Splitting methods for linear oscillators

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Consider a highly oscillatory system of the form (Ω symmetric)

$$\frac{d^2}{dt^2}q = -\Omega^2 q - U(q).$$

with Hamiltonian function

$$H(q,p) = \frac{1}{2}(p^T p + q^T \Omega^2 q + U(q).$$

Idea: Consider composition integrators based on the splitting

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

where $T(p) = \frac{1}{2}p^T p, \quad V(q) = \frac{1}{2}q^T \Omega^2 q.$

Goal: Construct methods to be used with relatively large τ.

For instance, the operator $e^{\tau(T+V+U)}$ can be replaced by

$$e^{\tau a_1 T} e^{\tau b_1 V} \dots e^{\tau a_m T} e^{\tau b_m V} e^{\tau U} e^{\tau b_m V} e^{\tau a_m T} \dots e^{\tau b_1 V} e^{\tau a_1 T} \quad (1)$$

where $a_1, b_1, \cdots, a_m, b_m \in \mathbb{R}$. In particular, if $e^{\frac{1}{2}\tau(T+V)}$ is well approximated by

$$e^{\tau b_m V} e^{\tau a_m T} \dots e^{\tau b_1 V} e^{\tau a_1 T} \quad (2)$$

then, (1) is an approximation of the method of Deuflhard (1979).

In principle, (1) might give a good integrator even if (2) is a poor approximation to $e^{\frac{1}{2}\tau(T+V)}$.

Of course, for $U = 0$ we get in particular

$$e^{\tau(T+V)} \approx e^{\tau a_1 T} e^{\tau b_1 V} \cdots e^{\tau a_m T} e^{\tau b_m V} e^{\tau b_m V} e^{\tau a_m T} \cdots e^{\tau b_1 V} e^{\tau a_1 T}. \quad (3)$$

Our present goal

Obtain efficient approximations of $e^{\tau(T+V)}$ of the form (3).

Future work:

- Approximate $e^{\tau(T+V+U)}$ by inserting exponentials of the form $e^{c_j \tau U}$ in (3).
- More generally, insert terms of the form $e^{c_j \tau U_j}$ with

  $$U_j(q) = U(P_j(\tau\Omega)q), \text{ where } P_j(z) \text{ is a polynomial in } z.$$

- Number of inserted terms $<<$ Number $2m$ of factors in (3).

When $T(p) = \frac{1}{2}p^T p,\ V(q) = \frac{1}{2}q^T \Omega^2 q$,

$$e^{\tau(T+V)} \to \begin{pmatrix} \cos(\tau\Omega) & \Omega^{-1}\sin(\tau\Omega) \\ -\Omega\sin(\tau\Omega) & \cos(\tau\Omega) \end{pmatrix}, \qquad (4)$$

$$e^{\tau T} \to \begin{pmatrix} I & \tau I \\ 0 & I \end{pmatrix}, \quad e^{\tau V} \to \begin{pmatrix} I & 0 \\ -\tau\Omega^2 & I \end{pmatrix},$$

Thus, in a splitting scheme, (4) is approximated by

$$\begin{pmatrix} I & 0 \\ -\tau b_m\Omega^2 & I \end{pmatrix}\begin{pmatrix} I & \tau a_m I \\ 0 & I \end{pmatrix}\cdots\begin{pmatrix} I & 0 \\ -\tau b_1\Omega^2 & I \end{pmatrix}\begin{pmatrix} I & \tau a_1 I \\ 0 & I \end{pmatrix}$$
$$= \begin{pmatrix} K_1(\tau\Omega) & \Omega^{-1}K_2(\tau\Omega) \\ -\Omega K_3(\tau\Omega) & K_4(\tau\Omega) \end{pmatrix}$$

$K_1(x)$ and $K_4(x)$ even, $K_2(x)$ and $K_3(x)$) odd.

