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ON LEAP-FROG-Chebyshev SCHEMES*

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Abstract. This paper is dedicated to the improvement of the efficiency of the leap-frog method for second order differential equations. In numerous situations the strict CFL condition of the leap-frog method is the main bottleneck that thwarts its performance. Based on Chebyshev polynomials new methods have been constructed that exhibit a much weaker CFL condition than the leap-frog method. However, these methods do not even approximately conserve the energy of the exact solution which can result in a bad approximation quality.

In this paper we propose two remedies to this drawback. For linear problems we show by using energy techniques that damping the Chebyshev polynomial leads to approximations which approximately preserve a discrete energy norm over arbitrary long times. Moreover, with a completely different approach based on generating functions, we propose to use special starting values that considerably improve the stability. We show that the new schemes arising from these modifications are of order two and can be modified to be of order four. These convergence results apply to semilinear problems. Finally, we discuss the efficient implementation of the new schemes and give generalizations to fully nonlinear equations.

Key words. time integration, Hamiltonian systems, wave equation, 2nd order ode, leap-frog method, CFL condition, Chebyshev polynomials, stability analysis, error analysis, energy techniques, generating functions

AMS subject classifications. Primary: 65L04, 65L20. Secondary: 65L05, 65L06, 65L70

1. Introduction. In this paper we are concerned with the second order differential equation

$$(1.1) \quad \ddot{\mathbf{q}}(t) = -\mathbf{L}\mathbf{q}(t) - g(\mathbf{q}(t)), \quad \mathbf{q}(0) = \mathbf{q}^0, \quad \dot{\mathbf{q}}(0) = \dot{\mathbf{q}}^0,$$

with a symmetric and positive definite matrix \mathbf{L} of large norm and a “nice” function g . Such equations are used to model a plurality of phenomena. Among others Hamiltonian problems and (spatially discretized) wave-type problems are described by (1.1).

The most natural approach to discretize (1.1) is to replace the second order time derivative by a centered second-order difference quotient — the well-known leap-frog (LF) scheme. Thanks to a variety of nice features such as symplecticity, time-reversibility [8] and an easy implementation the LF scheme serves as the standard time integrator for problems of the type (1.1).

However, its efficiency can be severely limited by the time step size restriction (CFL condition) arising from the large norm of \mathbf{L} . This forces a large number of evaluations of the nonlinear function g . In many situation such an evaluation is costly which renders the LF method prohibitively expensive.

The same issue arises for first order parabolic problems and explicit Runge–Kutta (RK) methods. In this setting Runge–Kutta–Chebyshev (RKC) methods [10, 16, 17, 18] have been found a remedy. First order RKC methods are constructed by using a scaled and shifted Chebyshev polynomial as stability function. This choice maximizes the stability region and thus alleviates the CFL condition compared to standard RK

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methods. Based on this idea higher order methods and further extensions, as, e.g., the ROCK family [1, 2], have been proposed.

In [6, 12] the authors applied analogous ideas to the linear case ($g \equiv 0$) of (1.1) and the LF method. In accordance with RKC schemes the resulting methods may be called leap-frog-Chebyshev (LFC) schemes. Unfortunately, these schemes suffer from stability problems. As numerical examples indicate they fail to reproduce the stability behavior of the exact solution. This can result in an energy drift and poor approximation quality.

The aim of this paper is to improve the LFC methods such that they generate approximations with the correct stability behavior and a good approximation grade. In fact, we propose the following two remedies to the aforementioned problem:

- Motivated by stabilized RKC methods [10, 16, 17, 18] we construct a damped version of the Chebyshev polynomial. Using an energy technique we show that this modified scheme nearly conserves a discrete energy and leads to uniformly bounded approximations over arbitrary long times.
- We replace the standard starting values based on a Taylor expansion of the exact solution by ones involving the Chebyshev polynomial and its derivative. With this modification we show via a generating functions technique the stability of the new scheme.

A main feature of the novel schemes emanating from these modifications is that their CFL condition is alleviated by a factor p compared to the LF method, if p is the degree of the Chebyshev polynomial.

Having these methods at hand, they can be combined, e.g., with the LF scheme for g to integrate the semilinear problem (1.1). As we will show in the course of this paper this multi rate method can be employed with an (approximately) p times larger time step than the LF method. This renders the method considerably more efficient than the LF scheme since it requires p times less evaluations of the nonlinearity g .

Our paper is organized as follows: In Section 2 we present a general two-step time integration method for (1.1) which comprises among others the LF and the LFC scheme. Section 3 is dedicated to linear problems. Here, we discuss the stability of the general scheme for $g \equiv 0$. We derive conditions which guarantee the stability of the scheme both in the standard and in the energy norm. Moreover, we construct the special starting value mentioned above and prove the stability of the resulting scheme. In Section 4 we present the error analysis. We show that the general scheme is of order two and can be adapted to converge with fourth order. Then, in Section 5 we show that all required assumptions apply for the LFC methods. Subsequently, we discuss in Section 6 the efficiency and the implementation of the LFC method and also generalize it to fully nonlinear problems. We conclude our paper in Section 7 with numerical examples. In particular, we look at the problems of the LFC methods in [6, 12] and show that our modifications overcome them.

2. A general class of two-step schemes. The LF scheme for the semilinear problem (1.1) is given by

$$(2.1a) \quad \mathbf{q}_{n+1} - 2\mathbf{q}_n + \mathbf{q}_{n-1} = -\tau^2 \mathbf{L}\mathbf{q}_n - \tau^2 g(\mathbf{q}_n),$$

$$(2.1b) \quad \mathbf{q}_0 = \mathbf{q}^0, \quad \mathbf{q}_1 = (\mathbf{I} - \frac{1}{2}\tau^2 \mathbf{L})\mathbf{q}^0 - \frac{1}{2}\tau^2 g(\mathbf{q}^0) + \tau \dot{\mathbf{q}}^0,$$

where $\tau > 0$ is the time step size and \mathbf{q}_n approximates the exact solution $\mathbf{q}(t_n)$ at time $t_n = n\tau$.

Our aim is to modify the “linear part” of the LF method such that the resulting scheme remains stable for larger time step sizes than the standard LF method (2.1).

For this purpose we use a polynomial P satisfying

$$(2.2) \quad P(0) = 0, \quad P'(0) = 1,$$

and propose the scheme

$$(2.3a) \quad \mathbf{q}_{n+1} - 2\mathbf{q}_n + \mathbf{q}_{n-1} = -P(\tau^2\mathbf{L})\mathbf{q}_n - \tau^2 g_n$$

$$(2.3b) \quad \mathbf{q}_0 = \mathbf{q}^0, \quad \mathbf{q}_1 = (\mathbf{I} - \frac{1}{2}P(\tau^2\mathbf{L}))\mathbf{q}^0 - \frac{1}{2}\tau^2 g_0 + \tau P'(\tau^2\mathbf{L})\dot{\mathbf{q}}^0,$$

where g_n is a suitable approximation to $g(\mathbf{q}(t_n))$. The obvious choice is to use $g_n = g(\mathbf{q}_n)$ but other choices are possible, e.g., filtered versions as in Gautschi-type methods [8, 9]. For such methods one could set $g_n = P(\tau^2\mathbf{L})g(\widehat{P}(\tau^2\mathbf{L})\mathbf{q}_n)$ with a suitable filter function \widehat{P} . Then, the scheme could be interpreted as a particular implementation of Gautschi-type methods, where the trigonometric matrix functions are approximated by special polynomials P and \widehat{P} , respectively.

In this paper we examine the general scheme (2.3a)–(2.3b) with particular attention to the choice

$$(2.3c) \quad P(z) = P_p(z) = 2 - \frac{2}{T_p(\nu_p)} T_p\left(\nu_p - \frac{z}{\alpha_p}\right), \quad \alpha_p = 2 \frac{T'_p(\nu_p)}{T_p(\nu_p)}.$$

Here, T_p denotes the p th Chebyshev polynomial of first kind, so that P_p is a polynomial of degree $p \geq 1$, and $\nu_p \geq 1$ is a damping parameter whose choice will be discussed later.

We note that (2.3c) is motivated by the construction of RKC methods [10, 16, 17, 18] and accordingly we name methods from the class (2.3a)–(2.3c) *leap-frog-Chebyshev* schemes. In particular, we discuss in this paper the method with $g \equiv 0$ and the multi rate case with $g_n = g(\mathbf{q}_n)$.

Let us remark that for $p = 1$ the LFC method (2.3a)–(2.3c) reduces to the standard LF method, i.e., $P(z) = P_1(z) = z$ for any choice of $\nu_p \geq 1$.

As already indicated above the general scheme (2.3a)–(2.3b) comprises the LF but also (for $g \equiv 0$) the modified equation leap-frog (modified LF) [15] method with

$$(2.4) \quad P_{\text{LF}}(z) = z, \quad P_{\text{modLF}}(z) = z - \frac{1}{12}z^2.$$

For $p > 1$, $\nu_p = 1$, $g \equiv 0$ and standard starting values (2.1b) the method (2.3a), (2.3c) has been constructed in [6, 12]. Unfortunately, as we will show in the next section, these methods suffer from stability issues. In particular, they are not suited to construct a stable multi rate method. We propose to remedy these problems by using the starting values (2.3b) which also involve P_p and its derivative P'_p . A second crucial modification is the use of a damping parameter $\nu_p > 1$. This approach follows the idea of damped RKC methods [10, 16, 17, 18]. In the next section, we show that these modifications lead to a stable scheme.

