Optimized splitting methods for linear oscillators

Ander Murua
Joint work with Sergio Blanes and Fernando Casas

Innsbruck, October 2008

Consider the linear time-dependent Shrödinger equations in semi-discrete form

$$i\frac{d}{dt}u = H_h u$$

(H_h a real symmetric matrix) obtained from a suitable space discretization, with discretization parameter h.
We consider splitting methods with the ODE system split in the form

$$\frac{d}{dt}\begin{pmatrix} p \\ q \end{pmatrix} = \overbrace{\begin{pmatrix} 0 & H_h \\ 0 & 0 \end{pmatrix}}^{A} \begin{pmatrix} p \\ q \end{pmatrix} + \overbrace{\begin{pmatrix} 0 & 0 \\ -H_h & 0 \end{pmatrix}}^{B} \begin{pmatrix} p \\ q \end{pmatrix}$$

where $u = q + ip$. In a splitting method, one replaces the operator $e^{\tau(A+B)}$ by a product of the form

$$e^{\tau(A+B)} \approx e^{\tau a_1 A} e^{\tau b_1 B} \cdots e^{\tau a_m A} e^{\tau b_m B}$$

with appropriately chosen $a_1, b_1, \cdots, a_m, b_m \in \mathbb{R}$.

Since

$$e^{\tau H_h} = e^{\tau(A+B)} = \begin{pmatrix} \cos(\tau H_h) & \sin(\tau H_h) \\ -\sin(\tau H_h) & \cos(\tau H_h) \end{pmatrix}, \qquad (1)$$

$$e^{\tau A} = \begin{pmatrix} I & \tau H_h \\ 0 & I \end{pmatrix}, \quad e^{\tau B} = \begin{pmatrix} I & 0 \\ -\tau H_h & I \end{pmatrix},$$

in a splitting scheme, (1) is approximated by

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

where $K_1(x)$ and $K_4(x)$ even polynomials, and $K_2(x)$ and $K_3(x)$ odd polynomials satisfying $K_1 K_4 - K_2 K_2 = 1$.

Stability restriction: $|\tau|\rho(H_h) < x_*$ with stability threshold x_* depending on $(a_1, b_1, \cdots, a_m, b_m) \in \mathbb{R}^{2m}$. Recall that $\rho(H_h) \to \infty$ as $h \to 0$.

Stability barrier: Relative stability threshold $\frac{x_*}{m} \leq 2$.

Assumption

There exists $k > 0$, $h_0 > 0$, $C_k > 0$ such that for all $h \leq h_0$

$$||H_h^k u(0)|| \leq C_k.$$

where $|| \cdot ||$ is the discrete L_2 norm.

Provided that the discrete energy is bounded

$$\frac{h}{2} u(0)^T H_h \overline{u(0)} \leq C \quad \text{for} \quad h \leq h_0,$$

our assumption holds at least for $k = 1/2$.

The stability matrix

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

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

Important: Any splitting method is uniquely determined by its stability matrix.

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

Given $x \in \mathbb{R}$, the following three conditions are equivalent:

1. $K(x)$ *is stable* ($K(x)^n$ *is bounded* $\forall n$)
2. $K(x)$ *is diagonalizable with eigenvalues with modulus one,*
3. $|p(x)| \leq 1$ *and there exists a* 2×2 *real 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 $\phi(x) = \arccos(p(x)) \in \mathbb{R}$.

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

Proposition

Consider a consistent symmetric splitting method with

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

The matrix $K(x)$ *is stable for a given* $x \in \mathbb{R}$ *if and only if there exist* $\phi(x), \gamma(x) \in \mathbb{R}$ *such that* $p(x) = \cos(\phi(x))$ *and* $K_2(x) = -\gamma(x)^2 K_3(x)$*. In that case,*

$$K(x) = \begin{pmatrix} \cos(\phi(x)) & \gamma(x)\sin(\phi(x)) \\ -\frac{\sin(\phi(x))}{\gamma(x)} & \cos(\phi(x)) \end{pmatrix} = \exp\begin{pmatrix} 0 & \gamma(x)\phi(x) \\ -\frac{\phi(x)}{\gamma(x)} & 0 \end{pmatrix}.$$

If the splitting method is of order $2n$, then

$$\phi(x) = x + \mathcal{O}(x^{2n+1}), \quad \gamma(x) = 1 + \mathcal{O}(x^{2n}), \quad \text{as} \quad x \to 0,$$

Symmetry implies that $\phi(-x) = -\phi(x)$ and $\gamma(-x) = \gamma(x)$.