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2. Splitting methods applied to systems of linear oscillators
   - Linear stability of splitting methods
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   - Efective efficiency diagrams for stability polynomials

The stability matrix and the stability polynomial

We define the stability matrix of a splitting method as

$$K(x) = \begin{pmatrix} 1 & 0 \\ -b_m x & 1 \end{pmatrix} \begin{pmatrix} 1 & a_m x \\ 0 & 1 \end{pmatrix} \cdots \begin{pmatrix} 1 & 0 \\ -b_1 x & 1 \end{pmatrix} \begin{pmatrix} 1 & a_1 x \\ 0 & 1 \end{pmatrix},$$

that is, the result of applying the method to the harmonic oscillator $\dot{q} = p$, $\dot{p} = -q$ with step-size $\tau = x$. Thus,

$$K(x) = \begin{pmatrix} K_1(x) & K_2(x) \\ K_3(x) & K_4(x) \end{pmatrix}.$$

where $K_1(x), K_4(x)$ (resp. $K_2(x), K_3(x)$) are even (resp. odd) an

$$\det K(x) = K_1(x) K_4(x) - K_2(x) K_3(x) = 1.$$

The stability polynomial of the method is defined as

$$p(x) = \frac{1}{2}\mathrm{tr}(K(x)) = \frac{1}{2}(K_1(x) + K_4(x)).$$

Proposition

$K(x)$ is stable ($K(x)^n$ is bounded $\forall n$) for a given $x \in \mathbb{R}$ if and only if any of the following two conditions hold

1. *The matrix $K(x)$ is diagonalizable with eigenvalues with modulus one,*
2. *$|p(x)| \leq 1$ and there exists a 2×2 matrix $Q(x)$ such that*

$$Q(x)^{-1}K(x)Q(x) = \begin{pmatrix} \cos(\Phi(x)) & \sin(\Phi(x)) \\ -\sin(\Phi(x)) & \cos(\Phi(x)) \end{pmatrix},$$

where $\Phi(x) = \arccos(p(x))$.

The stability threshold x_* is defined as the largest $x_* > 0$ such that the stability matrix $K(x)$ is stable $\forall x \in (-x_*, x_*)$.

Outline

Consider $\dot{q} = p, \quad \dot{p} = -\Omega^2 q$. If for the stability polynomial

$$p(x) = \cos(x) + \mathcal{O}(x^{2n+2}) \quad \text{as} \quad x \to 0,$$

then, there exists $\tilde{\Omega} = \Omega + \mathcal{O}(\tau^{2n})$ (as $\tau \to 0$) such that

$$\begin{pmatrix} I & 0 \\ -\tau b_m \Omega^2 & I \end{pmatrix} \begin{pmatrix} I & \tau a_m I \\ 0 & I \end{pmatrix} \cdots \begin{pmatrix} I & 0 \\ -\tau b_1 \Omega^2 & I \end{pmatrix} \begin{pmatrix} I & \tau a_1 I \\ 0 & I \end{pmatrix}$$

is similar to

$$\begin{pmatrix} \cos(\tau\tilde{\Omega}) & \tilde{\Omega}^{-1}\sin(\tau\tilde{\Omega}) \\ -\tilde{\Omega}\sin(\tau\tilde{\Omega}) & \cos(\tau\tilde{\Omega}) \end{pmatrix}$$

provided that $|\tau|\rho(\Omega) < x_*$.

Consider $\dot{u} = i\Omega u$. If we put $u = p + iq$, then

$$\dot{q} = \Omega p, \quad \dot{p} = -\Omega q.$$

Similarly to previous case, if $p(x) = \cos(x) + \mathcal{O}(x^{2n+2})$, then, there exists $\tilde{\Omega} = \Omega + \mathcal{O}(\tau^{2n})$ such that

$$\begin{pmatrix} I & 0 \\ -\tau b_m \Omega & I \end{pmatrix} \begin{pmatrix} I & \tau a_m \Omega \\ 0 & I \end{pmatrix} \cdots \begin{pmatrix} I & 0 \\ -\tau b_1 \Omega & I \end{pmatrix} \begin{pmatrix} I & \tau a_1 \Omega \\ 0 & I \end{pmatrix}$$

is similar to

$$\begin{pmatrix} \cos(\tau\tilde{\Omega}) & \sin(\tau\tilde{\Omega}) \\ -\sin(\tau\tilde{\Omega}) & \cos(\tau\tilde{\Omega}) \end{pmatrix}$$

provided that $|\tau|\rho(\Omega) < x_*$.

