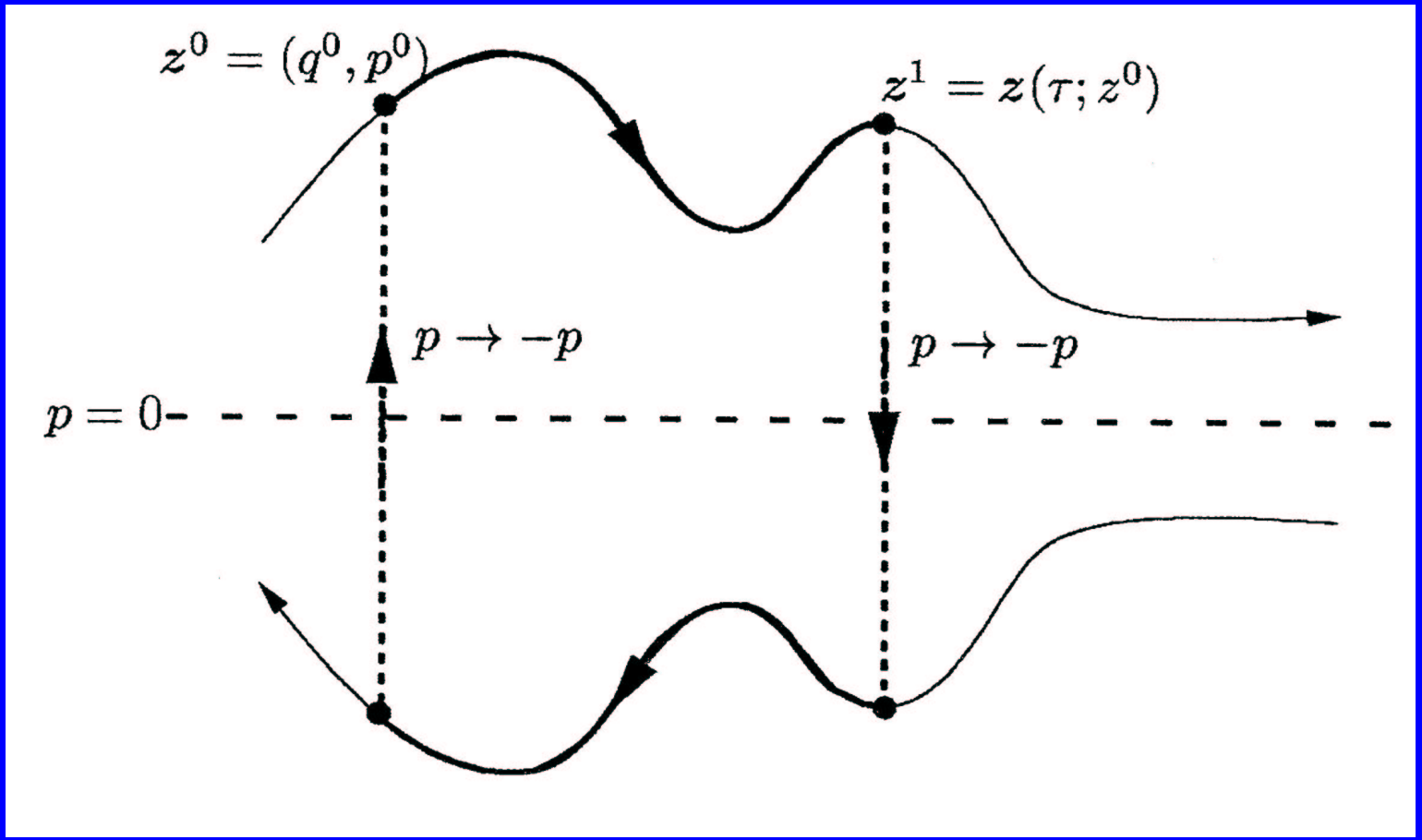
$$H(q,p) = \frac{p^T M^{-1} p}{2} + V(q)$$

is invariant under the a reflection symmetry $q \mapsto q, \quad p \mapsto -p$
The differential equations are, 1) before and 2) after $p \mapsto -p$

1) $\dot{q} = M^{-1}p, \quad \dot{p} = -\nabla_q V(q)$ 2) $\dot{q} = -M^{-1}p, \quad -\dot{p} = -\nabla_q V(q)$

If we now replace time t by $-t$ we get the original Hamiltonian system.
Hence with repect to q the solutions look the same backwards and forwards in time.