3. Linear stability. In this section we consider the associated linear homogeneous problem to (1.1), i.e.,

$$(3.1) \quad \ddot{\mathbf{q}}(t) = -\mathbf{L}\mathbf{q}(t), \quad \mathbf{q}(0) = \mathbf{q}^0, \quad \dot{\mathbf{q}}(0) = \dot{\mathbf{q}}^0.$$

Recall that $\mathbf{L} \in \mathbb{R}^{d \times d}$ is a symmetric, positive definite matrix w.r.t. a given inner product (\cdot, \cdot) , i.e., \mathbf{L} satisfies

$$(\mathbf{L}\mathbf{q}, \widehat{\mathbf{q}}) = (\mathbf{q}, \mathbf{L}\widehat{\mathbf{q}}), \quad (\mathbf{L}\mathbf{q}, \mathbf{q}) > 0, \quad \text{for all } \mathbf{q}, \widehat{\mathbf{q}} \in \mathbb{R}^d.$$

The solution

$$\mathbf{q}(t) = \cos(t\mathbf{L}^{1/2})\mathbf{q}^0 + t \operatorname{sinc}(t\mathbf{L}^{1/2})\dot{\mathbf{q}}^0, \quad \operatorname{sinc}(\zeta) = \frac{\sin \zeta}{\zeta},$$

of (3.1) satisfies

$$(3.2) \quad \|\mathbf{q}(t)\| \leq \|\mathbf{q}^0\| + t\|\dot{\mathbf{q}}^0\| \quad \text{and} \quad \|\|\mathbf{q}(t)\|\| = \|\|\mathbf{q}(0)\|\|$$

for all $t \geq 0$. Here, we denoted the *standard norm* by $\|\cdot\|^2 = (\cdot, \cdot)$ and the *energy norm* by

$$(3.3) \quad \|\|\mathbf{q}(t)\|\|^2 = \|\dot{\mathbf{q}}(t)\|^2 + \|\mathbf{q}(t)\|_{\mathbf{L}}^2, \quad \|\mathbf{q}\|_{\mathbf{L}}^2 = (\mathbf{L}\mathbf{q}, \mathbf{q}).$$

We show stability and error bounds in these norms by two completely different techniques, namely energy techniques and generating functions.

3.1. Stability in the energy norm. Before we start to study the stability of the recursion (2.3a), we introduce a short notation for differences and means:

$$\begin{aligned} [\mathbf{q}_{n+\frac{1}{2}}] &= \mathbf{q}_{n+1} - \mathbf{q}_n, & \{\mathbf{q}_{n+\frac{1}{2}}\} &= \frac{1}{2}(\mathbf{q}_{n+1} + \mathbf{q}_n), \\ \llbracket \mathbf{q}_n \rrbracket &= \mathbf{q}_{n+1} - 2\mathbf{q}_n + \mathbf{q}_{n-1}, & \{\!\!\{ \mathbf{q}_n \}\!\!\} &= \frac{1}{4}(\mathbf{q}_{n+1} + 2\mathbf{q}_n + \mathbf{q}_{n-1}). \end{aligned}$$

Using the identity

$$(3.5) \quad \mathbf{q}_n = \{\!\!\{ \mathbf{q}_n \}\!\!\} - \frac{1}{4}\llbracket \mathbf{q}_n \rrbracket,$$

we can write the recursion (2.3a) in the equivalent form

$$(3.6) \quad (\mathbf{I} - \frac{1}{4}\mathbf{P})\llbracket \mathbf{q}_n \rrbracket + \mathbf{P}\{\!\!\{ \mathbf{q}_n \}\!\!\} = 0, \quad \mathbf{P} = P(\tau^2\mathbf{L}).$$

From this form it is easy to see that this recursion has a preserved quantity.

LEMMA 3.1. *The iterates $(\mathbf{q}_n)_n$ obtained from the recursion (2.3a) with $g \equiv 0$ satisfy*

$$(3.7a) \quad \mathcal{M}_{\mathbf{q}, n+\frac{1}{2}} \equiv \mathcal{M}_{\mathbf{q}, \frac{1}{2}} \quad \text{for all } n = 1, 2, \dots,$$

where

$$(3.7b) \quad \mathcal{M}_{\mathbf{q}, n+\frac{1}{2}} = \left((\mathbf{I} - \frac{1}{4}\mathbf{P})[\mathbf{q}_{n+\frac{1}{2}}], [\mathbf{q}_{n+\frac{1}{2}}] \right) + \left(\mathbf{P}\{\mathbf{q}_{n+\frac{1}{2}}\}, \{\mathbf{q}_{n+\frac{1}{2}}\} \right).$$

Proof. The statement follows directly by taking the inner product of (3.6) with $\mathbf{q}_{n+1} - \mathbf{q}_{n-1}$. \square

Motivated by (3.3) we define the *discrete energy norm*

$$(3.8) \quad \|\|\mathbf{q}_{n+\frac{1}{2}}\|\|_{\tau}^2 = \left\| \left\| \frac{[\mathbf{q}_{n+\frac{1}{2}}]}{\tau} \right\| \right\|^2 + \|\|\{\mathbf{q}_{n+\frac{1}{2}}\}\|\|_{\mathbf{L}}^2 \approx \|\|\mathbf{q}(t_{n+\frac{1}{2}})\|\|^2.$$

It is easy to see that if $\mathcal{M}_{\mathbf{q}, n+\frac{1}{2}}$ is equivalent to the energy norm $\|\|\mathbf{q}_{n+\frac{1}{2}}\|\|_{\tau}^2$ then the recursion (2.3a) yields stable approximations for arbitrary starting values in the sense that there exists a constant C_{stb} such that

$$(3.9) \quad \|\|\mathbf{q}_{n+\frac{1}{2}}\|\|_{\tau} \leq C_{\text{stb}} \|\|\mathbf{q}_{\frac{1}{2}}\|\|_{\tau}, \quad n = 1, 2, \dots$$

Moreover, we will show in [Theorem 4.5](#) below that (under suitable assumptions) $\frac{1}{\tau^2} \mathcal{M}_{\mathbf{q}, n+\frac{1}{2}}$ coincides with $\|\mathbf{q}_{n+\frac{1}{2}}\|_{\tau}^2$ up to a second order perturbation, i.e., the recursion [\(2.3a\)](#) approximately preserves the discrete energy. This reflects the behavior of the exact solution which is also energy conserving, see [\(3.2\)](#).

The aforementioned of equivalence $\mathcal{M}_{\mathbf{q}, n+\frac{1}{2}}$ to $\|\mathbf{q}_{n+\frac{1}{2}}\|_{\tau}^2$ requires the following assumption.

ASSUMPTION 3.2. *We assume that there exist constants $\tau_{\text{CFL}}, m_1, m_2 > 0$ such that for all*

$$(3.10) \quad 0 < \tau \leq \tau_{\text{CFL}}$$

we have

$$(3.11) \quad m_1 \left\| \frac{[\mathbf{q}_{n+\frac{1}{2}}]}{\tau} \right\|^2 + m_2 \|\{\mathbf{q}_{n+\frac{1}{2}}\}\|_{\mathbf{L}}^2 \leq \frac{\mathcal{M}_{\mathbf{q}, n+\frac{1}{2}}}{\tau^2} \leq \left\| \frac{[\mathbf{q}_{n+\frac{1}{2}}]}{\tau} \right\|^2 + \|\{\mathbf{q}_{n+\frac{1}{2}}\}\|_{\mathbf{L}}^2.$$

The restriction [\(3.10\)](#) on the time step size is usually called a CFL condition.

THEOREM 3.3. *Let [Assumption 3.2](#) be satisfied. Then, for all $\tau \leq \tau_{\text{CFL}}$ the method consisting of the recursion [\(2.3a\)](#) and arbitrary starting values is stable. In fact, for all $n = 1, 2, \dots$ the iterates of this scheme are bounded by [\(3.9\)](#) with $C_{\text{stb}} = \min\{m_1, m_2\}^{-1/2}$.*

Proof. This follows directly from [\(3.7\)](#) and [\(3.11\)](#). \square

In the next lemma we give conditions on P that ensure [Assumption 3.2](#).

LEMMA 3.4. *[Assumption 3.2](#) is satisfied if*

$$(3.12) \quad m_1 \leq 1 - \frac{1}{4}P(z) \leq 1, \quad m_2 z \leq P(z) \leq z, \quad \text{for all } z \in [0, \beta^2],$$

with

$$(3.13) \quad \tau_{\text{CFL}}^2 = \frac{\beta^2}{\|\mathbf{L}\|}.$$

Proof. This follows by considering $\mathcal{M}_{\mathbf{q}, n+\frac{1}{2}}$ in the orthonormal eigenbasis of the matrix \mathbf{L} . \square

In the following we call the largest interval $[0, \beta^2]$ such that [\(3.12\)](#) holds true the *stability interval* of the method given by the recursion [\(2.3a\)](#) with arbitrary starting values.

Example 3.5. The LF method satisfies the second condition in [\(3.12\)](#) with $m_2 = 1$. However, the first condition requires $z \in [0, 4)$, i.e., the stability interval is $[0, 4\vartheta^2]$ with a $\vartheta < 1$. Then, we obtain $m_1 = 1 - \vartheta^2$ under the CFL condition [\(3.13\)](#) with $\beta^2 = \beta_{\text{LF}}^2 = 4\vartheta^2$.

The modified LF scheme fulfills the first condition in [\(3.12\)](#) for all $z \in [0, 12]$ with $m_1 = \frac{1}{4}$. However, the second condition requires that $z \in [0, 12)$, i.e., the stability interval is $[0, 12\vartheta^2]$ with $\vartheta < 1$. Then, we have $m_2 = 1 - \vartheta^2$ and $\beta_{\text{mLF}}^2 = 12\vartheta^2 = 3\beta_{\text{LF}}^2$. This means the modified LF method allows a $\sqrt{3} \approx 1.732$ times larger time step size than the LF method.

3.2. Stability in the standard norm. In this section we prove the stability of schemes relying on the recursion [\(2.3a\)](#) in the standard norm $\|\cdot\|$ with the generating functions technique. Our analysis shows that the choice [\(2.3b\)](#) of the starting value \mathbf{q}_1 yields a stable scheme even if [\(3.12\)](#) is only satisfied with $m_1 = m_2 = 0$.

