

Convolution-based Chebyshev Acceleration of Waveform Relaxation Methods

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Abstract

Waveform relaxation is a numerical method for solving large-scale systems of ordinary differential equations. In this paper, it is investigated whether the convergence of waveform relaxation can be accelerated by Chebyshev acceleration techniques. The Chebyshev method was originally developed for solving linear systems of equations, and can be generalised in a straightforward manner to the waveform case. It is shown that superior convergence results can be obtained from a related, convolution-based acceleration approach. A general convergence study of the convolution-based Chebyshev waveform relaxation method is presented, together with a discussion of several specific variants, some model problem analyses and numerical experiments.

Keywords : Chebyshev acceleration, convolution, waveform relaxation

AMS(MOS) Classification : 65F10, 65L05

CONVOLUTION-BASED CHEBYSHEV ACCELERATION OF WAVEFORM RELAXATION METHODS

JAN JANSSEN^{†‡} AND STEFAN VANDEWALLE^{†§}

Abstract. Waveform relaxation is a numerical method for solving large-scale systems of ordinary differential equations. In this paper, it is investigated whether the convergence of waveform relaxation can be accelerated by Chebyshev acceleration techniques. The Chebyshev method was originally developed for solving linear systems of equations, and can be generalised in a straightforward manner to the waveform case. It is shown that superior convergence results can be obtained from a related, convolution-based acceleration approach. A general convergence study of the convolution-based Chebyshev waveform relaxation method is presented, together with a discussion of several specific variants, some model problem analyses and numerical experiments.

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1. Introduction. Waveform relaxation (WR) or dynamic iteration is an iterative solution technique for systems of ordinary differential equations (ODEs) which was originally developed for the time-domain analysis of large-scale integrated circuits [10, 15]. Its key idea is to solve the given ODE system by integrating a sequence of subsystems in fewer variables. As such, the method can be regarded as the natural extension to systems of differential equations of the classical relaxation methods for solving systems of algebraic equations, with iteration vectors consisting of functions in time (waveforms) instead of scalar values.

WR methods have been used and discussed for a wide variety of problems, see e.g. [1, Chap. 7–9] and the references cited therein. Most convergence studies, however, concentrate on linear initial-value problems of the form

$$(1.1) \quad B\dot{u}(t) + Au(t) = f(t), \quad u(0) = u_0,$$

with $B, A \in \mathbb{C}^{d \times d}$ and B nonsingular. In those studies, an important goal has been to establish a quantitative comparison between the convergence behaviour of the waveform method for (1.1) and that of the associated relaxation method for the corresponding steady-state problem $Au = f$. We will refer to this classical relaxation method as *static* iteration; the WR method is often referred to as *dynamic* iteration. For the Jacobi and Gauss–Seidel methods, such a comparison was made for several model problems in [6, 13], showing the convergence rates of the waveform variants to be equal to those of the corresponding static iteration methods. A similar correspondence was expected for the WR method defined as the straightforward extension of the static successive overrelaxation (SOR) iteration. Yet, the resulting SOR WR method, based on multiplying a Gauss–Seidel like correction with a fixed overrelaxation parameter, only yields a marginal acceleration compared to the speed up obtained in the static SOR iteration case [8, 13]. These disappointing results led to the definition of the convolution SOR (CSOR) waveform method, in which the multiplication with a fixed SOR parameter is replaced by a convolution with a time-dependent kernel [4, 8, 16].

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This fix appeared to be a very effective one. Analysis showed that, for certain classes of problems, the optimal CSOR WR method attains an identical acceleration as the optimal SOR iteration for the corresponding steady-state problem [8].

In [11, 17], Lubich and Skeel successfully applied a similar convolution idea to the Chebyshev acceleration of the Picard iteration. In this paper, we analyse their result in the classical WR analysis framework (i.e. using Laplace-transform arguments) and we extend their result towards more general WR methods. Our paper is organised as follows. We summarise some important WR results and notations in §2. In §3, we briefly recall the results of [14], where it was shown that in the waveform case no essential speed up can be obtained by applying a standard polynomial acceleration technique, i.e., by taking linear combinations of the basic WR iterates. Our study of the convolution-based polynomial (Chebyshev) acceleration of WR methods is started in §4, where a general convergence analysis is derived. Some specific results for convolution-based Chebyshev acceleration of the Picard, Jacobi and Gauss–Seidel WR methods are presented in §5. In particular, we show that for certain problem classes, the convergence behaviour of the convolution Chebyshev WR method is similar to that of the corresponding static Chebyshev iteration method. Finally, we present some numerical results for a model heat flow problem in §6.

2. Basic WR results. In this section, we recall the asymptotic convergence behaviour of the basic WR methods for ODE system (1.1) in the normed linear spaces $L_p(0, \infty)$ with $1 \leq p \leq \infty$ [6]. It is shown that there is a correspondence between the convergence rates of the WR methods and those of the associated relaxation methods for the algebraic systems

$$(2.1) \quad (zB + A) \tilde{u}(z) = \tilde{f}(z) + Bu_0 ,$$

obtained by Laplace transforming (1.1). The ‘ $\tilde{\cdot}$ ’-notation is used here to denote a Laplace-transformed variable, as for instance in $\tilde{u}(z) = \int_0^\infty u(t)e^{-zt} dt$. We assume the systems (2.1) to be solvable for $\text{Re}(z) \geq 0$. This assumption, which is satisfied if all eigenvalues of $B^{-1}A$ have positive real parts, turns out to be a very natural one as it implies the boundedness and stability of the solution $u(t)$ to (1.1) if $f(t) \in L_p(0, \infty)$.

The basic WR iteration scheme for (1.1) is usually defined in terms of the splittings $B = M_B - N_B$ (with M_B nonsingular) and $A = M_A - N_A$, and is given by

$$(2.2) \quad M_B \dot{x}^{(n)}(t) + M_A x^{(n)}(t) = N_B \dot{x}^{(n-1)}(t) + N_A x^{(n-1)}(t) + f(t) , \quad n \geq 1 ,$$

with $x^{(n)}(0) = u_0$. Here $x^{(n)}(t)$ denotes the n -th approximation to $u(t)$. The initial approximation is usually selected as $x^{(0)}(t) = u_0$. The iteration can be rewritten as an explicit successive approximation scheme

$$(2.3) \quad x^{(n)}(t) = \mathcal{K} x^{(n-1)}(t) + \varphi(t) ,$$

where \mathcal{K} , the basic WR operator, consists of a matrix multiplication by $M_B^{-1}N_B$ and a Volterra convolution with a continuous kernel and

$$\varphi(t) = e^{-M_B^{-1}M_A t} (I - M_B^{-1}N_B) u_0 + \int_0^t e^{M_B^{-1}M_A(s-t)} M_B^{-1} f(s) ds ,$$

[6, §3.1]. The corresponding iteration for (2.1) is obtained by Laplace transforming (2.2), giving

$$(2.4) \quad \begin{aligned} \tilde{x}^{(n)}(z) &= \mathbf{K}(z) \tilde{x}^{(n-1)}(z) + \tilde{\varphi}(z) \\ &= (zM_B + M_A)^{-1} (zN_B + N_A) \tilde{x}^{(n-1)}(z) + \tilde{\varphi}(z) . \end{aligned}$$

This iteration corresponds to a splitting of the matrix $zB + A$ as $(zM_B + M_A) - (zN_B + N_A)$. The spectral radius of the waveform operator \mathcal{K} can be expressed in terms of the spectral radius of the symbol $\mathbf{K}(z)$, provided that the operator's convolution kernel belongs to $L_1(0, \infty)$ [6, Lemma 2.3]. This condition is satisfied if all eigenvalues of $M_B^{-1}M_A$ have positive real parts. In that case, one obtains

$$(2.5) \quad \rho(\mathcal{K}) = \sup_{\operatorname{Re}(z) \geq 0} \rho(\mathbf{K}(z)) = \sup_{z \in i\mathbb{R}} \rho(\mathbf{K}(z)) ,$$

the rightmost equality of which follows from the maximum principle. While this formula is strictly valid only if iterations on infinite-length time windows are considered, it is well-known that observed experimental convergence factors on (long enough) finite time intervals correspond very well to the values in the right-hand side of (2.5).