Proposition 2 implies that, provided that $|\tau|\rho(H_h) < x_*$, $u_j = q_j + ip_j \approx u(t_j)$ $(t_j = j\tau)$ obtained by applying the splitting method to $i\frac{d}{dt}u = H_h u$ satisfies

$$\begin{pmatrix} q_j \\ p_j \end{pmatrix} = \begin{pmatrix} \cos(t_j\tilde{H}_h) & \gamma(\tau H_h)\sin(t_j\tilde{H}_h) \\ -\gamma(\tau H_h)^{-1}\sin(t_j\tilde{H}_h) & \cos(t_j\tilde{H}_h) \end{pmatrix} \begin{pmatrix} q_0 \\ p_0 \end{pmatrix}$$

where $\tilde{H}_h = \frac{1}{\tau}\phi(\tau H_h) = H_h + \mathcal{O}(\tau^{2n})$ (as $\tau \to 0$). Equivalently,

$$\tilde{u}_j = \gamma(\tau H_h)^{-1/2} q_j + i\gamma(\tau H_h)^{1/2} p_j$$

is the exact solution $\tilde{u}_j = \tilde{u}(t_j)$ of

$$i\frac{d}{dt}\tilde{u} = \tilde{H}_h\tilde{u}, \quad \tilde{u}(0) = \tilde{u}_0,$$

In particular, the L_2 norm of $\tilde{u} = \tilde{q} + i\tilde{p}$ and the modified energy $\frac{1}{2}(\tilde{q}^T H_h\tilde{q} + \tilde{p}^T H_h\tilde{p})$ are conserved by the numerical integrator.

Lemma

Consider the numerical solution $u_j = q_j + ip_j \approx u(t_j)$ $(t_j = \tau\, n)$ *obtained by applying a symmetric splitting method to* $i\frac{d}{dt}u = H_h u$ *with* $u(0) = q_0 + ip_0$*, then*

$$\begin{aligned} ||u_j - u(t_j)|| &\leq ||n\,(\phi(\tau H_h) - \tau H_h)u(0)|| \\ &\quad + \max(||(\gamma(\tau H_h) - I)u(0)||, ||(\gamma(\tau H_h)^{-1} - I)u(0)||). \end{aligned}$$

Notation: For each $k <= 2n$ and $r < x_*$.

$$\begin{aligned} \mu_k(r) &= \sup_{-r\leq x\leq r} (r/x)^k |(\phi(x)/x - 1)|, \\ \nu_k(r) &= \sup_{-r\leq x\leq r} (r/x)^k \max(|(\gamma(x) - 1)|, |(\gamma(x)^{-1} - 1)|). \end{aligned}$$

Remark: Obviously, $\mu_k(\sigma r) \leq \sigma^k \mu_k(r)$ and $\nu_k(\sigma r) \leq \sigma^k \nu_k(r)$ if $0 < \sigma \leq 1$.

Theorem

Consider $i\frac{d}{dt}u = H_h u$ with $u(0) = q_0 + ip_0$ satisfying $||H_h^k u(0)|| \leq C_k$, and the numerical solution $u_j = q_j + ip_j \approx u(t_j)$ $(t_j = j\,\tau)$ of a splitting method of order $2n \geq k$ and stability threshold x_*. If $r = |\tau|\rho(H_h) < x_*$ then

$$||u_j - u(t_j)|| \quad \leq \quad C_k \left(|t|\mu_k(r) + \nu_k(r)\right) \rho(H_h)^{-k}.$$

Goal: Given $0 < r < 2$ and $k > 0$, construct optimized splitting methods to be used with a prescribed $|\tau| = r/\rho(\Omega)$ (under the assumptions of Theorem 4) that minimize $\mu_k(r) + \varepsilon\, \nu_k(r)$ for some $\epsilon > 0$:

- $\epsilon \approx 1$ for short term integration,
- $\epsilon << 1$ for long term integration.

Examples of known m-stage methods of order $2n$

- Values of relative stability threshold x_*/m,
- $(\mu_k(r\,m), \nu_k(r\,m))$ (for a few r and k) in the error estimate

$$||u_j - u(t_j)|| \quad \leq \quad C_k\left(|t|\mu_k(r\,m) + \nu_k(r\,m)\right)\rho(H_h)^{-k}$$

with step-size $\tau = \frac{r\,m}{\rho(H_h)}$.