THEOREM 3.6. *Assume P satisfies (3.12) with $m_1 = m_2 = 0$. Then, the scheme (2.3a), (2.3b) is stable for $\tau \leq \tau_{\text{CFL}}$ with τ_{CFL} given in (3.13). The iterates are bounded by*

$$(3.14) \quad \|\mathbf{q}_n\| \leq \|\mathbf{q}^0\| + P'_{\max} t_n \|\dot{\mathbf{q}}^0\|, \quad P'_{\max} = \max_{z \in [0, \beta^2]} |P'(z)|.$$

Proof. Following the generating functions technique we define the formal power series

$$\mathbf{q}(\zeta) = \sum_{n=0}^{\infty} \mathbf{q}_n \zeta^n.$$

Multiplying the recursion (2.3a) by ζ^{n+1} and summing over $n \geq 1$ we obtain

$$(3.15) \quad \boldsymbol{\varrho}(\zeta) \mathbf{q}(\zeta) = \mathbf{q}_0 + \zeta \mathbf{q}_1 - \zeta(2\mathbf{I} - \mathbf{P}) \mathbf{q}_0, \quad \boldsymbol{\varrho}(\zeta) = \zeta^2 \mathbf{I} - \zeta(2\mathbf{I} - \mathbf{P}) + \mathbf{I}.$$

The matrix-valued roots ζ_{\pm} of $\boldsymbol{\varrho}$ are given by

$$\zeta_{\pm} = \mathbf{I} - \frac{1}{2} \mathbf{P} \pm i \frac{1}{2} \sqrt{\mathbf{P}(4\mathbf{I} - \mathbf{P})},$$

where $i = \sqrt{-1}$ is the imaginary unit. By (3.12), we have $\|\zeta_{\pm}\| = 1$ so that we can write $\zeta_{\pm} = e^{\pm i \Phi}$ with a matrix Φ whose spectrum is contained in $[0, \pi]$. Clearly, this yields $\zeta_+ = \zeta_-^{-1}$ and thus

$$\boldsymbol{\varrho}(\zeta) = (\zeta \mathbf{I} - \zeta_+) (\zeta \mathbf{I} - \zeta_-) = (\mathbf{I} - \zeta \zeta_-) (\mathbf{I} - \zeta \zeta_+) = (\mathbf{I} - \zeta e^{-i \Phi}) (\mathbf{I} - \zeta e^{i \Phi}).$$

Using the Neumann series and the Cauchy product we have for $|\zeta| < 1$

$$\boldsymbol{\varrho}(\zeta)^{-1} = \sum_{n=0}^{\infty} e^{-in \Phi} \zeta^n \sum_{\ell=0}^n e^{2i \ell \Phi} = \sum_{n=0}^{\infty} \frac{\sin((n+1)\Phi)}{\sin \Phi} \zeta^n.$$

Here, the second equality follows with the geometric sum identity. Using this in (3.15) we deduce by comparing the coefficients of ζ^n that

$$(3.16) \quad \mathbf{q}_n = \frac{\sin((n+1)\Phi)}{\sin \Phi} \mathbf{q}^0 + \frac{\sin(n\Phi)}{\sin \Phi} \left(\mathbf{q}_1 - 2(\mathbf{I} - \frac{1}{2} \mathbf{P}) \mathbf{q}^0 \right),$$

where we further used $\mathbf{q}_0 = \mathbf{q}(0) = \mathbf{q}^0$. For the second starting value \mathbf{q}_1 , we employ the ansatz

$$(3.17) \quad \mathbf{q}_1 = a(\tau^2 \mathbf{L}) \mathbf{q}^0 + \tau b(\tau^2 \mathbf{L}) \dot{\mathbf{q}}^0,$$

where $a, b : [0, \infty) \rightarrow \mathbb{R}$ are suitable analytic functions satisfying the consistency conditions $a(0) = b(0) = 1$ and $a'(0) = -\frac{1}{2}$. Using $\mathbf{I} - \frac{1}{2} \mathbf{P} = \cos \Phi$ and a trigonometric identity, we infer

$$\mathbf{q}_n = \cos(n\Phi) \mathbf{q}^0 + \frac{\sin(n\Phi)}{\sin \Phi} \left((a(\tau^2 \mathbf{L}) - \cos \Phi) \mathbf{q}^0 + \tau b(\tau^2 \mathbf{L}) \dot{\mathbf{q}}^0 \right).$$

This motivates the choice $a(z) = 1 - \frac{1}{2} P(z)$ in (2.3b) since then $a(\tau^2 \mathbf{L}) = \cos \Phi$. The choice $b(z) = N'(z)$ is not so obvious. It is based on the observation that $|N'(z)/\sqrt{N(z)(4-N(z))}| \leq C$ for all $z \in (0, \beta^2)$ since by assumption the points z

where $N(z) \in \{0, 4\}$ are stationary points of N , i.e., $N'(z) = 0$. For this choice the expression simplifies to

$$\mathbf{q}_n = \cos(n\Phi)\mathbf{q}^0 + \tau \frac{\sin(n\Phi)}{\sin\Phi} \mathbf{P}'\dot{\mathbf{q}}^0.$$

Now, using that for all $\Phi \in \mathbb{R}$ we have $|\cos\Phi| \leq 1$ and $|\frac{\sin n\Phi}{\sin\Phi}| \leq n$ completes the proof. \square

In summary, we have seen that the recursion (2.3a) is stable under the CFL condition $\tau \leq \tau_{\text{CFL}}$ with τ_{CFL} given in (3.13), both in the standard and in the energy norm, if the polynomial P satisfies the conditions (3.12) with positive constants m_1, m_2 . However, for $m_1 = 0$ or $m_2 = 0$ this requires special starting values, e.g., (2.3b).

4. Error analysis. In the previous section we established the stability of the general scheme (2.3a), (2.3b). The aim of this section is to provide its error analysis. The outcome will be a convergence result in the energy norm $\|\cdot\|_\tau$ for the linear problem and a convergence result in the standard norm $\|\cdot\|$ for the semilinear case.

Let us denote the error of the scheme (2.3a), (2.3b) with

$$(4.1) \quad \mathbf{e}_n = \tilde{\mathbf{q}}_n - \mathbf{q}_n, \quad \tilde{\mathbf{q}}_n = \mathbf{q}(t_n),$$

where $\mathbf{q}(t)$ is the exact solution of (1.1). We denote bounds on derivatives of $\mathbf{q}(t)$ by

$$(4.2) \quad B_n^{(k)} = \max_{0 \leq t \leq t_n} \|\mathbf{q}^{(k)}(t)\|, \quad k = 1, 2, \dots$$

Our error analysis requires the following additional assumption.

ASSUMPTION 4.1. *There exist constants m_3, m_4, m'_3 and m'_4 such that for all $z \in [0, \beta^2]$ it holds*

$$(4.3a) \quad |P(z) - z| \leq m_3 z^2, \quad |P(z) - z + m_3 z^2| \leq m_4 z^3,$$

$$(4.3b) \quad |P'(z) - 1| \leq m'_3 z, \quad |P'(z) - 1 + m'_3 z| \leq m'_4 z^2.$$

This assumption implies that

$$(4.4a) \quad |Q(z)| \leq m_4, \quad Q(z) = \frac{P(z) - z + m_3 z^2}{z^3},$$

$$(4.4b) \quad |\hat{Q}(z)| \leq m'_4, \quad \hat{Q}(z) = \frac{P'(z) - 1 + m'_3 z}{z^2},$$

for all $z \in [0, \beta^2]$.

4.1. Error analysis in the energy norm for linear problems. In this section we restrict ourselves to linear problems (3.1). Then, we can prove the following error recursion.

LEMMA 4.2. *For $\mathbf{q} \in C^6(0, T)$ the error \mathbf{e}_n satisfies the recursion*

$$(4.5a) \quad \llbracket \mathbf{e}_n \rrbracket + \mathbf{P}\mathbf{e}_n = \mathbf{d}_n, \quad \mathbf{d}_n = \Delta_n + \delta_n^{(6)},$$

where

$$(4.5b) \quad \Delta_n = \left(\frac{1}{12} - m_3\right)\tau^4 \mathbf{q}^{(4)}(t_n) - \tau^6 Q(\tau^2 \mathbf{L})\mathbf{q}^{(6)}(t_n),$$

$$(4.5c) \quad \delta_n^{(k)} = \tau^{k-1} \int_{t_n}^{t_{n+1}} \kappa_{n,+}^{(k-1)}(t) \mathbf{q}^{(k)}(t) dt - \tau^{k-1} \int_{t_{n-1}}^{t_n} \kappa_{n,-}^{(k-1)}(t) \mathbf{q}^{(k)}(t) dt,$$

with $\kappa_{n,\pm}^{(\ell)}(t) = (t_{n\pm 1} - t)^\ell / (\ell! \tau^\ell)$. The defect is bounded by

$$(4.6) \quad \|\mathbf{d}_n\| \leq M_3 B_n^{(4)} \tau^4 + (m_4 + \frac{1}{60}) B_{n+1}^{(6)} \tau^6, \quad M_3 = \left| \frac{1}{12} - m_3 \right|.$$

Proof. We insert the exact solution $\tilde{\mathbf{q}}_n$ into the scheme (2.3a)

$$\llbracket \tilde{\mathbf{q}}_n \rrbracket + \mathbf{P} \tilde{\mathbf{q}}_n = \mathbf{d}_n,$$

which yields (4.5a) with a defect \mathbf{d}_n . In order to determine \mathbf{d}_n we use Taylor expansion and (3.1) to obtain

$$\llbracket \tilde{\mathbf{q}}_n \rrbracket = \tau^2 \ddot{\mathbf{q}}(t_n) + \frac{1}{12} \tau^4 \mathbf{q}^{(4)}(t_n) + \delta_n^{(6)} = -\tau^2 \mathbf{L} \tilde{\mathbf{q}}_n + \frac{1}{12} \tau^4 \mathbf{q}^{(4)}(t_n) + \delta_n^{(6)}.$$

This implies

$$\mathbf{d}_n = (\mathbf{P} - \tau^2 \mathbf{L}) \tilde{\mathbf{q}}_n + \frac{1}{12} \tau^4 \mathbf{q}^{(4)}(t_n) + \delta_n^{(6)},$$

which shows (4.5) by definition (4.4a) of Q . The bound follows directly from Assumption 4.1. \square

From the error recursion (4.5) we can derive an error bound in the energy norm.