Alternatively, one might be interested in the length of a time window $[0, T_r]$ wherein convergence is approximately geometric, with a given rate of decay r . This is especially interesting when \mathcal{K} is divergent or unbounded in $L_p(0, \infty)$. In that case, one investigates the operator \mathcal{K} in the exponentially weighted spaces $L_p^\alpha(0, \infty)$ with $\alpha > 0$ [6, Rem. 3.2]. If all eigenvalues of $M_B^{-1}M_A$ have real parts greater than $-\alpha$, then \mathcal{K} is a bounded operator in this weighted space (its convolution kernel belongs to $L_1^\alpha(0, \infty)$) and its spectral radius $\rho_\alpha(\mathcal{K})$ satisfies a formula similar to (2.5), with the suprema now taken over $\operatorname{Re}(z) \geq \alpha$ or $z \in \alpha + i\mathbb{R}$. Following Leimkuhler [9, §2.1], we may then set $T_r = 1/\alpha_r$, provided that

$$\alpha_r = \inf \{ \alpha \mid \mathcal{K} \text{ is bounded in } L_p^\alpha(0, \infty) \text{ and } \rho_\alpha(\mathcal{K}) < r \}$$

exists, and obtain

$$\left\| \mathcal{K}^n \left(x^{(0)}(t) - u(t) \right) \right\| \lesssim e r^n \left\| x^{(0)}(t) - u(t) \right\| .$$

Here, the symbol ' \lesssim ' means 'approximately bounded by' and $\|\cdot\|$ denotes the maximum norm on $[0, T_r]$. For obvious reasons, the window $[0, T_1]$ for $r = 1$ will be referred to as the window of (stable) convergence.

3. Polynomial acceleration of WR. As a first way to expedite the convergence of a sequence of iterates $\{x^{(i)}(t)\}$, generated by a classical WR method of the form (2.3), we consider a straightforward extension of the linear acceleration techniques for static iterations, see e.g. [3, Chap. 3] or [19, Chap. 11]. That is, we construct a new waveform sequence $\{u^{(i)}(t)\}$ by setting

$$(3.1) \quad u^{(n)}(t) = \sum_{i=0}^n v_{n,i} x^{(i)}(t) , \quad n \geq 0 .$$

The numbers $v_{n,i}$ are chosen such that $\sum_{i=0}^n v_{n,i} = 1$, which ensures consistency, i.e., $u^{(n)}(t) = u(t)$ for all $n \geq 0$ whenever the waveforms $x^{(i)}(t)$ equal the exact solution $u(t)$. By inserting (2.3), we can rewrite (3.1) as

$$u^{(n)}(t) = q_n(\mathcal{K}) u^{(0)}(t) + \varphi^{q_n}(t) ,$$

with $\varphi^{q_n}(t) = \sum_{i=1}^n v_{n,i} (\sum_{j=0}^{i-1} \mathcal{K}^j \varphi(t))$ and $q_n(s) = \sum_{i=0}^n v_{n,i} s^i$. In terms of this polynomial, the normalisation condition on the $v_{n,i}$ -values becomes $q_n(1) = 1$.

The symbol of the iteration operator $q_n(\mathcal{K})$ can be identified by Laplace transforming (3.1),

$$(3.2) \quad \begin{aligned} \tilde{u}^{(n)}(z) &= \sum_{i=0}^n v_{n,i} \tilde{x}^{(i)}(z) \\ &= q_n(\mathbf{K}(z)) \tilde{u}^{(0)}(z) + \tilde{\varphi}^{q_n}(z) . \end{aligned}$$

This expression corresponds to the polynomial acceleration of iteration (2.4) towards the solution of (2.1). If all eigenvalues of $M_B^{-1}M_A$ have positive real parts, the operator $q_n(\mathcal{K})$, a linear combination of powers of \mathcal{K} , consists of a matrix multiplication and a convolution with an L_1 -kernel. Hence, we have from [6, Lemma 2.3] that

$$(3.3) \quad \rho(q_n(\mathcal{K})) = \sup_{\operatorname{Re}(z) \geq 0} \rho(q_n(\mathbf{K}(z))) = \sup_{z \in i\mathbb{R}} \rho(q_n(\mathbf{K}(z))) .$$

The values $\rho(q_n(\mathcal{K}))$ and $\rho(q_n(\mathbf{K}(z)))$ yield convergence factors over n iterations. The corresponding asymptotic averaged spectral radii are defined by

$$\varrho(q_n(\mathcal{K})) = \lim_{n \rightarrow \infty} (\rho(q_n(\mathcal{K})))^{1/n} \quad \text{and} \quad \varrho(q_n(\mathbf{K}(z))) = \lim_{n \rightarrow \infty} (\rho(q_n(\mathbf{K}(z))))^{1/n} ,$$

see also e.g. [19, p. 299]. We have stuck to the notation of this latter reference, i.e., the left-hand sides contain a subscript n to emphasise the use of a sequence of polynomials $\{q_n(s)\}$. The ϱ -value depends on this *sequence* of polynomials, and not on a particular polynomial $q_n(s)$, of course. Combined with (3.3) these definitions immediately lead to

$$(3.4) \quad \varrho(q_n(\mathcal{K})) = \sup_{\operatorname{Re}(z) \geq 0} \varrho(q_n(\mathbf{K}(z))) = \sup_{z \in i\mathbb{R}} \varrho(q_n(\mathbf{K}(z))) .$$

The sequence of polynomials $\{q_n(s) \mid q_n(1) = 1\}$ that minimise (3.4) was studied in [14]. It was shown that only a marginal acceleration of the basic WR iteration is possible. Intuitively, this can be expected by the following argument. We know that $\varrho(q_n(\mathbf{K}(z)))$ is usually minimised in terms of a sequence of Chebyshev polynomials, chosen in terms of the eigenvalue distribution of $\mathbf{K}(z)$. As the eigenvalues are strongly dependent on z , one should not hope that any single polynomial will do well for all values of z in the closed right half complex plane. Better convergence results may be expected with a sequence of frequency-dependent polynomials, an idea which is addressed in the next section.

4. Convolution-based polynomial acceleration of WR.

4.1. Chebyshev acceleration in the frequency domain. The convergence of the basic waveform iterates in Laplace-transform space $\{\tilde{x}^{(i)}(z)\}$ can be improved by taking linear combinations of the latter iterates, that is, by setting

$$(4.1) \quad \tilde{u}^{(n)}(z) = \sum_{i=0}^n \tilde{\Upsilon}_{n,i}(z) \tilde{x}^{(i)}(z) .$$

Whereas the notation in equation (3.2) indicates that the same polynomial sequence $\{q_n(s)\}$ is used for all linear systems of the form (2.1), the notation in (4.1) suggests a different choice of coefficients for every value of z . By repeated insertion of (2.4), equation (4.1) can be rewritten as

$$(4.2) \quad \tilde{u}^{(n)}(z) = Q_n(z, \mathbf{K}(z)) \tilde{u}^{(0)}(z) + \tilde{\varphi}^{Q_n}(z) ,$$

with

$$\tilde{\varphi}^{Q_n}(z) = \sum_{i=1}^n \tilde{\Upsilon}_{n,i}(z) \left(\sum_{j=0}^{i-1} \mathbf{K}(z)^j \tilde{\varphi}(z) \right),$$

$Q_n(z, s) = \sum_{i=0}^n \tilde{\Upsilon}_{n,i}(z) s^i$ and $Q_n(z, 1) = 1$, which ensures that $\tilde{u}^{(n)}(z) = \tilde{u}(z)$ if $\tilde{x}^{(i)}(z) = \tilde{u}(z)$.

