Splitting methods for the time integration of wave equations

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Bilbao, July 2009

We are concerned with the application of splitting methods for the time-integration of wave equations, for instance

The semilinear wave equations

in a bounded $\Omega \subset \mathbb{R}^d$ with homogeneous Dirichlet boundary conds.

$$\begin{aligned} u_{tt} &= \Delta u + f(u) && \text{in} \quad \Omega \times \mathbb{R}, \\ u &= 0 && \text{in} \quad \partial\Omega \times \mathbb{R}, \\ u(0) &= u_0, \quad u_t(0) = v_0 && \text{in} \quad \Omega. \end{aligned}$$

We also consider

The semilinear wave equation with periodic boundary conditions

$$\begin{aligned} u_{tt} &= \Delta u + f(u) && \text{in} \quad \mathbb{T}^d \times \mathbb{R}, \\ u(0) &= u_0, \quad u_t(0) = v_0 && \text{in} \quad \mathbb{T}^d. \end{aligned}$$

Splitting methods

The simplest splitting method consists on approximating $e^{t\,L}$ by splitting the operator L as $X+Y$ and

$$e^{t\,(X+Y)} = \left(e^{\tau\,(X+Y)}\right)^m \approx \left(e^{\tau\,X} e^{\tau\,Y}\right)^m$$

with a small time-step $\tau = t/m$. Alternatively, one can use the

Strang splitting

$$e^{\tau\,(X+Y)} \approx e^{\frac{\tau}{2}\,X} e^{\tau\,Y} e^{\frac{\tau}{2}\,X}.$$

Using more general products of exponentials is also possible:

$$e^{\tau\,(X+Y)} \approx e^{\tau a_1 X} e^{\tau b_1 Y} \cdots e^{\tau a_m X} e^{\tau b_m Y}$$

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

How to split the semilinear wave equation?

- A possible option is splitting the wave equation as

$$u_{tt} = \Delta u, \quad \text{and} \quad u_{tt} = f(u),$$

- A better option, provided that $f(u) = \rho\, u + \mathcal{O}(u^2)$, is

$$u_{tt} = \Delta u + \rho\, u, \quad \text{and} \quad u_{tt} = f(u) - \rho\, u.$$

- A third option, based on rewritting the equations as

$$u_t = v, \quad v_t = \Delta u + f(u)$$

  and splitting it as

$$\left\{ \begin{array}{l} u_t = v, \\ v_t = 0, \end{array} \right. \quad \text{and} \quad \left\{ \begin{array}{l} u_t = 0, \\ v_t = \Delta u + f(u). \end{array} \right.$$

  But that only makes sense after spatial semidiscretization!

Semidiscretization in space

For a spatial grid $x_1, \ldots, x_N \in \Omega$, consider

$$q(t) \approx \begin{pmatrix} u(x_1,t) \\ \vdots \\ u(x_N,t) \end{pmatrix}, \quad p(t) \approx \begin{pmatrix} u_t(x_1,t) \\ \vdots \\ u_t(x_N,t) \end{pmatrix}$$

determined as the solutions of a

Semidiscretized problem

$$\frac{d}{dt} q = p, \qquad \frac{d}{dt} p = A\, q + g(q),$$

with initial values $q(0) = q_0, \quad p(0) = q_0.$

Here, $A \in \mathbb{R}^{N \times N}$ is such that

$$A\, q(t) \approx \begin{pmatrix} \Delta u(x_1,t) \\ \vdots \\ \Delta u(x_N,t) \end{pmatrix}, \quad \text{and} \quad g(q(t)) = \begin{pmatrix} f(u(x_1,t)) \\ \vdots \\ f(u(x_N,t)) \end{pmatrix}.$$