Time-reversible diagram



Given a Hamiltonian system with flow map Ψ_h such that

$$z(t+h) = z^{n+1} = \Psi_h z^n = \Psi_h z(t)$$

and a geometric integrator with map Φ_h then the integrator is said to be p^{th} order if

$$||\Psi_h(z) - \Phi_h(z)|| = O(p^{n+1})$$

It is possible to construct high order methods from low order methods by composition. This generally falls into two catagories, composition methods for seperable Hamiltonian systems and composition methods based on second order symmetric methods. These are generally based on the work by Yoshida.

The work by Yoshida is based on the following assumptions: Given a system with flows $exp(tX)$, where X denotes a vector field on some space with coordinates z, time t and system initial conditions z^0 i.e

$$\dot{z} = X(z) \Rightarrow z(t) = exp(tX)z^0$$

and, if we can write $X = A + B$, we have a map φ_τ such that

$$\varphi_\tau : z(t) \mapsto \hat{z} = exp(\tau A)exp(\tau B)(z(t)) = z(t+\tau) + O(\tau^2)$$

we can increase the order to p by composing several stages to get

$$exp(b_m tB)exp(a_m tA) \circ \cdots \circ exp(b_1 tB)exp(a_1 tA) = exp(t(A+B)) + O(t^{p+1})$$

with coefficients a_i, b_i calculated by using the Baker-Campbell-Hausdorf (BCH) equation.

BCH equation

The Baker-Campbell-Hausdorf (BCH) equation for two non-commutative operators X, Y is

$$exp(X)exp(Y) = exp(X + Y + \tfrac{1}{2}[X,Y] + \tfrac{1}{12}([X,X,Y] - [Y,Y,X]) + \tfrac{1}{24}[X,Y,Y,X] + \tfrac{1}{720}([Y,Y,Y,Y,X] + [\cdots]) + \cdots)$$

where:$[X,Y] := XY - YX$ is the commutator of X and Y.

This can be extended to a three term product:

$$exp(X)exp(Y)exp(X) = exp(2X + Y + \tfrac{1}{6}([Y,Y,X] - [X,X,Y]) + \tfrac{7}{360}[X,X,X,X,Y] + \cdots)$$

If we define a symmetric 2^{nd} order method as

$$S_{2^{nd}}(\tau) := exp(\tfrac{\tau}{2}A)exp(\tau B)exp(\tfrac{\tau}{2}A)$$
$$= exp(\tau\alpha_1 + \tau^3\alpha_3 + \tau^5\alpha_5 + \tau^7\alpha_7 + \cdots)$$

for some A, B where $\alpha_1 := A+B, \alpha_3 := \frac{1}{12}[B,B,A]-\frac{1}{24}[A,A,B])$, etc.

Note there are no even terms in τ as we would expect from the symmetric condition, hence any symmetric method is of order of 2 or greater.