The spectral radius of the iteration matrix in (4.2) is given by

$$(4.3) \quad \rho(Q_n(z, \mathbf{K}(z))) = \max_{\lambda \in \sigma(\mathbf{K}(z))} |Q_n(z, \lambda)|,$$

with $\sigma(\mathbf{K}(z))$ the spectrum of $\mathbf{K}(z)$. Since this spectrum is seldom known exactly, one will try to find polynomials $\{Q_n(z, s)\}$ that are small on a region containing $\sigma(\mathbf{K}(z))$. In particular, we assume the eigenvalues of $\mathbf{K}(z)$ to lie in a closed region $R(d(z), p(z), q(z), \phi(z))$, whose boundary equals the ellipse $E(d(z), p(z), q(z), \phi(z))$ centred around the complex point $d(z)$. This ellipse, illustrated in Figure 4.1, is given by

$$\left\{ \mu : \mu = d(z) + e^{i\phi(z)}(p(z) \cos(\theta) + iq(z) \sin(\theta)), \quad 0 \leq \theta < 2\pi \right\},$$

with semi-axes $p(z)$ and $q(z)$ that satisfy $p(z) \geq q(z) \geq 0$ and $-\pi/2 \leq \phi(z) < \pi/2$. When there is no confusion possible, we will denote this ellipse as $E(z)$, and $R(d(z), p(z), q(z), \phi(z))$ will be abbreviated as $R(z)$. The spectral radius (4.3) is then obviously bounded by the following number,

$$\bar{\rho}_R(Q_n(z, \mathbf{K}(z))) = \max_{\lambda \in R(z)} |Q_n(z, \lambda)|,$$

that is, for any $Q_n(z, s)$ we have that

$$\rho(Q_n(z, \mathbf{K}(z))) \leq \bar{\rho}_R(Q_n(z, \mathbf{K}(z))).$$

In order to determine the averaged convergence rate per iteration, we define the virtual asymptotic averaged spectral radius as

$$\bar{\rho}_R(Q_n(z, \mathbf{K}(z))) = \lim_{n \rightarrow \infty} (\bar{\rho}_R(Q_n(z, \mathbf{K}(z))))^{1/n}.$$

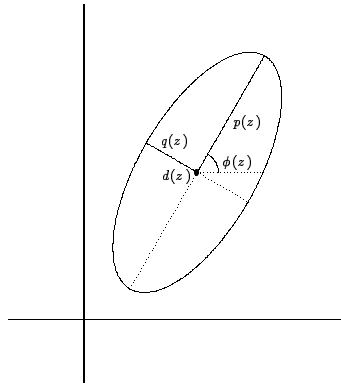


FIG. 4.1. An ellipse $E(d(z), p(z), q(z), \phi(z))$.

This number can be minimised by choosing $\{Q_n(z, s)\}$ as a sequence of scaled and translated Chebyshev polynomials of the first kind (in the variable s). The following theorem follows in a straightforward way from the paper by Manteuffel on the Chebyshev iteration for nonsymmetric linear systems [12].

THEOREM 4.1. *Assume $\sigma(\mathbf{K}(z))$ lies in the region $R(z)$, which does not contain the point 1 and for which $p(z) > q(z) > 0$. In terms of*

$$(4.4) \quad P_n^R(z, s) = \frac{T_n\left(\frac{s-d(z)}{c(z)}\right)}{T_n\left(\frac{1-d(z)}{c(z)}\right)},$$

with $T_n(\cdot)$ the n -th degree Chebyshev polynomial of the first kind and $c(z) = \sqrt{p^2(z) - q^2(z)}e^{i\phi(z)}$, we have

$$(4.5) \quad \bar{\rho}_R(P_n^R(z, \mathbf{K}(z))) \leq \bar{\rho}_R(Q_n(z, \mathbf{K}(z)))$$

for all polynomial sequences $\{Q_n(z, s) | Q_n(z, 1) = 1\}$. In particular,

$$(4.6) \quad \bar{\rho}_R(P_n^R(z, \mathbf{K}(z))) = \frac{p(z) + q(z)}{\left|1 - d(z) + \sqrt{(1 - d(z))^2 - c^2(z)}\right|},$$

where the branch for $\sqrt{\cdot}$ is chosen such that $\sqrt{(1 - d(z))^2} = 1 - d(z)$.

Proof. In [12], Manteuffel discusses the convergence of the Chebyshev-accelerated Richardson iteration for the nonsymmetric linear system $Ax = b$. His results apply immediately to our case with the provision that A and s in his paper are replaced by $I - \mathbf{K}(z)$ and $1 - s$. More precisely, equation (4.5) follows immediately from [12, Thms. 2.4 and 2.8]. Since $P_n^R(z, \lambda)$ is an analytic function of λ , its maximum modulus in region $R(z)$ is attained on the boundary. Consequently, $\bar{\rho}_R(P_n^R(z, \mathbf{K}(z)))$ is given by

$$\lim_{n \rightarrow \infty} \left(\max_{\lambda \in E(z)} |P_n^R(z, \lambda)| \right)^{1/n}.$$

For arbitrary $\lambda \notin [d(z) - c(z), d(z) + c(z)]$, that is, when λ is not on the interval connecting the focal points of the ellipse, one has

$$(4.7) \quad \lim_{n \rightarrow \infty} |P_n^R(z, \lambda)|^{1/n} = \frac{\left| \lambda - d(z) + \sqrt{(\lambda - d(z))^2 - c^2(z)} \right|}{\left| 1 - d(z) + \sqrt{(1 - d(z))^2 - c^2(z)} \right|},$$

which is shown to be constant for all $\lambda \in E(z)$ [12, Eqs. (3.1) and (2.13)]. The proof is then completed by inserting $\lambda = d(z) + p(z)e^{i\phi(z)}$ (the point on $E(z)$ which corresponds to $\theta = 0$) in the right-hand side of (4.7). \square

Similar results can be proven for degenerate cases of the region $R(z)$. When this region is chosen to be a disc with midpoint $d(z)$ and radius $p(z)(= q(z))$, the results of Theorem 4.1 remain valid in terms of the polynomials

$$(4.8) \quad P_n^R(z, s) = \left(\frac{s - d(z)}{1 - d(z)} \right)^n,$$

[12, Thm. 2.5]. The resulting iteration is then equivalent to the extrapolated method based on (2.4), see e.g. [3, Chap. 12, p. 335]; hence only moderate convergence acceleration can be achieved in such cases. For the other degenerate case, which occurs when

$\sigma(\mathbf{K}(z))$ lies on a closed line segment $R(d(z), p(z), 0, \phi(z)) = E(d(z), p(z), 0, \phi(z))$, we have the following theorem.

THEOREM 4.2. *If $\sigma(\mathbf{K}(z))$ lies on the line segment $R(d(z), p(z), 0, \phi(z))$, which does not contain the point 1, then the results of Theorem 4.1 remain valid with $q(z) = 0$ and $c(z) = p(z)e^{i\phi(z)}$.*

Proof. The optimality of the Chebyshev polynomials in the sense of (4.5) for a line segment follows from the equality of the polynomials (4.4) with $q(z) = 0$ and $c(z) = p(z)e^{i\phi(z)}$ and the normalised Faber polynomials for this line segment, see e.g. [2, Example 1]. Moreover, $P_n^R(z, \lambda)$ attains its maximum modulus on $R(d(z), p(z), 0, \phi(z))$ in the endpoints $\lambda = d(z) \pm p(z)e^{i\phi(z)}$. For these λ and the specified $q(z)$ and $c(z)$, the numerator of (4.4) evaluates to $T_n(\pm 1)$. Hence,

$$\bar{\varrho}_R(P_n^R(z, \mathbf{K}(z))) = \frac{1}{\lim_{n \rightarrow \infty} \left| T_n \left(\frac{1 - d(z)}{p(z)e^{i\phi(z)}} \right) \right|^{1/n}} .$$

Elaborating the latter equation (by using the techniques of [12]) leads immediately to (4.6) with $q(z) = 0$. \square

The problem of determining an optimal ellipse, that is, an ellipse surrounding $\sigma(\mathbf{K}(z))$ for which (4.6) is as small as possible, is addressed next.