Application of $e^{\tau(A+B)} = e^{\tau/2\,A} e^{\tau\,B} e^{\tau/2\,A}$ to the equations split as

$$\begin{cases} \frac{d}{dt} q = p, \\ \frac{d}{dt} p = 0, \end{cases} \quad \text{and} \quad \begin{cases} \frac{d}{dt} q = 0, \\ \frac{d}{dt} p = A\,q + g(q), \end{cases}$$

gives the

Leapfrog method

$(q_n, p_n) \approx (q(t_n), p(t_n))$ computed for $t_n = n\tau$ as follows:

$$\begin{aligned} p_{n-\frac{1}{2}} &= p_{n-1} + \frac{\tau}{2}\,(Aq_{n-1} + g(q_{n-1})), \\ q_n &= q_{n-1} + \tau\, p_{n-\frac{1}{2}}, \\ p_n &= p_{n-\frac{1}{2}} + \frac{\tau}{2}\,(Aq_n + g(q_n)), \end{aligned}$$

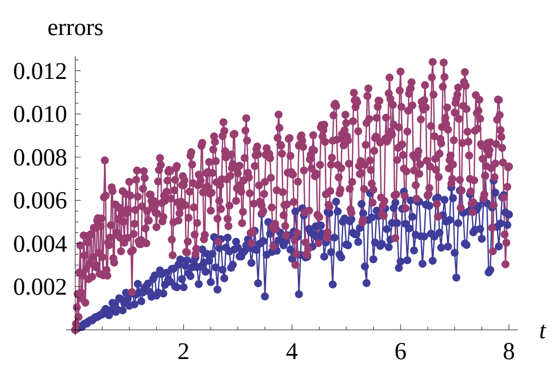
or in two step formulation, $q_1 = q_0 + \tau p_0 + \frac{\tau^2}{2}(Aq_0 + g(q_0))$ and

$$q_{n+1} - 2q_n + q_{n-1} = \tau^2(Aq_n + g(q_n)).$$

Central finite differences in space and leapfrog in time

Example: 1D-wave equation with homogeneous Dirichlet b.c.

$\Omega = (0,1)$, $f(u) = 2u - 4u^3$, $u_0(x) = \frac{1}{10+\sin^2(\pi x)}$, $v_0(x) = 0$,
$x_j = jh$, $(j = 1, \ldots, 15)$, $h = \frac{1}{16}$, $\tau = \frac{h}{2}$.
Space discretization errors and time discr. errors versus time:



Standard ODE error analysis: Consider a semidiscretized problem (for a fixed small h) and study errors as $\tau \to 0$.

We would like to analyze the full discretization error as $h, \tau \to 0$.

Approx. analysis of fully discretized solutions of small amplitude

Assume that

- $f(0) = 0$, so that for u with small amplitude, $f(u) \approx f'(0)u$,
- $-(A + f'(0)I)$ is diagonalizable with positive real eigenvalues. Then consider $B = (-(A + f'(0)I))^{1/2}$, and analyze leapfrog method applied to

$$\frac{d}{dt} q = p, \qquad \frac{d}{dt} p = -B^2 q,$$

If $\tau \leq \frac{2}{\rho(B)}$, then the numerical solution given by

$$q_{n+1} - 2q_n + q_{n-1} = -\tau^2 B^2 q_n$$

(where $q_1 = q_0 + \tau p_0 - \frac{\tau^2}{2} B^2 q_0$) lies in the trajectory of the

Modified problem

$$\frac{d}{dt}\tilde{q} = \tilde{p}, \qquad \frac{d}{dt}\tilde{p} = -\tilde{B}^2\, q,$$

with

$$\tilde{B} = \frac{2}{\tau} \arcsin(\frac{\tau}{2}\, B) = B + \frac{\tau^2}{24} B^3 + \cdots$$

and initial values

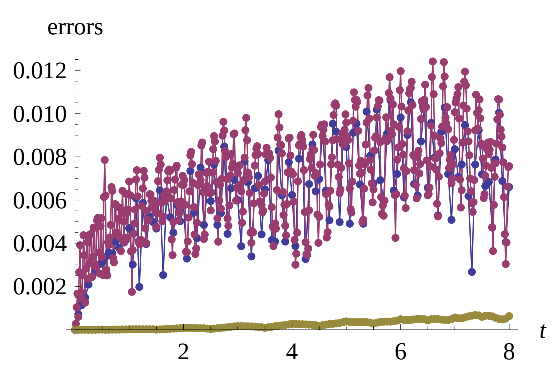
$$\tilde{q}(0) = q_0, \quad \tilde{p}(0) = (I - \frac{\tau^2}{4} B^2)^{-\frac{1}{2}}\, p_0 = p_0 - \frac{\tau^2}{8} B^2 p_0 + \cdots .$$

Central finite differences in space and leapfrog in time

Example: 1D-wave equation with homogeneous Dirichlet b.c.