Application to more general linear systems

Consider the expansion $x + \phi_3 x^3 + \phi_5 x^5 + \cdots$ in powers of x of $\Phi(x) = \arccos(p(x))$. Then, there exists $r > 0$ ($r \leq x_*$) such that the following holds for arbitrary linear systems of the form $\dot{q} = Mp, \quad \dot{p} = -Nq$:

$$\begin{pmatrix} I & 0 \\ -hb_m N & I \end{pmatrix} \begin{pmatrix} I & ha_m M \\ 0 & I \end{pmatrix} \cdots \begin{pmatrix} I & 0 \\ -hb_1 N & I \end{pmatrix} \begin{pmatrix} I & ha_1 M \\ 0 & I \end{pmatrix}$$

is similar to $\exp \begin{pmatrix} 0 & h\tilde{M} \\ -h\tilde{N} & 0 \end{pmatrix}$, where

$$\begin{aligned} \tilde{M} &= M(1 + \phi_3 h^2 (NM) + \phi_5 h^4 (NM)^2 + \cdots), \\ \tilde{N} &= N(1 + \phi_3 h^2 (MN) + \phi_5 h^4 (MN)^2 + \cdots), \end{aligned}$$

provided that the (non-necessarily diagonalizable) matrices NM and MN are such that $|\tau| \min(\sqrt{\rho(NM)}, \sqrt{\rho(MN)}) < r$.

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We are mainly interested in symmetric splitting methods, that is, $K(x)^{-1} = K(-x)$ (i.e. $K_1(x) = K_4(x)$).

Assume that $p(x)$ is an even polynomial satisfying that the smallest positive zero with odd multiplicit of $p(x)^2 - 1$ is x_*, and

$$p(x) = 1 - \frac{x^2}{2} + \mathcal{O}(x^4) \text{ as } x \to 0,$$

Then, there exists a finite number of symmetric stability matrices of the form

$$K(x) = \begin{pmatrix} p(x) & K_2(x) \\ K_3(x) & p(x) \end{pmatrix}$$

with stability interval $(-x_*, x_*)$.

All of them are similar to each other for $x \in (-x_*, x_*)$.

Consider the matrix

$$K(x) = \begin{pmatrix} 1 - \frac{1}{2}x^2 + \frac{1}{36}x^4 & x - \frac{2}{9}x^3 + \frac{1}{108}x^5 \\ -x + \frac{1}{12}x^3 & 1 - \frac{1}{2}x^2 + \frac{1}{36}x^4 \end{pmatrix}.$$

It is straightforward to check that it can be decomposed as

$$\begin{pmatrix} 1 & \frac{x}{3} \\ 0 & 1 \end{pmatrix}\begin{pmatrix} 1 & 0 \\ -\frac{x}{2} & 1 \end{pmatrix}\begin{pmatrix} 1 & \frac{x}{3} \\ 0 & 1 \end{pmatrix}\begin{pmatrix} 1 & 0 \\ -\frac{x}{2} & 1 \end{pmatrix}\begin{pmatrix} 1 & \frac{x}{3} \\ 0 & 1 \end{pmatrix}.$$

Let us now consider the matrix

$$K(x) = \begin{pmatrix} 1 - \frac{1}{2}x^2 + \frac{1}{24}x^4 & x - \frac{1}{4}x^3 + \frac{1}{48}x^5 \\ -x + \frac{1}{2}x^3 & 1 - \frac{1}{2}x^2 + \frac{1}{24}x^4 \end{pmatrix}. \qquad (5)$$