LEMMA 4.3. *Any optimal ellipse $E_{opt}(z)$ contains an eigenvalue of $\mathbf{K}(z)$. If $\sigma(\mathbf{K}(z))$ is collinear, the optimal ellipse $E_{opt}(z)$ equals the line segment linking the extremal eigenvalues of $\mathbf{K}(z)$.*

Proof. Suppose $\sigma(\mathbf{K}(z))$ is not collinear and let $E_1(z)$ be a surrounding ellipse that does not contain an eigenvalue of $\mathbf{K}(z)$. Then, there exists an elliptic region $R_2(z) \subsetneq R_1(z)$ (with the same midpoint and inclination angle as the first one) containing $\sigma(\mathbf{K}(z))$. More precisely, we have

$$(4.9) \quad \bar{\varrho}_{R_2}(P_n^{R_2}(z, \mathbf{K}(z))) \leq \bar{\varrho}_{R_2}(P_n^{R_1}(z, \mathbf{K}(z))) < \bar{\varrho}_{R_1}(P_n^{R_1}(z, \mathbf{K}(z))) .$$

The first equality follows from (4.5) with $P_n^{R_1}(z, \lambda)$ the polynomial (4.4) corresponding to the region $R_1(z)$, while the second (strict) inequality is an immediate consequence of the maximum principle. As a result, $E_1(z)$ cannot be optimal.

In the collinear case, we have, by a convexity argument, that any elliptic region $R(z)$ enclosing $\sigma(\mathbf{K}(z))$ must necessarily contain the line segment $R_{opt}(z)$. Hence, we have as in (4.9) that

$$\bar{\varrho}_{R_{opt}}(P_n^{R_{opt}}(z, \mathbf{K}(z))) \leq \bar{\varrho}_{R_{opt}}(P_n^R(z, \mathbf{K}(z))) < \bar{\varrho}_R(P_n^R(z, \mathbf{K}(z))) ,$$

and the proof is completed. \square

COROLLARY 4.4. *For an optimal ellipse, the virtual asymptotic averaged spectral radius is actually attained, i.e., we have*

$$(4.10) \quad \varrho(P_n^{R_{opt}}(z, \mathbf{K}(z))) = \bar{\varrho}_{R_{opt}}(P_n^{R_{opt}}(z, \mathbf{K}(z))) .$$

Proof. If $\sigma(\mathbf{K}(z))$ is not collinear, equation (4.10) is proved by noting that the optimal variant of (4.7) is constant for all $\lambda \in E_{opt}(z)$, at least one point of which belongs to $\sigma(\mathbf{K}(z))$ by Lemma 4.3. In the collinear case, (4.10) follows from the fact that $|P_n^{R_{opt}}(z, \lambda)|$ attains its maximum on $R_{opt}(z)$ in the endpoints of this interval, which are eigenvalues of $\mathbf{K}(z)$. \square

In general, Lemma 4.3 does not provide enough information to define the optimal ellipse in the case where the eigenvalues of $\mathbf{K}(z)$ are not collinear. Guided by one's intuition that such an ellipse should be as small as possible, and the knowledge that it should pass through at least one eigenvalue, one can then try to find a 'good' surrounding ellipse, for which (4.6) is close to its minimal value. This task turns out to be rather difficult as well.

Finally, iteration (4.1), where $\tilde{\Upsilon}_{n,i}(z)$ are the coefficients of the polynomials (4.4), can be transformed into a form that is more convenient for computation. Assume $q(z) < p(z)$, so that $c(z) \neq 0$. The transformation can be done by using the recurrence relation of the Chebyshev polynomials. It is easy to derive that

$$P_0(z, s) = 1, \quad P_1(z, s) = \tilde{\Gamma}(z)s - \tilde{\Gamma}(z) + 1,$$

$$P_n(z, s) = \tilde{\Lambda}_n(z) \left(\tilde{\Gamma}(z)s + 1 - \tilde{\Gamma}(z) \right) P_{n-1}(z, s) + (1 - \tilde{\Lambda}_n(z)) P_{n-2}(z, s), \quad n \geq 2,$$

where $\tilde{\Gamma}(z) = 1/(1 - d(z))$ and

$$\tilde{\Lambda}_n(z) = 2 \left(\frac{1 - d(z)}{c(z)} \right) \frac{T_{n-1} \left(\frac{1 - d(z)}{c(z)} \right)}{T_n \left(\frac{1 - d(z)}{c(z)} \right)}, \quad n \geq 2.$$

By applying the Chebyshev recurrence relation once more, one derives

$$\tilde{\Lambda}_n(z) = \begin{cases} \left(1 - \frac{1}{2}\sigma^2(z) \right)^{-1} & n = 2 \\ \left(1 - \frac{1}{4}\sigma^2(z) \tilde{\Lambda}_{n-1}(z) \right)^{-1} & n \geq 3 \end{cases},$$

with $\sigma^2(z) = c^2(z)/(1 - d(z))^2$, see also [3, Chap. 12]. It then follows from [3, Thm. 3-2.1] that (4.1) can be rewritten as

$$\tilde{u}^{(1)}(z) = \tilde{u}^{(0)}(z) + \tilde{\Gamma}(z) \left(\hat{\tilde{u}}^{(1)}(z) - \tilde{u}^{(0)}(z) \right)$$

$$(4.11) \quad \tilde{u}^{(n)}(z) = \tilde{u}^{(n-2)}(z) + \tilde{\Lambda}_n(z) \left[\tilde{\Gamma}(z) \left(\hat{\tilde{u}}^{(n)}(z) - \tilde{u}^{(n-1)}(z) \right) + \left(\tilde{u}^{(n-1)}(z) - \tilde{u}^{(n-2)}(z) \right) \right], \quad n \geq 2,$$

with

$$(4.12) \quad \hat{\tilde{u}}^{(n)}(z) = \mathbf{K}(z) \tilde{u}^{(n-1)}(z) + \tilde{\varphi}(z), \quad n \geq 1.$$

If $c(z) = 0$, it follows from (4.8) that $\tilde{\Gamma}(z) = 1/(1 - d(z))$ and $\tilde{\Lambda}_n(z) = 1$ for $n \geq 2$. As a result, (4.11) then becomes

$$\tilde{u}^{(n)}(z) = \tilde{u}^{(n-1)}(z) + \tilde{\Gamma}(z) \left(\hat{\tilde{u}}^{(n)}(z) - \tilde{u}^{(n-1)}(z) \right), \quad n \geq 1.$$

4.2. Convolution-based Chebyshev acceleration in the time domain.

By inverse Laplace transforming the z -dependent iteration scheme (4.1) for solving (2.1), we get

$$(4.13) \quad u^{(n)}(t) = \sum_{i=0}^n \int_0^t \Upsilon_{n,i}(t-s) x^{(i)}(s) ds = \sum_{i=0}^n \Upsilon_{n,i} \star x^{(i)}(t),$$

where the symbol ‘ \star ’ denotes convolution, and for which the normalisation condition (which ensures that $u^{(n)}(t) = u(t)$ if $x^{(i)}(t) = u(t)$) becomes $\sum_{i=0}^n \Upsilon_{n,i}(t) = \delta(t)$, with $\delta(t)$ the delta function. The $\Upsilon_{n,i}(t)$ are the inverse Laplace transforms of the z -dependent coefficients of the polynomial $Q_n(z, s)$. Method (4.13) is a convolution-based polynomial WR method. If the polynomials $Q_n(z, s)$ are of Chebyshev-type (4.4), inverse Laplace transforming (4.11)–(4.12) yields the mathematically equivalent iterative scheme

$$(4.14) \quad \begin{aligned} u^{(1)}(t) &= u^{(0)}(t) + \Gamma \star (\widehat{u}^{(1)} - u^{(0)})(t) \\ u^{(n)}(t) &= u^{(n-2)}(t) + \Lambda_n \star [\Gamma \star (\widehat{u}^{(n)} - u^{(n-1)}) + \\ &\quad (u^{(n-1)} - u^{(n-2)})](t), \quad n \geq 2. \end{aligned}$$