2^{nd} order method coefficients

Let $S_{2nd}(\tau) = exp(\tau\alpha_1 + \tau^2\alpha_2 + \tau^3\alpha_3 + \tau^4\alpha_4 + \tau^5\alpha_5 + \cdots)$
and $S_{2nd}(-\tau) = exp(-\tau\alpha_1 + \tau^2\alpha_2 - \tau^3\alpha_3 + \tau^4\alpha_4 - \tau^5\alpha_5 + \cdots)$

then $S_{2nd}(\tau)S_{2nd}(-\tau) = exp(2\tau^2\alpha_2 + O(\tau^3))$ by the BHC formula
But $S_{2nd}(\tau)S_{2nd}(-\tau) = 1$ hence $\alpha_2 = 0$
then $S_{2nd}(\tau)S_{2nd}(-\tau) = exp(2\tau^4\alpha_4 + O(\tau^5)) \Rightarrow \alpha_4 = 0$ etc.

Hence $\alpha_2 = \alpha_4 = \alpha_6 = \cdots = 0$ for all symmetric methods.

The 4^{th} order method is then constructed as follows:

$$S_{4^{th}}(\tau) := S_{2nd}(\tau x_1) S_{2nd}(\tau x_0) S_{2nd}(\tau x_1)$$

Then

$$S_{2nd}(\tau x_0) = exp(\tau x_0 \alpha_1 + \tau^3 x_0^3 \alpha_3 + \tau^5 x_0^5 \alpha_5 + \tau^7 x_0^7 \alpha_7 + \cdots)$$
$$S_{2nd}(\tau x_1) = exp(\tau x_1 \alpha_1 + \tau^3 x_1^3 \alpha_3 + \tau^5 x_1^5 \alpha_5 + \tau^7 x_1^7 \alpha_7 + \cdots)$$

Using the BCH formula we get

$$S_{4^{th}}(\tau) = exp(\tau(x_0 + 2x_1)\alpha_1 + \tau^3(x_0^3 + 2x_1^3)\alpha_3 + O(\tau^5))$$

To obtain the 4^{th} order method we must cancel the τ^3 term by solving $x_0 + 2x_1 = 1, \;\; x_0^3 + 2x_1^3 = 0$ and this yeilds exact values for the coefficients x_0 and x_1.

The process can be repeated to get higher order methods. It is possible to solve for the coefficients for fewer steps numerically.

In some N-body problems it can be an advantage to use a variable step size scheme so that smaller steps are used near to close approaches.

Given a Hamiltonian with differential equations

$$\dot{q} = \nabla_p H(q,p), \quad \dot{p} = -\nabla_q H(q,p)$$

and a Sundman time re-paramiterisation function $\frac{dt}{d\tau} = G(q,p)$ we can re-write the differential equations as

$$\dot{q}\frac{dt}{d\tau} = \frac{dq}{d\tau} = G(q,p)\nabla_p H(q,p), \quad \dot{p}\frac{dt}{d\tau} = \frac{dp}{d\tau} = -G(q,p)\nabla_q H(q,p)$$

This system is not Hamiltonian unless G is a constant function, but time reversibility is maintained if

$$G(q,p) = G(q,-p) \text{ and } G(q,p) > 0.$$

A typical G function could be $||q||^{\frac{3}{2}}$.

Re-paramiterised Verlet Method

A variable step method for system $H(q,p) = T(p) + V(q)$ with re-paramiterisation function $\frac{dt}{d\tau} = G(q,p)$

$$p^{n+\frac{1}{2}} = p^n - \tfrac{\tau}{2} G(q^n, p^n) \bigtriangledown_q V(q^n)$$
$$q^{n+\frac{1}{2}} = q^n + \tfrac{\tau}{2} G(q^n, p^n) \bigtriangledown_p T(p^{n+\frac{1}{2}})$$
$$q^{n+1} = q^{n+\frac{1}{2}} + \tfrac{\tau}{2} G(q^{n+1}, p^{n+1}) \bigtriangledown_p T(p^{n+\frac{1}{2}})$$
$$p^{n+1} = p^{n+\frac{1}{2}} - \tfrac{\tau}{2} G(q^{n+1}, p^{n+1}) \bigtriangledown_q V(q^{n+1})$$