Previous example with $h = \frac{1}{16}$ and $\tau = h$ (instead of $\tau = \frac{h}{2}$).

Space, time and full discretization errors versus time:



2nd order central finite differences with leapfrog in 1D

Stability requirement:

$$|\tau| \leq \frac{2}{\rho(B)} = \frac{h}{\sin(\frac{(1-h)\pi}{2})}, \quad (\text{for } f(u) = 0,)$$

hence, leapfrog scheme is stable for $\tau = h$.
Exceptional performance of full discretization for $\tau = h$:

- $\omega_k = k\pi \;\rightarrow\; \omega_k^h = \frac{2}{h}\sin(k\pi h/2) \;\rightarrow\; \omega_k^{h,\tau} = \frac{2}{\tau}\arcsin(\tau\omega_k^h/2)$.
  If $\tau = h$, then $\omega_k^{h,\tau} = k\pi$!
- Solutions of $u_{tt} = u_{xx}$ exactly satisfy

$$\frac{1}{\tau^2}(u(x,t+\tau) - 2u(x,t) + u(x,t-\tau)) = \frac{1}{h^2}(u(x+h,t) - 2u(x,t) + u(x-h,t))$$

for $\tau = h$.

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- Solutions of $u_{tt} = u_{xx}$ exactly satisfy

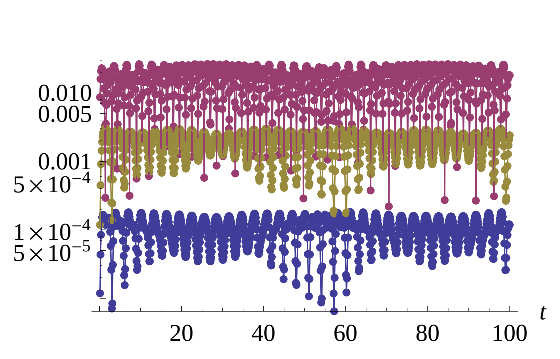
$$\begin{aligned} \frac{1}{\tau^2}(u(x,t+\tau) - 2u(x,t) + u(x,t-\tau)) &= \\ \frac{1}{h^2}(u(x+h,t) - 2u(x,t) + u(x-h,t)) & \end{aligned}$$

for $\tau = h$.

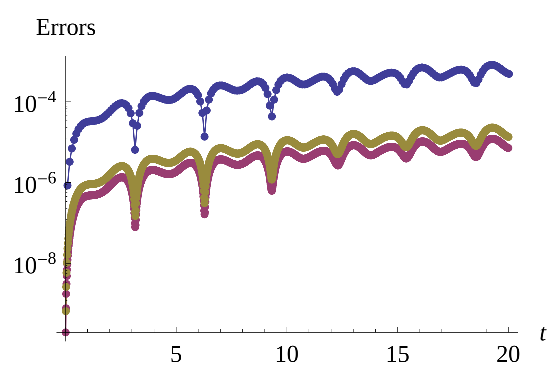
Fourier spectral collocation methods with leapfrog in time:

Example: 1D-wave equation with periodic boundary conditions

$x \in (0, 2\pi)$, $f(u) = \frac{u}{10} - 4u^3$, $u_0(x) = \frac{e^{\sin(x)}}{10}$, $v_0(x) = 0$, $h = \frac{2\pi}{16}$, $\tau = \frac{h}{4} < \frac{2}{\rho(B)} \approx \frac{2h}{\pi}$. Variation of discrete Hamiltonian, momentum and oscillatory energy:



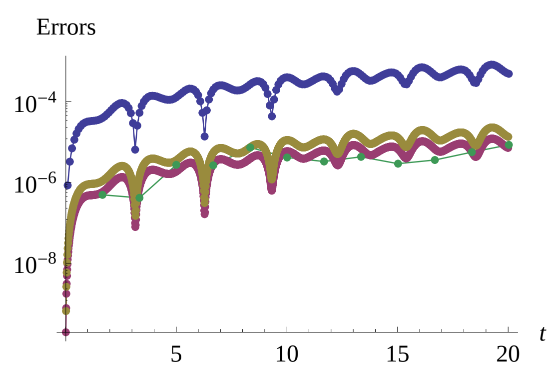
Fourier spectral collocation methods with leapfrog in time: Space discr. errors and time discr. errors (for $\tau = h/4$ and $\tau = h/24$) versus time:



Fourier spectral collocation methods with optimized splitting:

$$e^{\tau(X+Y)} \approx e^{\tau a_1 X} e^{\tau b_1 Y} \dots e^{\tau a_m X} e^{\tau b_m Y}.$$

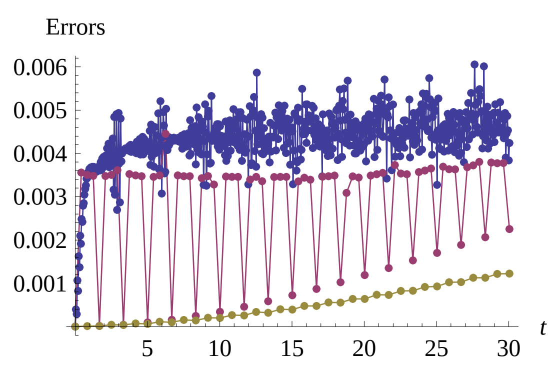
Time discr. error of new splitting method with $m = 17$ and $\tau = \frac{mh}{4}$



Fourier spectral collocation methods with optimized splitting methods for non-smooth data: $f(u) = 2u^3$, $n = 64$,

$$u_0(x) = \begin{cases} \frac{x}{20\pi} & \text{if } 0 \le x \le \pi \\ \frac{2\pi - x}{20\pi} & \text{if } \pi \le x \le 2\pi. \end{cases}, \qquad v_0(x) = 0$$

(i) Space discr. errors, (ii) time discr. errors for leapfrog with $\tau = h/2$ and (iii) another new method with $m = 17$ and $\tau = \frac{mh}{2}$.



Consider the problem

$$\frac{d}{dt} q = p, \qquad \frac{d}{dt} p = A\, q + g(q),$$

arising from the spatial semidiscretization of a wave equation.

Splitting scheme

$(q_n, p_n) \approx (q(t_n), p(t_n))$ computed for $t_n = n\tau$ as follows: Take $Q_0 = q_{n-1}$, $P_0 = p_{n-1}$, and compute for $j = 1, \ldots, m$

$$\begin{aligned} P_j &= P_{j-1} + a_j\, \tau\, (AQ_{j-1} + g(q_{j-1})), \\ Q_j &= Q_j + b_j\, \tau\, P_j, \end{aligned}$$

and take $(q_n, p_n) = (Q_m, P_m)$.

The coefficients a_j and b_j ($j = 1, \ldots, m$) appropriately chosen real numbers.

We want to analyse the application of the splitting method to

$$\frac{d}{dt}q = p, \qquad \frac{d}{dt}p = -B^2\, q,$$

where $B^2 = -(f'(0)I + A)$. We assume that B is symmetric positive definite.

- Obviously, $\rho(B) \to \infty$ as the spacial discretization converges to the continuous problem.
- For each splitting method, there exists $x^* \geq 0$ such that the scheme is stable if $\tau < \frac{x^*}{\rho(B)}$ ($x^* = 2$ for leapfrog).
- We want to apply a splitting method with $\tau = \frac{r}{\rho(B)}$ for fixed $r \leq x^*$. How are the time discretization errors as $\rho(B) \to \infty$?

It depends on the splitting method, and the (smoothness of the) initial data u_0, v_0.

We obtain estimates depending on

$$\begin{aligned} C_s &:= ||B^{s+1} q_0|| + ||B^s p_0|| \\ &\approx ||(f'(0)+\Delta)^{\frac{s+1}{2}} u_0|| + ||(f'(0)+\Delta)^{\frac{s}{2}} v_0||. \end{aligned}$$

Theorem

Given a splitting scheme with stability threshold x^*, for each $s > 0$ and each $r \in (0, x^*)$, there exist $\mu_s(r), \nu_s(r) > 0$ such that

$$||q_n - q(t_n)|| \leq \frac{C_s}{\rho(B)^s} (|t_n|\mu_s(r) + \nu_s(r)),$$

for $t_n = n\tau$ with $\tau = r/\rho(B)$.