Here, $\widehat{u}^{(n)}(t)$ is obtained by application of the unaccelerated WR method to $u^{(n-1)}(t)$, i.e.,

$$(4.15) \quad \widehat{u}^{(n)}(t) = \mathcal{K} u^{(n-1)}(t) + \varphi(t), \quad n \geq 1,$$

and the convolution kernels $\Gamma(t)$ and $\Lambda_n(t)$ are the inverse Laplace transforms of the functions $\widetilde{\Gamma}(z)$ and $\widetilde{\Lambda}_n(z)$. The iteration operator mapping $u^{(0)}(t)$ into $u^{(n)}(t)$ is identified in the next lemma.

LEMMA 4.5. *Assume that all eigenvalues of $M_B^{-1}M_A$ have positive real parts, $\Gamma(t) = \gamma \delta(t) + \gamma_c(t)$ and $\Lambda_i(t) = \lambda_i \delta(t) + (\lambda_i)_c(t)$ with $\gamma_c(t)$ and $(\lambda_i)_c(t)$ ($2 \leq i \leq n$) in $L_1(0, \infty)$. Then iteration (4.14)–(4.15) can be rewritten as*

$$(4.16) \quad u^{(n)}(t) = \mathcal{K}_n^{CH} u^{(0)}(t) + \varphi_n^{CH}(t),$$

where \mathcal{K}_n^{CH} consists of a matrix multiplication and a linear Volterra convolution with an $L_1(0, \infty)$ -kernel, and $\varphi_n^{CH}(t) = \sum_{i=1}^n (\Upsilon_{n,i} \star (\sum_{j=0}^{i-1} \mathcal{K}^j \varphi))(t)$ with $\Upsilon_{n,i}(t)$ the inverse Laplace transforms of the coefficients of (4.4).

Proof. The condition on the eigenvalues of $M_B^{-1}M_A$ ensures that the operator \mathcal{K} of the unaccelerated method is of the form $K + \mathcal{K}_c$, where K is a matrix and \mathcal{K}_c is a Volterra convolution operator whose kernel belongs to $L_1(0, \infty)$ [6, §3.1]. The nature of \mathcal{K}_n^{CH} follows as the space of such operators is closed under addition and convolution. \square

REMARK 4.1. The assumptions on $\Gamma(t)$ and $\Lambda_i(t)$ are satisfied when their Laplace transforms $\widetilde{\Gamma}(z)$ and $\widetilde{\Lambda}_i(z)$ are bounded and analytic in an open domain containing the closed right half of the complex plane, see [8, Rem. 3.1].

Under the assumptions of Lemma 4.5, the spectral radius of the operator \mathcal{K}_n^{CH} is given by

$$\rho(\mathcal{K}_n^{CH}) = \sup_{\operatorname{Re}(z) \geq 0} \rho(P_n^R(z, \mathbf{K}(z))) = \sup_{z \in i\mathbb{R}} \rho(P_n^R(z, \mathbf{K}(z))),$$

[6, Lemma 2.3]. The corresponding asymptotic averaged spectral radius is given by

$$(4.17) \quad \varrho(\mathcal{K}_n^{CH}) = \sup_{z \in i\mathbb{R}} \varrho(P_n^R(z, \mathbf{K}(z))),$$

and can be bounded by the virtual asymptotic averaged spectral radius

$$(4.18) \quad \sup_{z \in i\mathbb{R}} \bar{\varrho}_R(P_n^R(z, \mathbf{K}(z))) = \sup_{z \in i\mathbb{R}} \frac{p(z) + q(z)}{|1 - d(z) + \sqrt{(1 - d(z))^2 - c^2(z)}|},$$

where the equality follows from Theorem 4.1 if the ellipses $R(z)$ do not contain the point 1. Also, Corollary 4.4 implies that (4.17) equals (4.18) if the latter ellipses are optimal. In the remainder of the text, we shall often omit the subscript n in the notation of the operator \mathcal{K}_n^{CH} , which shall be referred to as the (convolution-based) Chebyshev WR operator.

5. Model problem analysis of Chebyshev–Picard, Chebyshev–Jacobi WR and Chebyshev–Gauss–Seidel WR. In this section, we shall discuss some specific results for the Chebyshev acceleration of several waveform relaxation variants and apply these results to the heat equation

$$(5.1) \quad \frac{\partial \mathbf{u}}{\partial t} - \Delta_m \mathbf{u} = 0, \quad x \in [0, 1]^m, \quad t > 0,$$

with Dirichlet boundary conditions and a given initial condition. If we discretise this equation in space using finite differences on a regular grid with mesh-size h , we obtain an ODE system (1.1) with $B = I$ and matrix A , which is given by the well-known 3-point, 5-point or 7-point central finite-difference stencil, respectively in the $m = 1$, $m = 2$ and $m = 3$ case. We also consider the finite-element discretisation of (5.1) for $m = 1$ with linear finite elements, yielding (1.1) with (in stencil notation)

$$(5.2) \quad B = \frac{h}{6} [1 \ 4 \ 1] \quad \text{and} \quad A = \frac{1}{h} [-1 \ 2 \ -1].$$

5.1. The Chebyshev–Picard method.

5.1.1. Discussion of the Picard method. The Picard method, which is only defined for ODE systems (1.1) with $B = I$, can be written as an iteration of the form (2.2) with $M_B = I$, $N_B = M_A = 0$ and $N_A = -A$. Consequently, $M_B^{-1}M_A$ equals the zero matrix and the corresponding operator \mathcal{K}^{PIC} can only be investigated in the weighted spaces $L_p^\alpha(0, \infty)$. For the finite-difference discretisation of equation (5.1), it is well-known that the eigenvalues of A are given by

$$\begin{aligned} 2(1 + \cos(i\pi h))/h^2, \quad i = 1, \dots, 1/h - 1 & \quad m = 1 \\ 2(2 + \cos(i\pi h) + \cos(j\pi h))/h^2, \quad i, j = 1, \dots, 1/h - 1 & \quad m = 2 \\ 2(3 + \cos(i\pi h) + \cos(j\pi h) + \cos(k\pi h))/h^2, \quad i, j, k = 1, \dots, 1/h - 1 & \quad m = 3 \end{aligned}$$

Hence, we derive

$$(5.3) \quad \sigma(\mathbf{K}^{\mathbf{PIC}}(z)) = \sigma\left(\frac{-A}{z}\right) \subset \left[\frac{-2m}{zh^2}(1 - \cos(\pi h)), \frac{-2m}{zh^2}(1 + \cos(\pi h)) \right]$$

and

$$\rho_\alpha(\mathcal{K}^{PIC}) = \sup_{z \in \alpha + i\mathbb{R}} \rho(\mathbf{K}^{\mathbf{PIC}}(z)) = \frac{2m}{\alpha h^2}(1 + \cos(\pi h)),$$

i.e., the spectral radius of \mathcal{K}^{PIC} equals that of $\mathbf{K}^{\mathbf{PIC}}(\alpha)$. The latter corresponds to the iteration matrix of the Richardson iteration $\alpha u^{(n)} = -A u^{(n-1)} + f$ for the linear system $(\alpha I + A)u = f$. The Picard method is obviously divergent in $L_p^\alpha(0, \infty)$ with $\alpha < 2m(1 + \cos(\pi h))/h^2$, and the window of stable convergence can be approximated by $[0, h^2/2m(1 + \cos(\pi h))]$. Since this window is very small, the Picard iteration does not have any practical use for the model heat problems. These results are illustrated for (5.1) with $m = 1$ and $h = 1/32$ in the left picture of Figure 5.1, where we plotted contourlines of $(\mathbf{K}^{\mathbf{PIC}}(z))$ in the complex plane. For this problem, the window of convergence equals $[0, 0.000245]$.