THEOREM 4.3. *Let $\mathbf{q} \in C^6(0, T)$ be the solution of (3.1) and let Assumptions 3.2 and 4.1 be satisfied. Then, for all $\tau \leq \tau_{\text{CFL}}$ and $t_{n+1} \leq T$ we have*

$$(4.7) \quad \frac{1}{C_{\text{stb}}} \|\mathbf{e}_{n+\frac{1}{2}}\|_\tau \leq C_2 \tau^2 + C_3 \tau^3 + C_4 \tau^4,$$

where

$$C_2 = M'_3 B_0^{(3)} + \frac{t_n}{\sqrt{m_1}} M_3 B_n^{(4)}, \quad C_3 = \frac{1}{2} M_3 B_0^{(4)}, \quad M'_3 = \left| \frac{1}{6} - m'_3 \right|,$$

and where C_{stb} is defined in Theorem 3.3. The constant C_4 only depends on t_n , the bounds $B_n^{(5)}$, $B_{n+1}^{(6)}$, and the constants in Assumption 4.1.

Proof. This first part of the proof is inspired by [4, Lemma 2.6] and [11, Section 2.4].

Using (3.5), we write (4.5a) in the equivalent form

$$(4.8) \quad (\mathbf{I} - \frac{1}{4} \mathbf{P}) \llbracket \mathbf{e}_n \rrbracket + \mathbf{P} \{\mathbf{e}_n\} = \mathbf{d}_n.$$

Taking the inner product of (4.8) with $\mathbf{e}_{n+1} - \mathbf{e}_{n-1}$ we obtain

$$\begin{aligned} \mathcal{M}_{\mathbf{e}_{n+\frac{1}{2}}} - \mathcal{M}_{\mathbf{e}_{n-\frac{1}{2}}} &= (\mathbf{d}_n, \mathbf{e}_{n+1} - \mathbf{e}_{n-1}) \leq \|\mathbf{d}_n\| \left(\|\llbracket \mathbf{q}_{n+\frac{1}{2}} \rrbracket\| + \|\llbracket \mathbf{q}_{n-\frac{1}{2}} \rrbracket\| \right) \\ &\leq \frac{1}{\sqrt{m_1}} \|\mathbf{d}_n\| \left(\sqrt{\mathcal{M}_{\mathbf{e}_{n+\frac{1}{2}}}} + \sqrt{\mathcal{M}_{\mathbf{e}_{n-\frac{1}{2}}}} \right), \end{aligned}$$

where $\mathcal{M}_{\mathbf{e}_{n+\frac{1}{2}}}$ was defined in (3.7b) and where we used (3.11) for the last estimate. This is equivalent to

$$\sqrt{\mathcal{M}_{\mathbf{e}_{n+\frac{1}{2}}}} - \sqrt{\mathcal{M}_{\mathbf{e}_{n-\frac{1}{2}}}} \leq \frac{1}{\sqrt{m_1}} \|\mathbf{d}_n\|.$$

Summing this inequality and again applying (3.11) yields

$$(4.9) \quad \frac{1}{C_{\text{stb}}} \|\mathbf{e}_{n+\frac{1}{2}}\|_{\tau} \leq \frac{1}{\tau} \|\mathbf{e}_1\| + \frac{1}{\sqrt{m_1}} \frac{1}{\tau} \sum_{\ell=1}^n \|\mathbf{d}_{\ell}\|.$$

Here, we further used that that by $\mathbf{q}_0 = \mathbf{q}^0$ we have $\mathbf{e}_0 = 0$ and thus $\mathcal{M}_{\mathbf{e}, \frac{1}{2}} = \|\mathbf{e}_1\|^2$.

It remains to bound $\|\mathbf{e}_1\|$. A Taylor expansion of $\mathbf{q}(\tau)$ shows

$$\mathbf{e}_1 = \frac{1}{2}(\mathbf{P} - \tau^2 \mathbf{L} + \frac{1}{12} \tau^4 \mathbf{L}^2) \mathbf{q}(0) + \tau(\mathbf{I} - \frac{1}{6} \tau^2 \mathbf{L} - \mathbf{P}') \dot{\mathbf{q}}(0) + \tau^4 \int_0^{\tau} \kappa_{0,+}^{(4)}(t) \mathbf{q}^{(5)}(t) dt.$$

By (4.4), we find

$$\begin{aligned} \mathbf{e}_1 &= \frac{1}{2} \left(\frac{1}{12} - m_3 \right) \tau^4 \mathbf{q}^{(4)}(0) + \left(\frac{1}{6} - m'_3 \right) \tau^3 \mathbf{q}^{(3)}(0) \\ &\quad - \frac{1}{2} Q(\tau^2 \mathbf{L}) \tau^6 \mathbf{q}^{(6)}(0) - \widehat{Q}(\tau^2 \mathbf{L}) \tau^5 \mathbf{q}^{(5)}(0) + \tau^4 \int_0^{\tau} \kappa_{0,+}^{(4)}(t) \mathbf{q}^{(5)}(t) dt. \end{aligned}$$

Using the bounds in (4.4) we obtain

$$\|\mathbf{e}_1\| \leq M'_3 B_0^{(3)} \tau^3 + \frac{1}{2} M_3 B_0^{(4)} \tau^4 + m'_4 B_0^{(5)} \tau^5 + \frac{1}{24} B_1^{(5)} \tau^5 + \frac{1}{2} m_4 B_0^{(6)} \tau^6.$$

Inserting this bound and (4.6) into (4.9) completes the proof. \square

Theorem 4.3 shows that in general the scheme (2.3a), (2.3b) with a polynomial P satisfying (3.12) and (4.3) is of order two and how the error constants depend on the assumptions on P . In particular, we see that if the polynomial P satisfies (4.3) with

$$(4.10) \quad m_3 = \frac{1}{12} \quad \text{and} \quad m'_3 = \frac{1}{6}$$

we have error constants $M_3 = M'_3 = 0$. Then, the resulting scheme satisfies the bound (4.7) with constants $C_2 = C_3 = 0$ and thus is a fourth order scheme. Moreover, for $0 < m_3 < \frac{1}{6}$ and $0 < m'_3 < \frac{1}{3}$, the error constants M_3 and M'_3 are smaller than the ones of the LF scheme, where $M_3 = \frac{1}{12}$ and $M'_3 = \frac{1}{6}$. This results in smaller errors, as will be confirmed in our numerical examples in Section 7.

The second order error bound can also be proved under the weaker regularity conditions $\mathbf{q} \in C^4(0, T)$.

COROLLARY 4.4. *Let the assumptions of Theorem 4.3 be fulfilled for $\mathbf{q} \in C^4(0, T)$. Then, for all $\tau \leq \tau_{\text{CFL}}$ and $t_{n+1} \leq T$ we have*

$$(4.11) \quad \frac{1}{C_{\text{stb}}} \|\mathbf{e}_{n+\frac{1}{2}}\|_{\tau} \leq \widehat{C}_2 \tau^2 + \widehat{C}_3 \tau^3,$$

where

$$\widehat{C}_2 = m'_3 B_0^{(3)} + \frac{t_n}{\sqrt{m_1}} \left(m_3 + \frac{1}{3} \right) B_{n+1}^{(4)}$$

and \widehat{C}_3 only depends on m_3 and on the bounds $B_1^{(3)}$ and $B_0^{(4)}$.

Proof. The statement follows as in the proof of Theorem 4.3 with two minor changes. We write the defect in (4.5) as

$$\mathbf{d}_n = (\mathbf{P} - \tau^2 \mathbf{L}) \widetilde{\mathbf{q}}_n + \delta_n^{(4)},$$

and the error \mathbf{e}_1 as

$$\mathbf{e}_1 = \frac{1}{2}(\mathbf{P} - \tau^2 \mathbf{L})\mathbf{q}^0 + \tau(\mathbf{I} - \mathbf{P}')\dot{\mathbf{q}}^0 + \tau^2 \int_0^\tau \kappa_{0,+}^{(2)} \mathbf{q}^{(3)}(t) dt.$$

By (4.3) this yields $\|\mathbf{d}_n\| \leq (m_3 + \frac{1}{3})B_{n+1}^{(4)}\tau^4$ and $\|\mathbf{e}_1\| \leq m'_3 B_0^{(3)}\tau^3 + \frac{1}{2}m_3 B_0^{(4)}\tau^4 + \frac{1}{2}B_1^{(3)}\tau^3$. Inserting these bounds in (4.9) proves the error bound. \square

Let us end this section on the linear error analysis by proving that the recursion (2.3a) nearly preserves the discrete energy by showing that it is order two close to the preserved quantity $\mathcal{M}_{\mathbf{q}, \frac{1}{2}} = \mathcal{M}_{\mathbf{q}, n+\frac{1}{2}}$.

THEOREM 4.5. *We consider the method (2.3a), (2.3b) with a polynomial P satisfying (3.12) and (4.3a). Then, we have*

$$\left| \|\mathbf{q}_{n+\frac{1}{2}}\|_\tau - \frac{\mathcal{M}_{\mathbf{q}, n+\frac{1}{2}}}{\tau^2} \right| \leq C\tau^2.$$

Proof. We have

$$\tau^2 \|\mathbf{q}_{n+\frac{1}{2}}\|_\tau^2 - \mathcal{M}_{\mathbf{q}, n+\frac{1}{2}} = \frac{1}{4}(\mathbf{P}[\mathbf{q}_{n+\frac{1}{2}}], [\mathbf{q}_{n+\frac{1}{2}}]) - ((\mathbf{P} - \tau^2 \mathbf{L})\{\mathbf{q}_{n+\frac{1}{2}}\}, \{\mathbf{q}_{n+\frac{1}{2}}\}).$$

Using (3.12) and (4.3a) we can bound this by

$$0 \leq \|\mathbf{q}_{n+\frac{1}{2}}\|_\tau^2 - \frac{\mathcal{M}_{\mathbf{q}, n+\frac{1}{2}}}{\tau^2} \leq \frac{1}{4}\tau^2 \left\| \frac{[\mathbf{q}_{n+\frac{1}{2}}]}{\tau} \right\|^2 + m_3 \tau^2 \|\mathbf{L}\{\mathbf{q}_{n+\frac{1}{2}}\}\|^2,$$

which proves the result. \square

4.2. Error analysis in the standard norm for semilinear problems. In this section we prove an error bound for the scheme (2.3a), (2.3b) for semilinear problems (1.1). We assume that $g : \mathbb{R}^d \rightarrow \mathbb{R}^d$ is a Lipschitz-continuous function with

$$(4.12) \quad \|g(\mathbf{q}) - g(\hat{\mathbf{q}})\| \leq L_g \|\mathbf{q} - \hat{\mathbf{q}}\|, \quad \text{for all } \mathbf{q}, \hat{\mathbf{q}} \in \mathbb{R}^d.$$

THEOREM 4.6. *Let $\mathbf{q} \in C^4(0, T)$ and let Assumptions 3.2 and 4.1 be satisfied. Then, for all $\tau \leq \tau_{\text{CFL}}$ and $t_n \leq T$ we have*

$$(4.13) \quad \|\mathbf{e}_n\| \leq (C_1 t_n + C_d t_n^2) e^{L_g t_n^2} \tau^2.$$

The constants C_1, C_d are independent of \mathbf{L}, n , and τ .