Similar estimates can be obtained for $||p_n - p(t_n)||$.

For the leapfrog method, given $0 \leq s \leq 2$ and $r < x^* = 2$,

$$\begin{aligned} \mu_s(r) &= \sup_{0<x\leq r} \left| \left(\tfrac{r}{x}\right)^s \left(\tfrac{2}{x} \arcsin\left(\tfrac{x}{2}\right) - 1\right) \right|, \\ \nu_s(r) &= \sup_{0<x\leq r} \left| \left(\tfrac{r}{x}\right)^s \sqrt{1 - \tfrac{x^2}{4}} \right|. \end{aligned}$$

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We obtain estimates depending on

$$C_s := ||B^{s+1} q_0|| + ||B^s p_0|| \approx ||(f'(0) + \Delta)^{\frac{s+1}{2}} u_0|| + ||(f'(0) + \Delta)^{\frac{s}{2}} v_0||.$$

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For the leapfrog method, given $0 \leq s \leq 2$ and $r < x^* = 2$,

$$\mu_s(r) = \sup_{0 < x \leq r} \left| \left(\frac{r}{x}\right)^s \left(\frac{2}{x} \arcsin\left(\frac{x}{2}\right) - 1\right) \right|,$$

$$\nu_s(r) = \sup_{0 < x \leq r} \left| \left(\frac{r}{x}\right)^s \sqrt{1 - \frac{x^2}{4}} \right|.$$

Given a splitting scheme with coefficients $a_1, b_1, \ldots, a_m, b_m$, there exist $x^* \geq 0$ and two even functions $\kappa(x)$ and $\gamma(x)$ such that, if B is symmetric positive definite and $|\tau|\rho(B) \leq x^*$, then

$$q_n = \tilde{q}(n\tau), \quad p_n = \gamma(\tau B)\tilde{p}(n\tau),$$

where $(\tilde{q}(t), \tilde{p}(t))$ is the exact solution of

$$\frac{d}{dt}\tilde{q} = \tilde{p}, \qquad \frac{d}{dt}\tilde{p} = -\tilde{B}^2\, q,$$

with $\tilde{B} = \kappa(\tau B)B$ and initial values

$$\tilde{q}(0) = q_0, \quad \tilde{p}(0) = \gamma(\tau B)^{-1}\, p_0.$$

Furthermore, the theorem above holds with

$$\begin{aligned} \mu_s(r) &= \sup_{0<x\leq r} \left| \left(\tfrac{r}{x}\right)^s (\kappa(x) - 1) \right|, \\ \nu_s(r) &= \sup_{0<x\leq r} \left| \left(\tfrac{r}{x}\right)^s (\gamma(x) - 1) \right|. \end{aligned}$$

Work in progress

- Construction of optimized splitting methods with relatively large number m of factors with optimized values of $\mu_s(r) + \epsilon\, \nu_s(r)$ for prescribed m, s, r, ϵ.
- Testing/analysis of methods for (weakly) non-linear wave equations, and eventually adapt the optimization criteria (Conjecture: Small coefficients $|a_j|, |b_j|$ required, in addition to small $\mu_s(r) + \epsilon\, \nu_s(r)$).
- Apply and adapt optimized splitting methods to other linear problems of the form

  $$\frac{d}{dt} q = M\, p, \quad \frac{d}{dt} p = -N\, q$$

  with all eigenvalues in the imaginary axis: Schrödinger, Maxwel.
- ...

Parameters for known splitting methods with m stages and order $2n$

- Relative stability threshold x^*/m,
- Values for $(\mu_s(r\,m), \nu_s(r\,m))$ in the error estimate

$$||q_n - q(t_n)|| \quad \leq \quad \frac{C_s}{\rho(B)^s} \left(|t_n|\mu_s(r\,m) + \nu_s(r\,m)\right)$$

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

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