It is easy to check that (5) coincides with

$$\begin{pmatrix} 1 & \frac{1}{2}x \\ 0 & 1 \end{pmatrix}\begin{pmatrix} 1 & 0 \\ -x + \frac{1}{12}x^3 & 1 \end{pmatrix}\begin{pmatrix} 1 & \frac{1}{2}x \\ 0 & 1 \end{pmatrix}$$

Proposition

Given a 2×2 matrix $K(x)$ with polynomial entries satisfying that $\det K(x) \equiv 1$, $K_2(x)$ and $K_3(x)$ are odd polynomials, and $K_1(x)$ and $K_4(x)$ are even polynomials with $K_1(0) = K_4(0) = 1$, there exists a unique decomposition of $K(x)$ of the form

$$\begin{pmatrix} 1 & 0 \\ B_m(x) & 1 \end{pmatrix} \begin{pmatrix} 1 & A_m(x) \\ 0 & 1 \end{pmatrix} \cdots \begin{pmatrix} 1 & 0 \\ B_1(x) & 1 \end{pmatrix} \begin{pmatrix} 1 & A_1(x) \\ 0 & 1 \end{pmatrix},$$

where $A_j(x), B_j(x)$ ($j = 1, \ldots, m$) are odd polynomials in x with

$$A_j(x) \neq 0, \quad B_{j-1}(x) \neq 0, \quad j = 2, \ldots, m.$$

That factorization corresponds to a generalized splitting method. If $K(x)$ is the stability matrix of a standard splitting method, then $A_j(x) = a_j x$ and $B_j(x) = -b_j x$. Any splitting method is uniquely determined by its stability matrix!

Outline

We want to obtain accurate symmetric schemes with large stability intervals $(-x_*, x_*)$.

A family of stability matrices

Given $m, n \geq 1$, $l \geq 0$, such that $m \geq 2n + l - 1$, we consider $p(x) = K_1(x)$ of degree $2m$ and $K_2(x)$ and $K_3(x)$ of degrees $2m + 1$ and $2m - 1$ resp., satisfying that

$$K_1(x)^2 - K_2(x)K_3(x) = 1, \qquad K_1(x) = \cos(x) + \mathcal{O}(x^{2n+2}),$$
$$K_2(x) = \sin(x) + \mathcal{O}(x^{2n+1}), \qquad K_3(x) = -\sin(x) + \mathcal{O}(x^{2n+1}),$$

and there exist $x_j \approx j\pi$, $j = 1, \ldots, l$, such that

$$\begin{aligned} K_1(x_j) &= (-1)^j, \quad K_1'(x_j) = 0, \\ K_2(x_j) &= 0, \qquad K_3(x_j) = 0. \end{aligned}$$

There are $m - (2n + l - 1)$ free parameters.

Let us consider the Chebyshev norm $||\cdot||_I$ defined by

$$||f(x)||_I = \int_{-1}^{1} \left(1-x^2\right)^{-1/2} f\left(\frac{(2I+1)\pi x}{2}\right)^2 dx.$$

Determine the free parameters of $K(x)$ in such a way that

$$\left|\left|\frac{K_1(x)-\cos(x)}{x^{2n+2}}\right|\right|_I^2 + \left|\left|\frac{K_2(x)-\sin(x)}{x^{2n+1}}\right|\right|_I^2 + \left|\left|\frac{K_3(x)+\sin(x)}{x^{2n+1}}\right|\right|_I^2$$

is minimized (equivalent to minimizing in the least square sense the coefficients of their Chebyshev series expansion).
This is a nonlinearly constrained minimization problem that has (for moderate m) a high number of local minima. Good initial guesses are required for the numerical search.

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Assume that $m \geq 2(n+l) - 1$.