Proof. Analogously to Lemma 4.2 and Corollary 4.4 the error \mathbf{e}_n satisfies the recursion

$$(4.14) \quad \mathbf{e}_{n+1} - (2\mathbf{I} - \mathbf{P})\mathbf{e}_n + \mathbf{e}_{n-1} = \mathbf{d}_n + \mathbf{r}_n, \quad \mathbf{r}_n = -\tau^2(g(\tilde{\mathbf{q}}_n) - (\mathbf{q}_n)),$$

with

$$(4.15) \quad \mathbf{e}_0 = 0, \quad \|\mathbf{e}_1\| \leq C_1 \tau^3, \quad \|\mathbf{d}_n\| \leq C_d \tau^4, \quad \|\mathbf{r}_n\| \leq \tau^2 L_g \|\mathbf{e}_n\|.$$

By the same procedure as for the proof of Theorem 3.6 we have

$$\mathbf{e}_n = \frac{\sin(n\Phi)}{\sin \Phi} \mathbf{e}_1 + \sum_{\ell=0}^{n-1} \frac{\sin((n-\ell-1)\Phi)}{\sin \Phi} (\mathbf{d}_\ell + \mathbf{r}_\ell).$$

Since $\left| \frac{\sin n\Phi}{\sin \Phi} \right| \leq n$ for all $\Phi \in \mathbb{R}$ and using the bounds (4.15) we obtain

$$(4.16) \quad \|\mathbf{e}_n\| \leq (C_1 t_n + C_d t_n^2) \tau^2 + L_g t_n \tau \sum_{\ell=0}^{n-1} \|\mathbf{e}_\ell\|.$$

The statement now follows from a discrete Gronwall lemma. \square

COROLLARY 4.7. *For linear problems ($g \equiv 0$), we have $\|\mathbf{e}_n\| \leq (C_1 t_n + C_d t_n^2) \tau^2$, so that the error only grows quadratically in t_n .*

5. Error and stability analysis of LFC methods. In this section we show that the LFC method (2.3a)–(2.3c) satisfies the assumptions of Sections 3 and 4.

THEOREM 5.1. *Let $p > 1$ and $\nu_p > 1$. The polynomial P_p defined in (2.3c) satisfies Assumptions 3.2 and 4.1 with*

$$(5.1a) \quad m_1 = \frac{1}{2} \left(1 - \frac{1}{T_p(\nu_p)} \right), \quad m_2 = 4 \frac{m_1}{\beta_p^2}, \quad \beta^2 = \beta_p^2 = \alpha_p(\nu_p + 1),$$

$$(5.1b) \quad m_3 = \frac{T_p''(\nu_p)}{\alpha_p^2 T_p(\nu_p)}, \quad m_4 = \frac{T_p'''(\nu_p)}{3\alpha_p^3 T_p(\nu_p)},$$

$$(5.1c) \quad m'_3 = 2m_3, \quad m'_4 = 3m_4.$$

Remark 5.2. (i) For $p = 2, \dots, 5$ the following choices of ν_p fulfill (4.10):

$$\nu_2 = \frac{\sqrt{6}}{2} \approx 1.224745, \quad \nu_3 \approx 1.029086, \quad \nu_4 \approx 1.008261, \quad \nu_5 \approx 1.003233,$$

and thus give a fourth order scheme. In the case of $p = 2$ and $\nu_2 = \frac{\sqrt{6}}{2}$ we retrieve the modified LF method, see (2.4).

(ii) We have the following limits,

$$\begin{aligned} \lim_{\nu_p \rightarrow 1} \alpha_p &= 2p^2, & \lim_{\nu_p \rightarrow \infty} \alpha_p &= 0, & \lim_{\nu_p \rightarrow 1} \beta_p^2 &= 4p^2, & \lim_{\nu_p \rightarrow \infty} \beta_p^2 &= 2p, \\ \lim_{\nu_p \rightarrow 1} m_1 &= 0, & \lim_{\nu_p \rightarrow \infty} m_1 &= \frac{1}{2}, & \lim_{\nu_p \rightarrow 1} m_2 &= 0, & \lim_{\nu_p \rightarrow \infty} m_2 &= \frac{1}{p}, \end{aligned}$$

and

$$\begin{aligned} \lim_{\nu_p \rightarrow 1} m_3 &= \frac{p^2 - 1}{12p^2}, & \lim_{\nu_p \rightarrow \infty} m_3 &= \frac{p - 1}{4p}, \\ \lim_{\nu_p \rightarrow 1} m_4 &= \frac{(p^2 - 1)(p^2 - 4)}{360p^4}, & \lim_{\nu_p \rightarrow \infty} m_4 &= \frac{(p - 1)(p - 2)}{24p^2}, \end{aligned}$$

see also Figure 5.1. This means the stability constants m_1, m_2 improve and the CFL condition degrades with larger ν_p . Moreover, we see that the error constant M_3 defined in (4.6) depends on the size of ν_p .

Proof. Throughout this proof we change between the coordinates

$$x = \nu_p - \frac{z}{\alpha_p} \in [-1, \nu_p] \quad \text{and} \quad z = \alpha_p(\nu_p - x) \in [0, \beta_p^2].$$

(a) We have to prove that the inequalities (3.12) hold true with constants (5.1a):

(i) First inequality: It is well-known that for $\nu_p \geq 1$ we have

$$-1 \leq T_p(x) \leq T_p(\nu_p), \quad \text{for } x \in [-1, \nu_p],$$

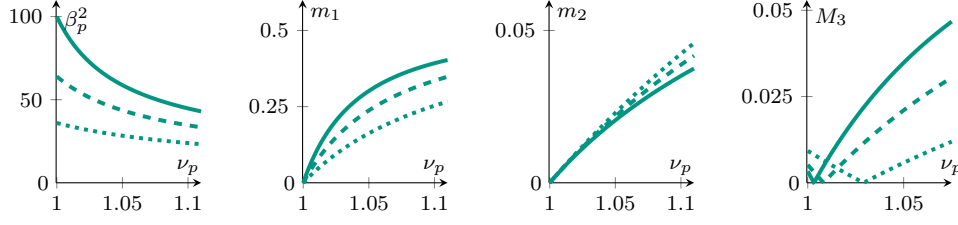


Fig. 5.1: Dependence of β_p^2 , m_1 , m_2 and $M_3 = |\frac{1}{12} - m_3|$ on ν_p for $p = 3, 4, 5$ (dotted, dashed, solid).

see also [Figures 5.2a](#) and [5.2b](#). This is equivalent to

$$\frac{1}{2} \left(1 - \frac{1}{T_p(\nu_p)} \right) \leq 1 - \frac{1}{4} P_p(x) \leq 1, \quad \text{for } x \in [-1, \nu_p],$$

which is the desired bound with m_1 given in [\(5.1a\)](#).

(ii) Second inequality: For the lower bound note that T_p is bounded by the line ℓ_T through $(-1, 1)$ and $(\nu_p, T_p(\nu_p))$ (the blue line in [Figures 5.2a](#) and [5.2b](#)), i.e., for $x \in [-1, \nu_p]$, we have

$$\begin{aligned} T_p(x) &\leq \ell_T(x) = T_p(\nu_p) + \frac{1 - T_p(\nu_p)}{1 + \nu_p} (\nu_p - x) \\ &= T_p(\nu_p) + \frac{1 - T_p(\nu_p)}{\beta_p^2} \alpha (\nu_p - x). \end{aligned}$$

From this we obtain

$$P_p(z) \geq \frac{2}{\beta_p^2} \left(1 - \frac{1}{T_p(\nu_p)} \right) z = \ell_P(z), \quad \text{for } z \in [0, \beta_p^2],$$

which is the claimed bound (see also the blue line in [Figures 5.2c](#) and [5.2d](#)).

For the upper bound we use that

$$T_p'(x) \leq T_p'(1), \quad \text{for } x \in [-1, 1],$$

see, e.g., [\[7, Thm 2.1\]](#) or the original work [\[13\]](#). Because T_p' is monotonically increasing on $[1, \infty)$ we deduce that

$$T_p'(x) \leq T_p'(\nu_p), \quad \text{for } x \in [-1, \nu_p].$$

Integrating from x to ν_p gives

$$T_p(\nu_p) - T_p(x) \leq T_p'(\nu_p)(\nu_p - x),$$

and from this we obtain

$$P_p(z) \leq \frac{T_p'(\nu_p)}{T_p(\nu_p)} (\nu_p - x) = \alpha_p (\nu_p - x) = z.$$

(b) We have to show the inequalities [\(4.3a\)](#) with constants [\(5.1b\)](#): Markov brothers' inequality, see, e.g., [\[7, Thm 2.2\]](#) or the original work [\[14\]](#), states that

$$(5.2) \quad T_p^{(n)}(x) \leq T_p^{(n)}(\nu_p) \quad \text{for } x \in [-1, \nu_p], \quad n \in \mathbb{N}.$$

Using $n = 2$ in this inequality and integrating it twice from x to ν_p we obtain

$$T_p(\nu_p) - T_p(x) \geq T'_p(\nu_p)(\nu_p - x) - \frac{T''_p(\nu_p)}{2}(\nu_p - x)^2.$$

Choosing $n = 3$ and integrating three times we get

$$T_p(\nu_p) - T_p(x) \leq T'_p(\nu_p)(\nu_p - x) - \frac{T''_p(\nu_p)}{2}(\nu_p - x)^2 + \frac{T'''_p(\nu_p)}{6}(\nu_p - x)^3.$$

From these two inequalities we conclude

$$P_p(z) \geq z - m_3 z^2, \quad P_p(z) \leq z - m_3 z^2 + m_4 z^3,$$

and together with the second bound of (3.12)

$$0 \geq P_p(z) - z \geq -m_3 z^2, \quad 0 \leq P_p(z) - z + m_3 z^2 \leq m_4 z^3.$$

(c) It remains to show (4.3b) with constants (5.1c): We have

$$P'_p(z) = \frac{2}{\alpha_p T_p(\nu_p)} T'_p(x) = \frac{1}{T'_p(\nu_p)} T'_p(x).$$

By (5.2) with $n = 1$ it holds $P'_p(z) - 1 \leq 0$. Integrating (5.2) with $n = 2$ once from x to ν_p we obtain

$$T'_p(\nu_p) - T'_p(x) \leq T''_p(\nu_p)(\nu_p - x).$$

Moreover, by integrating (5.2) with $n = 3$ twice we get

$$T'_p(\nu_p) - T'_p(x) \geq T''_p(\nu_p)(\nu_p - x) - \frac{T'''_p(\nu_p)}{2}(\nu_p - x)^2.$$

So, we can conclude

$$2m_3 z \leq P'_p(z) - 1 \leq 0, \quad 0 \leq P'_p(z) - 1 + 2m_3 z \leq 3m_4 z^2.$$

This finishes the proof. \square

In the next corollary we show the convergence of the LFC scheme.