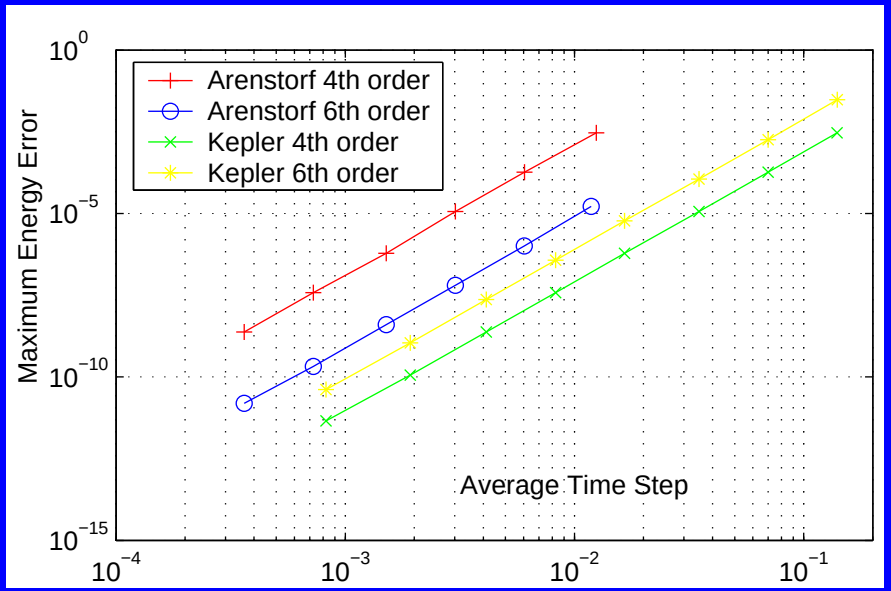
resulting in implicit terms for q^{n+1} and p^{n+1}. It is common to use $G = G(q)$, here only the equation for q^{n+1} is implicit.
To get an explicit method we need to use the Adaptive Verlet method.

Variable step method, with re-paramiterisation function $\frac{dt}{d\tau} = G(q,p)$, scalar variables $g^n,\ g^{n+1}$

$$p^{n+\frac{1}{2}} = p^n - \frac{\tau}{2} g^n \bigtriangledown_q V(q^n)$$
$$q^{n+\frac{1}{2}} = q^n + \frac{\tau}{2} g^n \bigtriangledown_p T(p^{n+\frac{1}{2}})$$
$$\frac{1}{g^{n+1}} + \frac{1}{g^n} = \frac{2}{G(q^{n+\frac{1}{2}}, p^{n+\frac{1}{2}})}$$
$$q^{n+1} = q^{n+\frac{1}{2}} + \frac{\tau}{2} g^{n+1} \bigtriangledown_p T(p^{n+\frac{1}{2}})$$
$$p^{n+1} = p^{n+\frac{1}{2}} - \frac{\tau}{2} g^{n+1} \bigtriangledown_q V(q^{n+1})$$

This method is 2^{nd} order, explicit and time-reversible.

We want to use the Adaptive Verlet method as the base method for higher order schemes to get time re-paramiterisation. Numerical experiments with 4^{th} and 6^{th} order composition schemes gave 4^{th} order for both schemes.



Backward Error Analysis of the Adaptive Verlet method

A backward error analysis of the variable step size method for Hamiltonian system

$$\dot{q} = M^{-1}p, \quad \dot{p} = F(q)$$

is given in a paper by Stephane Cirilli, Ernst Hairer and Benedict Leimkukler. The method can be formally written as

$$q^n = \tilde{q}(t_n)+(-1)^n\hat{q}(t_n), p^n = \tilde{p}(t_n)+(-1)^n\hat{p}(t_n), g^n = \tilde{g}(t_n)+(-1)^n\hat{g}(t_n)$$