Find $\hat{K}_1(x)$, $\hat{K}_2(x)$, $\hat{K}_3(x)$ of degrees $2m$, $2m+1$, and $2m-1$ resp., such that

$$\left|\left|\frac{K_1(x) - \cos(x)}{x^{2n+2}}\right|\right|_l^2$$

is minimized under the constraints

$$\begin{aligned} \hat{K}_1(x)^2 - \hat{K}_2(x)\hat{K}_3(x) &= 1, & \hat{K}_1(x) &= \cos(x) + \mathcal{O}(x^{2n+2}), \\ \hat{K}_2(x) &= \sin(x) + \mathcal{O}(x^3), & \hat{K}_3(x) &= -\sin(x) + \mathcal{O}(x^3), \\ \hat{K}_1(j\pi) = (-1)^j, \ \hat{K}_1'(j\pi) &= 0, & \hat{K}_2(j\pi) = 0, \ \hat{K}_3(j\pi) &= 0. \end{aligned}$$

All the local minima of that minimization problem can be explicitly obtained.

A family of stability polynomials

We construct a stability polynomial $p_{n,l}(x)$ for arbitrary $n, l \geq 0$, as follows:

$$p_{n,l}(x) = 1 + \sum_{j=1}^{n} (-1)^j \frac{x^{2j}}{(2j)!} + x^{2n+2} \sum_{j=0}^{2l} d_j x^{2j}$$

where the coefficients d_j are uniquely determined by the requirement that

$$p_{n,l}(j\pi) = (-1)^j, \quad p'_{n,l}(j\pi) = 0, \quad j = 1, \ldots, l.$$

Note the interpolatory nature of $p_{n,l}(x)$, as

$$\cos(j\pi) = (-1)^j, \quad \cos'(j\pi) = -\sin(j\pi) = 0, \quad \forall j \geq 1.$$

A more general family of stability polynomials

For $n, k, l \geq 0$, $k = m - 2(n+l) - 1$,

$$p_{n,l,k}(x) = p_{n,l}(x) + x^{2n+2} \prod_{j=1}^{l} (x^2 - (j\pi)^2)^2 \sum_{i=0}^{k} e_i x^{2i},$$

where the e_i are uniquely determined by requiring that

$$\|\frac{p_{n,l,k}(x) - \cos(x)}{x^{2n+2}}\|_l$$

is minimized. Each local minimum of the neighbouring constrained minimization problem corresponds to one different $\hat{K}(x)$ having $p_{n,l,k}(x)$ as stability polynomial. One can choose among them the best candidates as initial guesses in the numerical search to obtain the local minimia of the original constrained minimization problem (either by a Newton-type iteration or by using a continuation algorithm).

Outline

The long-term error accuracy of splitting methods applied to linear systems is related to the difference

$$\begin{pmatrix} \cos(\Phi(x)) & \sin(\Phi(x)) \\ -\sin(\Phi(x)) & \cos(\Phi(x)) \end{pmatrix} - \begin{pmatrix} \cos(x) & \sin(x) \\ -\sin(x) & \cos(x) \end{pmatrix},$$

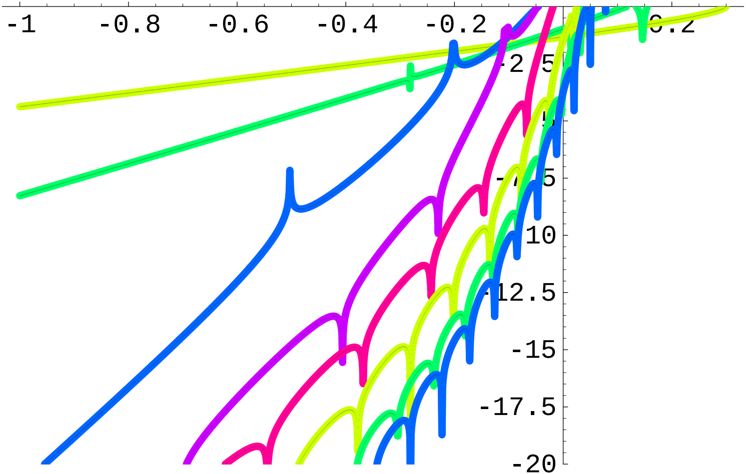
where $\Phi(x) = \arccos(p(x))$, that is, the long-term effective error corresponds to $|\Phi(x) - x|$. To fairly compare of method with different number $2m$ of factors, we consider