COROLLARY 5.3. *For $p > 1$ and $\nu_p > 1$, we consider the LFC scheme (2.3a)–(2.3c).*

- (a) *If the exact solution of (3.1) satisfies $\mathbf{q} \in C^4(0, T)$, then the error is bounded by (4.11).*
- (b) *If the exact solution of (3.1) satisfies $\mathbf{q} \in C^6(0, T)$, then the error is bounded by (4.7).*
- (c) *Let g fulfill (4.12). If the exact solution of (1.1) satisfies $\mathbf{q} \in C^4(0, T)$, then the error is bounded by (4.13).*

The constants are given in Theorem 5.1.

Proof. Theorem 5.1 shows that the assumptions of Theorem 4.3 and Corollary 4.4 are satisfied. \square

Let us end this section by remarking that it is possible to slightly increase the stability bound β_p^2 given in (5.1a). However, this degrades either m_1 or m_2 depending on whether the polynomial degree p is odd or even. The next lemma gives the details.

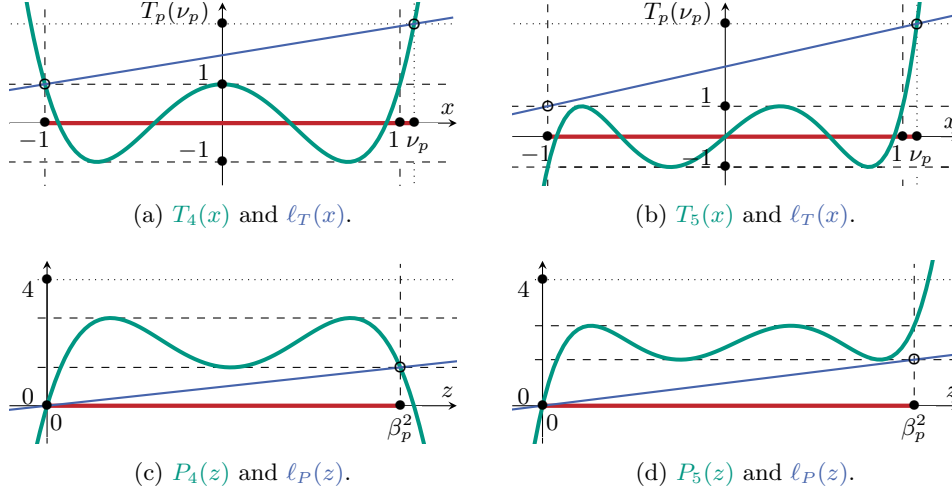


Fig. 5.2: Illustration of the Chebyshev polynomial $T_p(x)$ and the line $\ell_T(x)$ (top) and of the LFC polynomial $P_p(z)$ and the line $\ell_P(z)$ (bottom) for $p = 4, 5$.

LEMMA 5.4. *Let $p > 1$, $\nu_p > 1$ and $\theta \in (\frac{1}{\nu_p}, 1)$. Moreover, let*

$$(5.3) \quad \widehat{m}_1 = \frac{1}{2} \left(1 - \frac{T_p(\theta\nu_p)}{T_p(\nu_p)} \right), \quad \widehat{m}_2 = 4 \frac{\widehat{m}_1}{\widehat{\beta}_p^2}, \quad \widehat{\beta}_p^2 = \alpha_p \nu_p (1 + \theta).$$

Then, P_p satisfies Assumption 3.2 with $\widehat{\beta}_p^2$, m_1 and \widehat{m}_2 if p is even, and $\widehat{\beta}_p^2$, \widehat{m}_1 and m_2 if p is odd, respectively. The bounds from Assumption 4.1 stay true with the constants (5.1b), (5.1c) for $z \in [0, \widehat{\beta}_p^2]$.

Remark 5.5. (i) For $\theta = \frac{1}{\nu_p}$ we obtain $\widehat{m}_1 = m_1$, $\widehat{m}_2 = m_2$ and $\widehat{\beta}_p^2 = \beta_p^2$.
(ii) For $\theta = 1$ we get $\widehat{m}_1 = \widehat{m}_2 = 0$.

Proof. We show how the proof of Theorem 5.1 has to be adapted. For $\theta \in [\frac{1}{\nu_p}, 1)$ we define $\widehat{\nu}_p = \theta\nu_p \in [1, \nu_p]$, so that we have the coordinates

$$x = \nu_p - \frac{z}{\alpha_p} \in [-\widehat{\nu}_p, \nu_p] \quad \text{and} \quad z = \alpha_p(\nu_p - x) \in [0, \widehat{\beta}_p^2].$$

Modifications of part (a)(i): For p even the considerations for the lower bound hold true for $x \in [-\widehat{\nu}_p, \nu_p]$ while for p odd we have

$$-T_p(\widehat{\nu}_p) \leq T_p(x) \leq T_p(\nu_p), \quad \text{for } x \in [-\widehat{\nu}_p, \nu_p].$$

This yields (3.12) with \widehat{m}_1 .

Modifications of part (a)(ii): For p odd all considerations for the lower and the upper bound hold true for $x \in [-\widehat{\nu}_p, \nu_p]$. For p even, T_p is bounded by the line $\widehat{\ell}$ through $(-\widehat{\nu}_p, T_p(\widehat{\nu}_p))$ and $(\nu_p, T_p(\nu_p))$, whence

$$T_p(x) \leq \widehat{\ell}_T(x) = T_p(\nu_p) + \frac{T_p(\widehat{\nu}_p) - T_p(\nu_p)}{\widehat{\beta}_p^2} \alpha(\nu_p - x), \quad \text{for } x \in [-\widehat{\nu}_p, \nu_p],$$

and thus

$$P_p(z) \geq \frac{2}{\widehat{\beta}_p^2} \left(1 - \frac{T_p(\widehat{\nu}_p)}{T_p(\nu_p)}\right) z, \quad \text{for } z \in [0, \widehat{\beta}_p^2].$$

This is the desired bound. The proof for the upper bound holds true for $x \in [-\widehat{\nu}_p, \nu_p]$.

Parts (b) and (c) remain unchanged since (5.2) stays true for $x \in [-\widehat{\nu}_p, \nu_p]$. \square

6. Efficiency, implementation, and generalizations of the LFC method.

In this section we discuss the efficiency and the implementation of the LFC method (2.3a)–(2.3c) for semilinear differential equations and we generalize it to fully nonlinear problems.

6.1. Semilinear LFC method. In Algorithm 6.1 we present an efficient implementation of the n th time step of the LFC method (2.3a)–(2.3c) to integrate the semilinear problem (1.1).

Algorithm 6.1 Leap-frog-Chebyshev scheme for (1.1).

- 1: $\widetilde{P}_0 = 0, \widetilde{P}_1 = \frac{2}{\alpha_p \nu_p} \tau^2 \mathbf{L} \mathbf{q}_n$
 - 2: **for** $k = 2, \dots, p$ **do**
 - 3: $\widetilde{P}_k = 2\nu_p \frac{T_{k-1}(\nu_p)}{T_k(\nu_p)} \widetilde{P}_{k-1} + \frac{2}{\alpha_p} \frac{T_{k-1}(\nu_p)}{T_k(\nu_p)} \tau^2 \mathbf{L} (2\mathbf{q}_n - \widetilde{P}_{k-1}) - \frac{T_{k-2}(\nu_p)}{T_k(\nu_p)} \widetilde{P}_{k-2}$
 - 4: **end for**
 - 5: $\mathbf{q}_{n+1} = 2\mathbf{q}_n - \mathbf{q}_{n-1} - \widetilde{P}_p - \tau^2 g(\mathbf{q}_n)$
-

The parameters α_p and $T_0(\nu_p), \dots, T_p(\nu_p)$ have to be precomputed only once by means of the Chebyshev recursions. Hence, each time step requires p matrix-vector multiplications with \mathbf{L} and one evaluation of g . As we show below this makes the algorithm attractive in applications where on the one hand the evaluation of g is expensive compared to a matrix-vector multiplication by \mathbf{L} but on the other hand the time step is restricted by a CFL condition dominated by \mathbf{L} .

We compare the CFL conditions of the standard LF scheme and the general recursion (2.3a) for the special case of a linear function g , i.e., $g(\mathbf{q}) = \mathbf{G}\mathbf{q}$, where \mathbf{G} is a symmetric and positive semidefinite matrix with $\|\mathbf{G}\| \ll \|\mathbf{L}\|$.

LEMMA 6.1. *Let $g(\mathbf{q}) = \mathbf{G}\mathbf{q}$ and assume that the CFL conditions*

$$(6.1) \quad \tau^2 \|\mathbf{L}\| \leq \beta^2, \quad \tau^2 \|\mathbf{G}\| \leq 4\vartheta^2, \quad \vartheta^2 \in (0, m_1),$$

are satisfied. Then, the recursion (2.3a) with P satisfying Assumption 3.2 is stable with bound

$$(6.2) \quad \min\{m_1 - \vartheta^2, m_2\} \|\mathbf{q}_{n+\frac{1}{2}}\|_\tau^2 \leq \left\| \frac{[\mathbf{q}_{\frac{1}{2}}]}{\tau^2} \right\|^2 + \|\{\mathbf{q}_{\frac{1}{2}}\}\|_{\mathbf{L}+\mathbf{G}}^2.$$

Remark 6.2. Note that the CFL conditions (6.1) can only be satisfied if $m_1 > 0$. For LFC methods this requires a sufficiently large damping parameter $\nu_p > 1$ to allow for a reasonable ϑ .