where $t_n = n\tau$ and

$$\begin{aligned}
\tilde{q}' &= \tilde{g}M^{-1}\tilde{p} + \tau^2\tilde{Q}_2(.) + \cdots, & \hat{q} &= \tau^2\hat{Q}_2(.) + \cdots \\
\tilde{p}' &= \tilde{g}F(\tilde{q}) + \tau^2\tilde{P}_2(.) + \cdots, & \hat{p} &= \tau^2\hat{P}_2(.) + \cdots, \\
\tilde{g} &= G(\tilde{q},\tilde{p}) + \tau^2\tilde{G}_2(.) + \cdots, & \hat{g}' &= \hat{G}(.) + \tau^2\hat{G} + 2(.) + \cdots,
\end{aligned}$$

All of the expansions are formal and in even powers of τ.

We can re-write these equations as

$$z^n = \tilde{z}^n + (-1)^n \hat{z}^n = F_n(\bar{z}^n)$$

for some function F_n, where

$$z^n = \begin{pmatrix} q^n \\ p^n \\ g^n \end{pmatrix}, \tilde{z}^n = \begin{pmatrix} \tilde{q}^n \\ \tilde{p}^n \\ \tilde{g}^n \end{pmatrix}, \hat{z}^n = \begin{pmatrix} \hat{q}^n \\ \hat{p}^n \\ \hat{g}^n \end{pmatrix}, \bar{z}^n = \begin{pmatrix} \tilde{q}^n \\ \tilde{p}^n \\ \hat{g}^n \end{pmatrix}$$

Since the differential equations for $\tilde{z}$ are a perturbation of the origional system there exists a mapping Φ_τ such that

$$\tilde{z}^{n+1} = \Phi_\tau \tilde{z}^n$$

We can also show that F_n has an inverse, hence there is a mapping $\Psi_\tau^n = F_{n+1} \circ \Phi_\tau \circ F_n^{-1}$ such that $z^{n+1} = \Psi_\tau^n z^n$.

Since, if $\hat{z} \neq 0$, $F_n \neq F_{n+1}$ but $F_n = F_{n+2k}, \quad k \in Z, \quad \forall n$. Also from the above analasis $\hat{z} = O(\tau^4)$ hence

$$\Psi_\tau^n = \Psi_\tau^{n+1} + O(\tau^4)$$

If we substutute this back into Yoshida's equations we get

$$\begin{aligned} S_{2^{nd}}(\tau x_0) &= exp(\tau x_0 \alpha_1 + \tau^3 x_0^3 \alpha_3 + \tau^5 x_0^5 \alpha_5 + \tau^7 x_0^7 \alpha_7 + \cdots) \\ S_{2^{nd}}(\tau x_1) &= exp(\tau x_1 \alpha_1 + \tau^3 x_1^3 \alpha_3 + \tau^5 x_1^5 \alpha_5 + \tau^7 x_1^7 \alpha_7 + \cdots) + O(\tau^4) \\ &= exp(\tau x_1 \alpha_1 + \tau^3 x_1^3 \alpha_3 + \tau^5 x_1^5 \alpha_5 + O(\tau^4)) \\ &= exp(\tau x_1 \alpha_1 + \tau^3 x_1^3 \alpha_3 + \tau^5 x_1^5 \alpha_5 + O(\tau^5)) \end{aligned}$$

since the method is symmetrical.

From this we can see that the τ^5 term cannot be eliminated and hence we cannot get methods with orders above 4^{th}.