Method	Leapfrog	Yoshida	Blanes & Moan
m	1	4	6
$2n$	2	4	4
x_*/m	2	0.393	0.482
$(\mu_2(\frac{5m}{4}), \nu_2(\frac{5m}{4}))$	$(0.078, 0.27)$	(∞, ∞)	(∞, ∞)
$(\mu_2(m), \nu_2(m))$	$(0.0472, 0.155)$	(∞, ∞)	(∞, ∞)
$(\mu_2(\frac{3m}{10}), \nu_2(\frac{3m}{10}))$	$(0.0037, 0.011)$	$(0.186, 0.230)$	$(0.0002, 0.003)$
$(\mu_4(\frac{3m}{10}), \nu_4(\frac{3m}{10}))$	(∞, ∞)	$(0.186, 0.230)$	$(0.0002, 0.003)$

For practical purposes, we replace the ∞-norm of functions defined in $[-r, r]$ by the norm $|| \cdot ||_r$ defined by

$$||u||_r^2 = \int_{-1}^{1} \left(1 - x^2\right)^{-1/2} u\,(r\,x)^2 \;dx.$$

Recall that, if

$$u(x) = \widehat{u}_0 + 2 \sum_{k=1}^{\infty} \widehat{u}_k \, T_k(x/r)$$

is the Chebyshev series expansion of $u(x)$ in the interval $[-r, r]$, (with the Chebyshev polynomials $T_k(x) = \cos(k \arccos(x))$,) then

$$||u||_r = \sqrt{\pi \left(\widehat{u}_0^2 + 2 \sum_{k=1}^{\infty} \widehat{u}_k^2 \right)}.$$

Theorem 4 motivates us for considering the following optimized splitting methods: Given $r \in \mathbb{R}^+$, $n, m \in \mathbb{Z}^+$ with $m \geq 2n-1$, consider the set $\mathcal{S}(r,m,n)$ of stability matrices $K(x)$ of $(2n)$th order symmetric splitting methods with m stages with $x_* > r$.

Optimization of splitting methods for linear system

Given $r, \varepsilon \in \mathbb{R}^+$, $m, n, k \in \mathbb{Z}^+$ with $m \geq 2n-1$ and $k \leq 2n$, determine $K(x)$ in $S(r,m,n)$ that minimizes

$$\left|\left|(\phi(x)/x - 1)(r/x)^k\right|\right|_r + \varepsilon \left|\left|(\gamma(x) - 1)(r/x)^k\right|\right|_r. \tag{2}$$

Difficulty: The objective function is very ill-conditioned with respect to the coefficients of the polynomials $p(x), K_2(x), K_3(x)$ of $K(x)$ (where $K(x) = p(x)^2 - K_2(x)K_3(x) = 1$).

Optimal stability polynomials

Given $r \in \mathbb{R}^+$, $k, m \in \mathbb{Z}^+$, consider the even polynomial(s) of degree $2m$ with minimal value of $||\delta||_r$, where

$$\delta(x) = (\kappa(x) - 1)x^{-k} = (\arccos(p(x)) - x)x^{-k-1}.$$

Observe that $||\delta||_r$ is a well defined finite real number for an even polynomial $p(x)$, if and only if the following two conditions hold:

- $|p(x)| \leq 1$ for $x \in [-r, r]$,
- $p(x) = \cos(x) + \mathcal{O}(x^{k+2})$.

The optimal stability polynomial $p(x)$ must then be of the form

$$p(x) = \sum_{j=0}^{[(k+1)/2]} \frac{(-1)^j}{(2j)!} x^{2j} + x^{k+2} q(x). \qquad (3)$$

Remark: These conditions can fail for arbitrarily small perturbation of the coefficients of a polynomial $p(x)$ satisfying them.

Optimization procedure to construct second-order symmetric splitting methods to apply when $||H_h^2 u(0)|| \leq C_2$:

1. Choose $m \geq 3$ and $r < 2m$, and find a polynomial $p(x)$ of degree $2m$ that minimizes

$$||(\arccos(p(x))/x - 1)(r/x)^2||_r.$$

2. Choose among all odd polynomials $K_2(x) = x + \mathcal{O}(x^3)$ and $K_3(x) = -x + \mathcal{O}(x^3)$ satisfying $p(x)^2 - 1 = K_2(x)K_3(x)$, the pair (K_2, K_3) that minimizes

$$\nu_2(r) \;=\; \sup_{-r \leq x \leq r} (r/x)^2 \max(|(\gamma(x) - 1)|, |(\gamma(x)^{-1} - 1)|)$$

where $\gamma(x) = \sqrt{-K_2(x)/K_3(x)}$.