Proof. For the scheme (2.3) we have

$$\begin{aligned} \mathcal{M}_{\mathbf{q}, n+\frac{1}{2}} &= \left((\mathbf{I} - \frac{1}{4}\mathbf{P})[\mathbf{q}_{n+\frac{1}{2}}, [\mathbf{q}_{n+\frac{1}{2}}]] \right) + (\mathbf{P}\{\mathbf{q}_{n+\frac{1}{2}}\}, \{\mathbf{q}_{n+\frac{1}{2}}\}) \\ &\quad - \frac{1}{4}(\tau^2 \mathbf{G}[\mathbf{q}_{n+\frac{1}{2}}, [\mathbf{q}_{n+\frac{1}{2}}]]) + (\tau^2 \mathbf{G}\{\mathbf{q}_{n+\frac{1}{2}}\}, \{\mathbf{q}_{n+\frac{1}{2}}\}). \end{aligned}$$

The first two terms can be treated with [Assumption 3.2](#) using the first CFL condition in [\(6.1\)](#) and for the last two terms we can use the second CFL condition in [\(6.1\)](#) and the fact that \mathbf{G} is positive semidefinite to obtain

$$(m_1 - \vartheta^2) \left\| \frac{[\mathbf{q}_{n+\frac{1}{2}}]}{\tau^2} \right\|^2 + m_2 \|\{\mathbf{q}_{n+\frac{1}{2}}\}\|_{\mathbf{L}}^2 \leq \frac{\mathcal{M}_{\mathbf{q}, n+\frac{1}{2}}}{\tau^2} \leq \left\| \frac{[\mathbf{q}_{n+\frac{1}{2}}]}{\tau^2} \right\|^2 + \|\{\mathbf{q}_{n+\frac{1}{2}}\}\|_{\mathbf{L}+\mathbf{G}}^2.$$

The assertion follows similar to the proof of [Theorem 3.3](#). \square

Let $\|\mathbf{L}\| = r\|\mathbf{G}\|$ with a factor $r \gg 1$. For $p^2 \lesssim r$ the first CFL condition in [\(6.1\)](#) limits the time step size, whereas for $p^2 \gtrsim r$ the second CFL condition applies. This means that a larger polynomial degree p of P in [\(2.3a\)](#) improves the CFL condition until $p \approx \sqrt{r}$. A further increase of the polynomial degree does not alleviate the CFL condition anymore.

So, let $p^2 \lesssim r$. Then, the CFL condition of the recursion [\(2.3a\)](#) and of the LF method are

$$\tau^2 \lesssim \frac{4p^2}{r\|\mathbf{G}\|} \quad \text{and} \quad \tau^2 \lesssim \frac{4}{(r+1)\|\mathbf{G}\|},$$

respectively. The fraction is $\frac{r+1}{r}p^2 \sim p^2$ since we assume $r \gg 1$. Thus, the recursion [\(2.3a\)](#) allows an (approximately) p times larger time step than the LF method.

In summary, we conclude that N time steps of the LFC method (via [Algorithm 6.1](#)) cost

pN matrix vector multiplications with $\mathbf{L} + N$ evaluations of g .

Due to its stricter CFL condition the LF method has to perform pN time steps with costs

pN matrix vector multiplications with $\mathbf{L} + pN$ evaluations of g .

We see that the effort on the ‘‘linear part’’ are equal for the LFC and the LF method, but the evaluations of the nonlinearity g can be (considerably) reduced by using the LFC method.

6.2. Nonlinear LFC method. In this section we derive the LFC method for the nonlinear problem

$$(6.3) \quad \ddot{\mathbf{q}}(t) = -f(\mathbf{q}), \quad \mathbf{q}(0) = \mathbf{q}^0, \quad \dot{\mathbf{q}}(0) = \dot{\mathbf{q}}^0.$$

This requires a recursion for P_p inspired by RKC methods [\[16\]](#) which we provide in the next lemma.

LEMMA 6.3. *The polynomial*

$$P_{k,p}(z) = 2 - \frac{2}{T_k(\nu_p)} T_k\left(\nu_p - \frac{z}{\alpha_p}\right)$$

satisfies the recursion

$$\begin{aligned} P_{0,p}(z) &= 0, \\ P_{1,p}(z) &= \frac{2}{\alpha_p \nu_p} z, \\ T_k(\nu_p) P_{k,p}(z) &= 2\nu_p T_{k-1}(\nu_p) P_{k-1,p}(z) \\ &\quad + \frac{2}{\alpha_p} T_{k-1}(\nu_p) z (2 - P_{k-1,p}(z)) - T_{k-2}(\nu_p) P_{k-2,p}(z), \end{aligned}$$

for $k = 2, \dots, p$.

Proof. The result follows easily from the recursion of Chebyshev polynomials. \square

Lemma 6.3 and $P_p(z) = P_{p,p}(z)$ imply the following algorithm to implement one time-step of the LFC scheme for nonlinear ordinary differential equations (6.3). One time step requires p evaluations of f as the main cost.

Algorithm 6.2 Leap-frog-Chebyshev scheme for (6.3).

- 1: $\tilde{P}_0 = 0, \tilde{P}_1 = \frac{2}{\alpha_p \nu_p} \tau^2 f(\mathbf{q}_n)$
 - 2: **for** $k = 2, \dots, p$ **do**
 - 3: $\tilde{P}_k = 2\nu_p \frac{T_{k-1}(\nu_p)}{T_k(\nu_p)} \tilde{P}_{k-1} + \frac{2}{\alpha_p} \frac{T_{k-1}(\nu_p)}{T_k(\nu_p)} (2\tau^2 f(\mathbf{q}_n) - \tau^2 f(\tilde{P}_{k-1})) - \frac{T_{k-2}(\nu_p)}{T_k(\nu_p)} \tilde{P}_{k-2}$
 - 4: **end for**
 - 5: $\mathbf{q}_{n+1} = 2\mathbf{q}_n - \mathbf{q}_{n-1} - \tilde{P}_p$
-

7. Numerical examples. In our last section we illustrate our theoretical findings on LFC schemes by numerical examples. It turns out that already the most simple examples show the lack of stability for general starting values or for the undamped case $\nu_p = 1$. All implementations have been performed in Python. The codes will be made available by the authors on request.

7.1. Harmonic oscillator. We consider the harmonic oscillator

$$(7.1) \quad \ddot{q}(t) = -\omega^2 q(t), \quad q(0) = q^0, \quad \dot{q}(0) = \dot{q}^0,$$

where $\omega > 0$ is a fixed frequency. Recall that the solution q satisfies (3.2) and in particular it preserves the energy.

Now, we examine the LFC method (2.3a), (2.3c) with the standard starting values (2.1b) obtained from Taylor expansion and the new ones we proposed in (2.3b).

In Figure 7.1 we present the results for $\omega^2 = 4$, $\mathbf{q}^0 = 2$ and $\dot{\mathbf{q}}^0 = 1$. We used the fifth order polynomial P_5 in (2.3c) without damping ($\nu = 1$) and employ a range of time steps τ so that the product $0 \leq \tau^2 \omega^2 \leq \beta_5^2 = 100$. In Figure 7.1a we depict the (discrete) energy norm of the approximations \mathbf{q}_n obtained with starting value (2.3b). For this choice the energy norm stays bounded independent of the simulation time. In contrary, for the standard choice (2.1b) illustrated in Figure 7.1b we observe resonance effects appearing at $z = \tau^2 \omega^2$ where $P_p(z) = 4$ or $P_p(z) = 0$. This fits perfectly to our analysis because these values force $m_1 = 0$ or $m_2 = 0$ in (3.12), respectively, and thus prevent a stability result as obtained in Theorem 3.3.

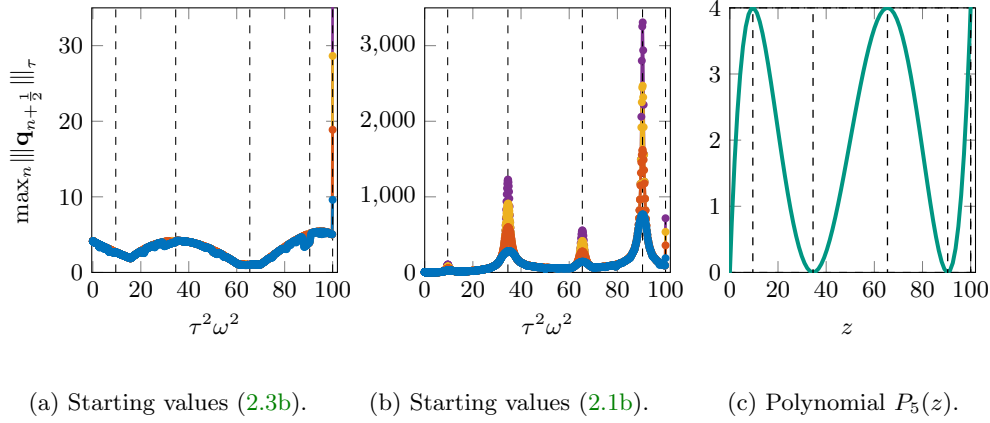


Fig. 7.1: Time integration of the harmonic oscillator with the LFC recursion (2.3a), (2.3c) and different starting values \mathbf{q}_1 . We ran the simulation for $N = 5, 10, 15$ and 20 time steps.