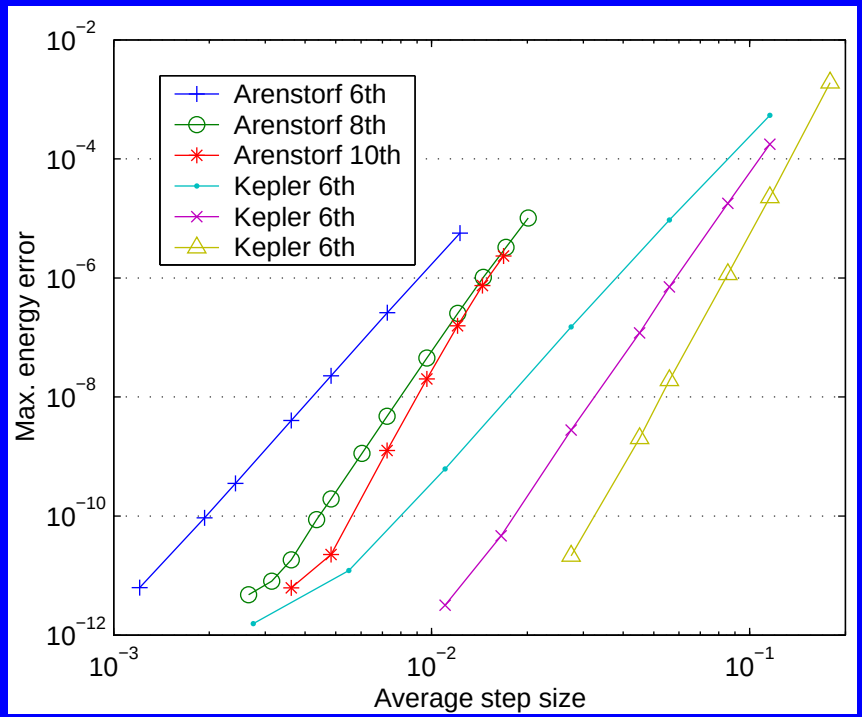
Using a method which changes during sucessive steps gives rise to elements that are not canceled using the Yoshida approach. The first solution is to compose the odd and even steps to create a new method on which to base a composition scheme i.e.

$$\Phi_\tau = \Psi_{\frac{\tau}{2}}^{n+1} \circ \Psi_{\frac{\tau}{2}}^{n}$$

Since Φ_τ now contains both the odd and even terms for n it has no dependence on n. Methods generated in this manner display $6^{th}, 8^{th}$ and 10^{th} order behavior.

This solution also works for higher order methods of fewer steps than the 3^{n-1} required by the exact solutions shown earlier in the text, where the coeficients are calculated numerically.

Results from Solution 1.



For methods based on coefficients which are calculated exactly, as in the above analasis, another solution is possible. If we look at the combination of two such steps we get, for the 6^{th} order method from above

$$\begin{aligned} S_{6^{th}}(\tau) \circ S_{6^{th}}(\tau) = & \, exp(\tau\gamma_1 + \tau^5(x_0^5\gamma_5^2 + 2x_1^5\gamma_5^1) \\ & + O(\tau^7))exp(\tau\gamma_1 + \tau^5(x_0^5\gamma_5^1 + 2x_1^5\gamma_5^2) + O(\tau^7)) \\ & = exp(2\tau\gamma_1 + \tau^5(x_0^5 + 2x_1^5)(\gamma_5^2 + \gamma_5^1) + O(\tau^7)) \\ & = exp(2\tau\gamma_1 + O(\tau^7)) \qquad \text{since } (x_0^5 + 2x_1^5) = 0. \end{aligned}$$

which gives a 6^{th} order method provided that any relevent output is taken at an even step number. This can be extended to higher orders.

Conclusion

From this we can see that it is possible to produce high order, explicit methods with a time transformation.

These methods have applications where high accuracy is required in systems where near approches can occur, where the work can be reduced by the time transformation.

A potential application of the methods is to the understanding of Near Earth Objects (NEOs), i.e. small asteroids that exist in Earth-crossing orbits. It is estimated that only about half of the objects that present a real danger to the earth have been identified.

Acknowledgements

Book:
Benedict Leimkukler, Sabastian Reich
Numerical Methods for Hamiltonian Systems

Papers:
Haruo Yoshida,
Construction of higher order symplectic integrators,

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Asymptotic Error Analysis of the Adaptive Verlet Method

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