5.1.2. Chebyshev acceleration of the Picard method. The Picard method can be accelerated quite well by the convolution-based Chebyshev approach, which is perhaps somewhat surprising. One of the virtues of the Picard method is that for its acceleration, we only need a good/optimal ellipse surrounding $\sigma(A)$; the multiplication of this ellipse by $-1/z$ is expected to lead to a good/optimal ellipse for the symbol $\mathbf{K}^{\text{PIC}}(z) = -A/z$ at other values of $z \neq 0$ too. More precisely, for the heat equation Lemma 4.3 implies that the line segment given in (5.3) is the optimal ellipse surrounding $\sigma(\mathbf{K}^{\text{PIC}}(z))$ for $z \neq 0$. We prove the following statement for the asymptotic averaged spectral radius of the resulting optimal Chebyshev–Picard operator $\mathcal{K}^{\text{CH-PIC,opt}}$ in $L_p(0, \infty)$.

LEMMA 5.1. *Consider the model problem (5.1), discretised using finite differences. Then, if we consider $\mathcal{K}^{\text{CH-PIC,opt}}$ as an operator in $L_p(0, \infty)$ with $1 \leq p \leq \infty$, we have*

$$(5.4) \quad \varrho(\mathcal{K}^{\text{CH-PIC,opt}}) = \frac{\cos(\pi h)}{1 + \sqrt{1 - \cos^2(\pi h)}} \approx 1 - \pi h .$$

Proof. First note that $A = \mathbf{K}^{\text{PIC}}(-1)$. By using (5.3), the parameters of the optimal line segment $E_{\text{opt}}(z)$ surrounding $\sigma(\mathbf{K}^{\text{PIC}}(z))$ equal $d_{\text{opt}}(z) = -d_{\text{opt}}(-1)/z = -2m/zh^2$ and $c_{\text{opt}}(z) = c_{\text{opt}}(-1)/z = 2m \cos(\pi h)/zh^2$. Hence, Theorem 4.1 implies for $z \neq 0$

$$(5.5) \quad P_n^{R_{\text{opt}}}(z, \mathbf{K}^{\text{PIC}}(z)) = \frac{T_n\left(\frac{\mathbf{K}^{\text{PIC}}(z) - d_{\text{opt}}(z)}{c_{\text{opt}}(z)}\right)}{T_n\left(\frac{1 - d_{\text{opt}}(z)}{c_{\text{opt}}(z)}\right)} = \frac{T_n\left(\frac{d_{\text{opt}}(-1) - A}{c_{\text{opt}}(-1)}\right)}{T_n\left(\frac{z + d_{\text{opt}}(-1)}{c_{\text{opt}}(-1)}\right)} .$$

Since the (zero) eigenvalues of $M_B^{-1}M_A$ do not have positive real parts, we cannot apply Lemma 4.5 in order to prove that the optimal Chebyshev–Picard operator $\mathcal{K}^{\text{CH-PIC,opt}}$ consists of a matrix multiplication and an L_1 -convolution part. Yet, the conditions of Lemma 4.5 are not necessary to this end, and we shall adopt a different approach here. That is, we observe that $z = 0$ is a removable singularity of $P_n^{R_{\text{opt}}}(z, \mathbf{K}^{\text{PIC}}(z))$, or, more precisely, that the rightmost expression of (5.5) is bounded and analytic for $\text{Re}(z) \geq 0$. As in Remark 4.1, its inverse Laplace transform $\mathcal{K}^{\text{CH-PIC,opt}}$ then consists of a matrix multiplication and an L_1 -convolution part. Using Corollary 4.4, we have as in (4.17)–(4.18) that

$$(5.6) \quad \varrho(\mathcal{K}^{\text{CH-PIC,opt}}) = \sup_{z \in i\mathbb{R}} \varrho(P_n^{R_{\text{opt}}}(z, \mathbf{K}^{\text{PIC}}(z))) .$$

Since the optimal line segment does not contain the point 1 for $z \neq 0$, Theorem 4.1 implies that

$$(5.7) \quad \varrho(P_n^{R_{\text{opt}}}(z, \mathbf{K}^{\text{PIC}}(z))) = \frac{2m \cos(\pi h)}{\left|zh^2 + 2m + \sqrt{(zh^2 + 2m)^2 - (2m \cos(\pi h))^2}\right|}$$

for $z = i\xi$, $\xi \neq 0$. For $z = 0$, the polynomial (5.5) can be rewritten as the optimal Chebyshev polynomial for accelerating the convergence of the static Richardson iteration $u^{(n)} = (I - A)u^{(n-1)} + f$, which equals

$$(5.8) \quad \frac{T_n\left(\frac{(I-A) - (1 - d_{\text{opt}}(-1))}{c_{\text{opt}}(-1)}\right)}{T_n\left(\frac{1 - (1 - d_{\text{opt}}(-1))}{c_{\text{opt}}(-1)}\right)} .$$

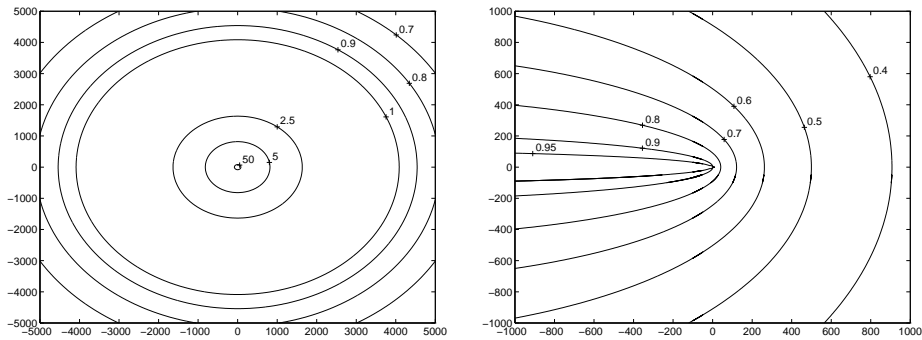


FIG. 5.1. Contourlines of $\rho(\mathbf{K}^{\text{PIC}}(z))$ - left picture - and $\rho(P_n^{\text{Rot}}(z, \mathbf{K}^{\text{PIC}}(z)))$ - right picture - for (5.1) with $m = 1$, discretised using finite differences with $h = 1/32$.

Application of Theorem 4.1 to the latter polynomial leads exactly to the right-hand side of (5.7), evaluated at $z = 0$.

Finally, we remark that the supremum in (5.6) for the function in (5.7) is attained at the origin. Hence, the proof is completed by inserting $z = 0$ in (5.7) and calculating a series expression for small h . \square

This lemma is illustrated in the right picture of Figure 5.1, where we plotted contourlines of $\rho(P_n^{\text{Rot}}(z, \mathbf{K}^{\text{PIC}}(z)))$ for the one-dimensional heat equation with $h = 1/32$.

5.1.3. Relation to previously published work by Lubich and Skeel. In [11, 17], Lubich and Skeel already discussed a related Chebyshev–Picard method. They define a shifted Picard iteration in terms of

$$(5.9) \quad \dot{u}^{(n)}(t) + \mu_n u^{(n)}(t) = f(t) - Au^{(n-1)}(t) + \mu_n u^{(n-1)}(t), \quad u^{(n)}(0) = u_0,$$

with $\mu_n = d - c\xi_n$ and $n = 1, 2, \dots, N$. Here, $\xi_n = \cos((2n - 1)\pi/2N)$ denote the zeros of $T_N(\cdot)$, while d and c are the usual parameters of an ellipse that was chosen to enclose the spectrum of A .