7.2. Wave equation. Next, we consider the homogeneous wave equation with homogeneous Dirichlet boundary conditions in the unit square $\Omega = (0, 1)^2$,

$$(7.2a) \quad \begin{aligned} \ddot{q}(t, x, y) &= \Delta q(t, x, y) - d q(t, x, y), & (x, y) \in \Omega, \quad t \in [0, T], \\ q(t, x, y) &= 0, & (x, y) \in \partial\Omega, \quad t \in [0, T], \\ q(0, x, y) &= q^0(x, y), \quad \dot{q}(0, x, y) = \dot{q}^0(x, y), & (x, y) \in \Omega, \end{aligned}$$

with a parameter $d \geq 0$. As initial data we choose

$$(7.2b) \quad q^0(x, y) = \sin(\pi x) \sin(\pi y), \quad \dot{q}^0(x, y) = \sqrt{2\pi^2 + d} \sin(\pi x) \sin(\pi y).$$

Then, the solution of (7.2) is given by

$$(7.3) \quad q(t, x, y) = \sin(\pi x) \sin(\pi y) (\cos(t\sqrt{2\pi^2 + d}) + \sin(t\sqrt{2\pi^2 + d})).$$

We discretize (7.2) with a symmetric interior penalty discontinuous Galerkin method [3], [5, Chapter 4] using piecewise polynomials of degree three on an unstructured mesh with 312 triangles with smallest and largest diameter 0.0301 and 0.0744, respectively. This results in the following system of odes

$$(7.4) \quad \mathbf{M}\ddot{\mathbf{q}}(t) = -\mathbf{A}\mathbf{q}(t) - d\mathbf{M}\mathbf{q}(t) \quad \mathbf{q}(0) = \mathbf{q}^0, \quad \dot{\mathbf{q}}(0) = \dot{\mathbf{q}}^0.$$

The block diagonal mass matrix \mathbf{M} and the stiffness matrix \mathbf{A} are symmetric (w.r.t. the standard Euclidean inner-product) and positive definite. The boundary condition in (7.2a) is enforced through \mathbf{A} .

Because the mass matrix is block-diagonal it can be inverted at low costs. Thus, (7.2) can be written in the form (1.1) with $\mathbf{L} = -\mathbf{M}^{-1}\mathbf{A}$ and $g(\mathbf{q}) = d\mathbf{q}$. Note that \mathbf{L} is symmetric w.r.t. the inner-product $(\mathbf{q}, \hat{\mathbf{q}}) = \mathbf{q}^T \mathbf{M} \hat{\mathbf{q}}$.

In the following, we integrate (7.4) with the LFC method (2.3a)–(2.3c) until the final time $T = 4.2$ and consider the error

$$(7.5) \quad \mathbf{e}_{h,n} = \mathbf{q}_h(t_n) - \mathbf{q}_n$$

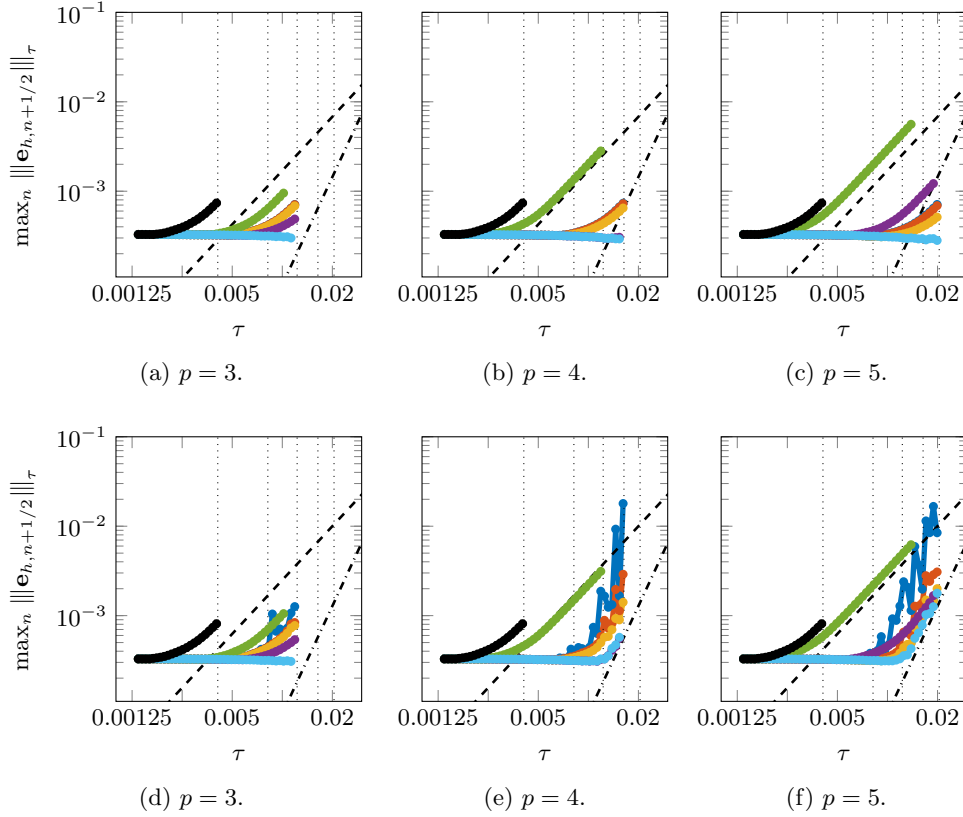


Fig. 7.2: Error of the LFC method (2.3a), (2.3c) plotted over time steps τ for starting values (2.3b) (top) and starting values (2.1b) (bottom). The polynomial degree p is 3, 4 and 5 (left to right). For ν_p we used the following choices: $\nu_p = 1$, $\nu_p = 1.0001$, $\nu_p = 1.0001$, $\nu_p = 1.01$, $\nu_p = 1.1$, ν_p from Remark 5.2 (4th order scheme). The solid black line stems from the LF method. The black dashed lines represent $25\tau^2$ and $8000\tau^4$. The dotted lines correspond to integer multiples of the maximum stable time step size τ_{LF} of the LF method, i.e., $m\tau_{LF}$, with $m = 1, \dots, 5$.

between the $L^2(\Omega)$ -orthogonal projection $\mathbf{q}_h(t)$ of the exact solution onto the discontinuous Galerkin space and the LFC iterate \mathbf{q}_n . We distinguish the cases $d = 0$ and $d > 0$.

7.2.1. Wave equation with $d = 0$. We are in the situation of Section 4.1 and in particular of Theorem 4.3. To show the validity of these elaborations we plot in Figure 7.2a–Figure 7.2c the error (7.5) of the LFC method for polynomial degrees $p = 3, 4, 5$ and different choices of the damping parameter ν_p .

We observe that the LFC method allows us to choose an approximately p times larger time step compared to the LF method (see the dashed lines which mark integer multiples of the maximum stable time step of the LF method). If we use more damping the maximum stable time step gets smaller since β_p^2 is a monotonically decreasing function of the damping parameter ν_p , see also Figure 5.1. Moreover, one can clearly

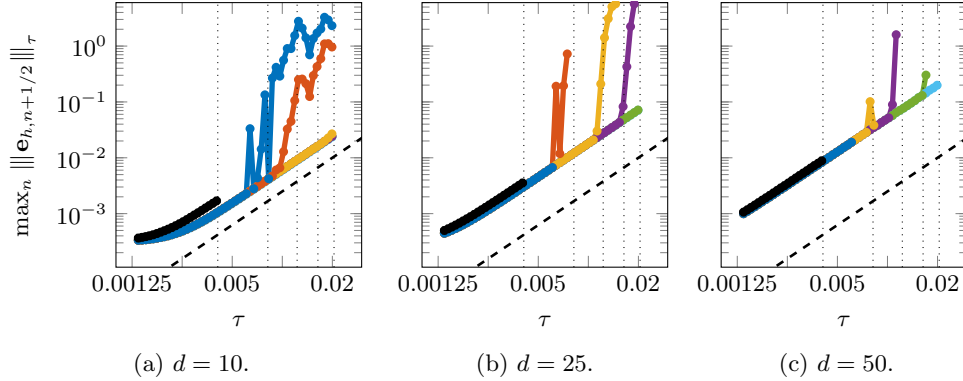


Fig. 7.3: Error of the LFC method (2.3a)–(2.3c) plotted over time steps τ for different values of d . We used polynomial degree $p = 5$ and damping parameters $\nu_p = 1$, $\nu_p = 1.00001$, $\nu_p = 1.00005$, $\nu_p = 1.0001$, $\nu_p = 1.00025$, $\nu_p \approx 1.003233$ (4th order scheme). The solid black line stems from the LF method and the black dashed line represent $25\tau^2$. The dotted lines correspond to integer multiples of the maximum stable time step size τ_{LF} of the LF method, i.e., $m\tau_{\text{LF}}$, with $m = 1, \dots, 5$.

see the effects of the value of ν_p on the error constant. In particular, we observe that a choice of ν_p near the value which gives a fourth order scheme (see (4.10) and Remark 5.2) yields a remarkably better error constant compared to the LF method and consequently clearly smaller errors.

We can confirm the second order convergence rate of the general LFC method. However, the fourth order achieved via (4.10) cannot be visible in this example since the time discretization error is so small that it is already dominated by the space discretization error.

As comparison we give in Figure 7.2d–Figure 7.2f the error of the LFC recursion (2.3a), (2.3c) supplemented with the standard fifth order starting value

$$(7.6) \quad \mathbf{q}_1 = \mathbf{q}^0 + \tau \dot{\mathbf{q}}^0 - \frac{1}{2} \tau^2 \mathbf{L} \mathbf{q}^0 - \frac{1}{6} \tau^3 \mathbf{L} \dot{\mathbf{q}}^0 + \frac{1}{24} \tau^4 \mathbf{L}^2 \mathbf{q}^0.$$

We clearly see larger errors compared to the LFC method (2.3a)–(2.3c). In particular, the undamped case $\nu_p = 1$ suffers from stability problems. However, with enough damping this can be controlled and we even can confirm the fourth order convergence rate achieved by the choice (4.10) of ν_p .

7.2.2. Wave equation with $d > 0$. Last, we consider the case $d > 0$ as a model problem for the semilinear equation (1.1) to show the effects of the LFC method (2.3a)–(2.3c) discussed in Section 6.1. In Figure 7.3 we plotted the error (7.5) for $d = 10, 25, 50$, polynomial degree $p = 5$ and different values of ν_p . As stated in Lemma 6.1 and Remark 6.2 we observe that without enough damping the LFC method cannot achieve a p times larger time than the LF scheme. The larger d is the more damping we have to use. However, if ν_p is sufficiently large we observe an almost p times larger maximum stable time step size and second order convergence.

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