3. Find $(a_1, b_1, \cdots, a_m, b_m) \in \mathbb{R}^{2m}$ of a splitting method having $K(x)$ as stability matrix (if it exists, it is unique).

Example: Coefficients $\mu_2(rm)$ for long term integration with step-size $\tau = \frac{r\,m}{\rho(H_h)}$ of

$$i\frac{d}{dt}u = H_h u$$

under the assumption $||H_h^2 u(0)|| \le C_2$ in the estimate

$$||u_j - u(t_j)|| \quad \le \quad C_2\left(|t|\mu_2(r\,m) + \nu_2(r\,m)\right)\rho(H_h)^{-2}.$$

Method of order 2 with $m = 19$ optimized for r=5/4m

Method	Leapfrog	Optimized method
m	1	19
$2n$	2	2
x_*/m	2	1.352
$\mu_2(\frac{5m}{4})$	0.078	$1.044\ 10^{-6}$
$\mu_2(m)$	0.0472	$6.68\ 10^{-7}$
$\mu_2(\frac{3m}{10})$	0.0037	$6.01\ 10^{-8}$

Work in progress

- Construction of optimized symmetric splitting methods with large number $2m$ of compositions of different order $2n$ under the assumptions $||H_h^k u(0)|| \leq C_k$ with $k \leq 2n$.
- Theoretical and experimental comparison of our splitting methods with truncated Chebyshev series expansions of e^{ix} in $x \in [-r, r]$.
- Extension of results with linear systems of the form

$$\frac{d}{dt} q = M_h p, \quad \frac{d}{dt} p = -N_h q$$

(Maxwel equations, wave equations ...)
- Generalization of splitting methods for the Shrödinger equation with time-dependent potential, i.e.,

$$i \frac{d}{dt} u = H_h(t) u.$$

Under the assumptions of Proposition 2, let $0 = x_0 < x_1 < \cdots < x_l < x_*$ be all the non-negative zeroes of the polynomial $p(x)^2 - 1 = K_2(x)K_3(x)$ in the interval $[0, x_*]$. In what follows we adopt the following

Assumption

Each zero x_j $(0 \leq j \leq l)$ of the stability polynomial in the interval $[0, x_*)$ is a zero of multiplicity m_j for both $K_2(x)$ and $K_3(x)$.

Otherwise, $\gamma(x)$ or $\gamma(x)^{-1}$ is unbounded in a neighbourhood of x_j. Such an additional assumption tipically holds with $m_j = 1$, if

$$K(x) \approx \begin{pmatrix} \cos(x) & \sin(x) \\ -\sin(x) & \cos(x) \end{pmatrix} \quad \text{for} \quad x_l \leq x \leq x_l,$$

in which case $x_j \approx j\pi$, $K_2'(x_j) \approx -\cos(j\pi) = (-1)^{j+1}$ and $K_3'(x_j) \approx \cos(j\pi) = (-1)^j$ for $j = 1, \ldots, l$.
Then, $\phi(x)$ and $\gamma(x)$ are uniquely defined for $x \in (-x_*, x_*)$.

A parametrization of stability polynomials

Given $r \in \mathbb{R}$ and $m, n, l, k \in \mathbb{Z}^+$ with $m \geq n + 2l$ and $k \leq 2n$.
For each $(\widehat{\theta}_1, \ldots, \widehat{\theta}_{m-n-l}) \in \mathbb{R}^{m-n-l}$, consider the odd polynomial $\theta(x)$ of degree $2(m-l)-1$ of the form

$$\theta(x) = x\left(1 + (x/r)^{2n} \sum_{j=1}^{m-n-l} \widehat{\theta}_j T_{2(j-1)}(x/r)\right).$$

We determine an even polynomial $p(x)$ of degree $2m$ of the form

$$p(x) = \sum_{j=0}^{n} \frac{(-1)^j}{(2j)!} x^{2j} + (x/r)^{2n+2} q(x)$$

that minimize $||\epsilon||_r$, where $\epsilon(x) = (p(\theta(x)) - \cos(x))(r/x)^{2n+2}$, under the following constraints: For $j = 1, \ldots, l$,

$$p(\alpha_j) = (-1)^j, \quad p'(\alpha_j) = 0, \quad \text{where} \quad \alpha_j = \theta(j\pi).$$