By Laplace transformation of (5.9) we can check that the resulting waveform $u^{(N)}(t)$ corresponds to the N -th waveform of our scheme (4.14)–(4.15), with $d(z) = -d/z$ and $c(z) = c/z$ and $\phi(z) = \text{Arg}(c(z))$ for $z \neq 0$. Hence, for this particular selection of the ellipses $E(z)$, both methods give similar results (after N steps).

Assume that the ellipse E surrounding $\sigma(A)$ has a major semi axis that is parallel to one of the coordinate axes. For these choices of this ellipse, Lubich proved that in $L_p(0, T)$, the Chebyshev–Picard method for $\dot{u}(t) + Au(t) = f(t)$ gives at least the same error reduction as the Chebyshev acceleration of the Richardson method $\frac{1}{T}u^{(n)} = -Au^{(n-1)} + f$ for the static linear system

$$(5.10) \quad \left(\frac{1}{T}I + A \right) u = f,$$

[11, p. 537]. For the reader’s convenience, we rewrite the result (for the case that the major axis of E lies on the real axis) in our notations. The other case is completely similar.

LEMMA 5.2. *Consider an ODE system $\dot{u} + Au = f$. Suppose that the major axis of the ellipse chosen to enclose $\sigma(A)$ lies on the real axis of the complex plane. Then,*

the resulting Chebyshev–Picard iteration satisfies

$$(5.11) \quad \left\| u^{(n)}(t) - u(t) \right\|_{L_p(0,T)} \leq e \left\| P_n^R \left(\frac{1}{T}, \mathbf{K}^{\text{PIC}} \left(\frac{1}{T} \right) \right) \right\| \cdot \left\| u^{(0)}(t) - u(t) \right\|_{L_p(0,T)}$$

for $1 \leq p \leq \infty$ and $0 < T \leq \infty$.

Observe that for $T = \infty$, $P_n^R(0, \mathbf{K}^{\text{PIC}}(0))$ has to be interpreted as in (5.8) as the scaled and translated Chebyshev polynomial corresponding to the matrix $I - A$. As such, the latter lemma, applied to the finite-difference discretisation of (5.1) with $T = \infty$ and with the ellipse E surrounding $\sigma(A)$ equal to the optimal line segment $[2(1 - \cos(\pi h))/h^2, 2(1 + \cos(\pi h))/h^2]$, can be regarded as the norm equivalent of Lemma 5.1.

5.2. The Chebyshev–Jacobi WR method.

5.2.1. The $B = I$ -case. In terms of the classical splitting $A = D_A - L_A - U_A$ with D_A , L_A and U_A the diagonal, lower triangular and upper triangular part of A , respectively, the Jacobi WR method is defined as iteration (2.2) with $M_B = I$, $N_B = 0$, $M_A = D_A$ and $N_A = L_A + U_A$. If we suppose in addition that D_A has a constant positive diagonal $D_A = d_a I$ ($d_a > 0$), we have

$$(5.12) \quad \mathbf{K}^{\text{JAC}}(z) = \frac{d_a}{z + d_a} D_A^{-1} (L_A + U_A) = \frac{d_a}{z + d_a} \mathbf{K}^{\text{JAC}}(0),$$

with $\mathbf{K}^{\text{JAC}}(0)$ the static Jacobi iteration matrix. We then only need a good/optimal ellipse surrounding $\sigma(\mathbf{K}^{\text{JAC}}(0))$ to define the resulting Chebyshev–Jacobi WR method for this problem.

In terms of the asymptotic averaged spectral radius, we can prove the following relation between the optimal Chebyshev–Jacobi WR method and the corresponding static iteration for $Au = f$.

LEMMA 5.3. *Consider an ODE system $\dot{u}(t) + Au(t) = f(t)$. Assume A is consistently ordered with constant positive diagonal $D_A = d_a I$ ($d_a > 0$) and the eigenvalues of $\mathbf{K}^{\text{JAC}}(0)$ are real with $\mu_1 = \rho(\mathbf{K}^{\text{JAC}}(0)) < 1$. Then, if we consider $\mathcal{K}^{\text{CH-JAC,opt}}$ as an operator in $L_p(0, \infty)$, we have*

$$(5.13) \quad \varrho(\mathcal{K}^{\text{CH-JAC,opt}}) = \varrho(P_n^{\text{Ropt}}(0, \mathbf{K}^{\text{JAC}}(0))) = \frac{\mu_1}{1 + \sqrt{1 - \mu_1^2}}.$$

Proof. Since A is consistently ordered, the eigenvalues of $\mathbf{K}^{\text{JAC}}(0)$ occur in opposite pairs and Lemma 4.3 implies that $E_{\text{opt}}(z) = \frac{d_a}{z + d_a} E_{\text{opt}}(0) = \frac{d_a}{z + d_a} [-\mu_1, \mu_1]$. Since this line segment does not contain the point 1 for $\text{Re}(z) \geq 0$, Theorem 4.1 and (4.10) imply that for these z

$$(5.14) \quad \varrho(P_n^{\text{Ropt}}(z, \mathbf{K}^{\text{JAC}}(z))) = \frac{|\mu_1(z)|}{1 + \sqrt{1 - \mu_1^2(z)}},$$

with $\mu_1(z) = \frac{d_a}{z + d_a} \mu_1$. In addition,

$$\tilde{\Gamma}_{\text{opt}}(z) = 1 \quad \text{and} \quad (\tilde{\Lambda}_{\text{opt}})_n(z) = \frac{2}{\mu_1(z)} \frac{T_{n-1}\left(\frac{1}{\mu_1(z)}\right)}{T_n\left(\frac{1}{\mu_1(z)}\right)}$$

are bounded and analytic functions for $\operatorname{Re}(z) \geq 0$, so that we may apply Lemma 4.5 and (4.17)–(4.18). The proof is completed by noting that the supremum of (5.14) taken over $z \in i\mathbb{R}$ is attained at $z = 0$. \square

Finally, we can apply Lemma 5.3 to the finite-difference discretisation of the heat equation (5.1), since their matrices A satisfy the conditions of the latter lemma with $\mu_1 = \cos(\pi h)$.

COROLLARY 5.4. *Consider the heat equation (5.1), discretised using finite differences. Then, if we consider $\mathcal{K}^{CH-JAC,opt}$ as an operator in $L_p(0, \infty)$, we have*

$$(5.15) \quad \varrho(\mathcal{K}^{CH-JAC,opt}) = \frac{\cos(\pi h)}{1 + \sqrt{1 - \cos^2(\pi h)}} \approx 1 - \pi h .$$

This result is illustrated in the left picture of Figure 5.2, where we plotted contourlines of $\varrho(P_n^{R,opt}(z, \mathbf{K}^{JAC}(z)))$ for the two-dimensional heat equation with finite differences and $h = 1/32$.

It may be verified by elementary Laplace-transform techniques that the N -th WR iterate from the general Chebyshev–Jacobi variant of (4.14)–(4.15) can also be obtained from a ‘shifted’ Jacobi iteration, i.e.,

$$\frac{1}{d_a} \dot{u}^{(n)}(t) + (1 - \mu_n) u^{(n)}(t) = (\mathbf{K}^{JAC}(0) - \mu_n) u^{(n-1)}(t) + \frac{1}{d_a} f(t) , \quad u^{(n)}(0) = 0 ,$$

with $\mu_n = d(0) + c(0)\xi_n$ and $n = 1, 2, \dots, N$. As before, ξ_n denote the zeros of $T_N(\cdot)$, while $d(0)$ and $c(0)$ are the parameters of the ellipse $E(0)$ that was chosen to enclose the spectrum of $\mathbf{K}^{JAC}(0)$. As in the Picard case, we can relate the error reduction of the Chebyshev–Jacobi WR method for $\dot{u}(t) + Au(t) = f(t)$ in $L_p(0, T)$ to that of the Chebyshev–Jacobi method for (5.10) for a particular choice of the ellipse $E(0)$.