$$|\Phi(mx) - mx|$$

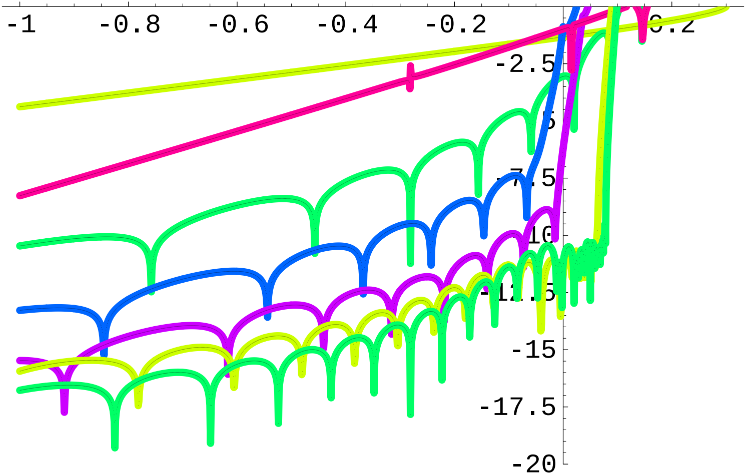
That is, we compare a method with $2m$ factors applied with step-size τ to m steps of Störmer-Verlet with step-size τ/m.

We show diagrams in double logarithmic scale. That is, $\log_{10}(|mx - \arccos(p(mx))|)$ versus $\log_{10}(x)$.

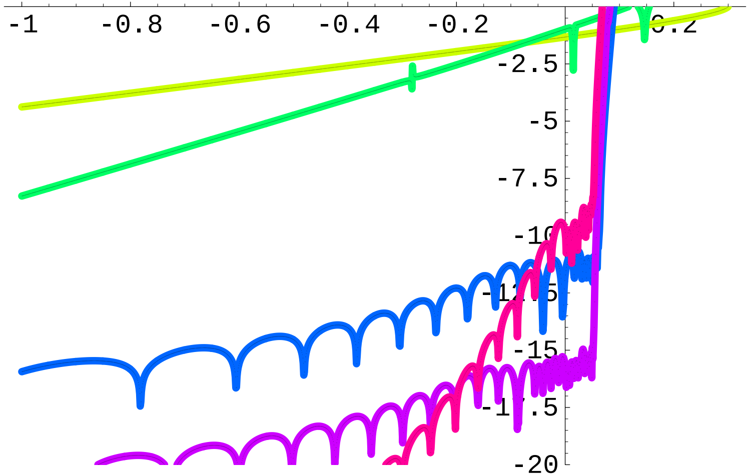
Leapfrog $m = 2$, optimal stability method with $n = 3$, $m = 6$ (Gray & McLachlan), and $p_{n,l}(x)$ for $n = 10$, and $l = 3, 6, 10, 14, 16$ $(m = 10 + 2l)$



Leapfrog $m = 2$, optimal stability method with $n = 3$, $m = 6$ (Gray & McLachlan), and $p_{n,l,k}(x)$ for $n = 1,\ k = 9$, and $l = 4, 6, 8, 14, 16$ $(m = 10 + 2l)$



Leapfrog ($m = 2$), optimal stability method $n = 3$ and $m = 6$ (Gray & McLachlan), and $p_{1,14,9}(x)$ ($m = 38$), $p_{1,18,13}(x)$, and $p_{7,18,7}(x)$ ($m = 50$).



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