LEMMA 5.5. *Consider an ODE system $\dot{u}(t) + Au(t) = f(t)$ with $D_A = d_a I$ ($d_a > 0$), and assume that the major axis of the ellipse $E(0)$ chosen to enclose $\sigma(\mathbf{K}^{JAC}(0))$ lies on the real axis of the complex plane. Then, the resulting Chebyshev–Jacobi WR iteration satisfies*

$$(5.16) \quad \left\| u^{(n)}(t) - u(t) \right\|_{L_p(0, T)} \leq e \left\| P_n^R \left(\frac{1}{T}, \mathbf{K}^{JAC} \left(\frac{1}{T} \right) \right) \right\| \cdot \left\| u^{(0)}(t) - u(t) \right\|_{L_p(0, T)}$$

for $1 \leq p \leq \infty$ and $0 < T \leq \infty$.

Proof. The parameters of the ellipse $E(z)$ surrounding $\sigma(\mathbf{K}^{JAC}(z))$ can be written in terms of those of the ellipse $E(0)$, that is, $d(z) = \frac{d_a}{z+d_a}d(0)$ and $c(z) = \frac{d_a}{z+d_a}c(0)$. Hence,

$$P_n^R(z, \mathbf{K}^{JAC}(z)) = \frac{T_n \left(\frac{\mathbf{K}^{JAC}(z) - d(z)}{c(z)} \right)}{T_n \left(\frac{1 - d(z)}{c(z)} \right)} = \frac{T_n \left(\frac{\mathbf{K}^{JAC}(0) - d(0)}{c(0)} \right)}{T_n \left(\frac{\frac{z+d_a}{d_a} - d(0)}{c(0)} \right)} ,$$

while the polynomial of the corresponding static Chebyshev–Jacobi method for (5.10) is given by $P_n^R(1/T, \mathbf{K}^{JAC}(1/T))$. The rest of the proof is an immediate extension of the proof of Lemma 5.2, given in [11, p. 537]. \square

5.2.2. The $B \neq I$ -case. The Jacobi WR method for (1.1) is given by iteration (2.2) with

$$M_B = D_B , \quad M_A = D_A , \quad N_B = L_B + U_B \quad \text{and} \quad N_A = L_A + U_A .$$

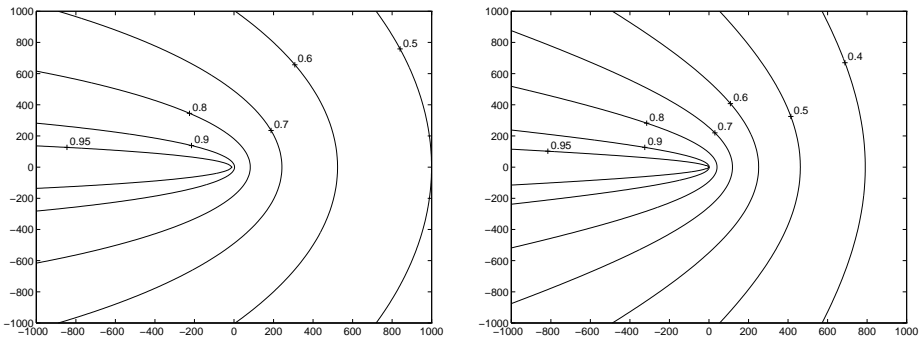


FIG. 5.2. Contourlines of $\rho(P_n^{Ropt}(z, \mathbf{K}^{JAC}(z)))$ for (5.1) with $m = 2$, discretised using finite differences - left picture - and $m = 1$, discretised using linear finite elements - right picture - with $h = 1/32$.

The symbol $\mathbf{K}^{JAC}(z)$ equals $(zD_B + D_A)^{-1}(z(L_B + U_B) + (L_A + U_A))$, and in general we cannot explicitly relate its eigenvalue distribution to that of $\mathbf{K}^{JAC}(0)$ as in equation (5.12). For the one-dimensional heat equation (5.1), discretised using linear finite elements, we can prove the following lemma.

LEMMA 5.6. Consider the one-dimensional heat equation (5.1), discretised using linear finite elements. Then, if we consider $\mathcal{K}^{CH-JAC,opt}$ as an operator in $L_p(0, \infty)$, we have

$$(5.17) \quad \rho(\mathcal{K}^{CH-JAC,opt}) = \frac{\cos(\pi h)}{1 + \sqrt{1 - \cos^2(\pi h)}} \approx 1 - \pi h .$$

Proof. From (5.2), we derive that

$$\sigma(\mathbf{K}^{JAC}(z)) = \left\{ \frac{-2zh^2 + 12}{4zh^2 + 12} \cos(j\pi h) \mid j = 1, \dots, 1/h - 1 \right\} .$$

Hence, Lemma 4.3 implies that $E_{opt}(z) = [-\mu_1(z), \mu_1(z)]$ with $\mu_1(z) = \frac{2zh^2 - 12}{4zh^2 + 12} \cos(\pi h)$. The rest of the proof is similar to the proof of Lemma 5.3, and a series expression is calculated for small values of h . \square

We provide contourlines of $\rho(P_n^{Ropt}(z, \mathbf{K}^{JAC}(z)))$ for $h = 1/32$ in the right picture of Figure 5.2. Since its supremum over $\text{Re}(z) \geq 0$ or $z \in i\mathbb{R}$ is attained at $z = 0$, the optimal Chebyshev–Jacobi WR method behaves as its static counterpart for the linear system $Au = f$.

5.2.3. Comparison to the CSOR WR method. We can now compare the convergence behaviour of the optimal Chebyshev–Jacobi WR method to that of other waveform variants for ODE systems that satisfy the conditions of Lemma 5.3. More precisely, we have

$$\rho(\mathcal{K}^{JAC}) = \mu_1 \quad \text{and} \quad \rho(\mathcal{K}^{CSOR,opt}) = \frac{\mu_1^2}{(1 + \sqrt{1 - \mu_1^2})^2} ,$$

see [6] and [8, Thm. 3.9]. These results, which may be applied e.g. to the finite-difference discretisation of the heat equation (5.1) by setting $\mu_1 = \cos(\pi h)$, imply

that the Chebyshev–Jacobi WR method is substantially faster than the unaccelerated Jacobi variant, but only half as fast as the optimal CSOR WR method.

Similar results may be obtained for the one-dimensional heat equation discretised using linear finite elements, treated in Lemma 5.6. Again, the optimal Chebyshev–Jacobi WR is much faster than its unaccelerated Jacobi variant (with spectral radius $\cos(\pi h)$ [6]) but only half as fast as the optimal CSOR WR method (with spectral radius $\cos^2(\pi h)/(1 + \sqrt{1 - \cos^2(\pi h)})^2$ [8, Thm. 5.2]).

This observation for model problems with collinear spectra of their Jacobi symbols also holds in a more general way. We recall that the CSOR WR method for (1.1) is a straightforward extension of the static SOR iteration, except that the multiplication with an overrelaxation parameter ω is replaced by a convolution with a time-dependent overrelaxation function $\Omega(t)$. The symbol of the method is given by

$$(5.18) \quad \mathbf{K}^{\text{CSOR}}(z) = \left(z \left(\frac{1}{\tilde{\Omega}(z)} D_B - L_B \right) + \left(\frac{1}{\tilde{\Omega}(z)} D_A - L_A \right) \right)^{-1} \cdot \left(z \left(\frac{1 - \tilde{\Omega}(z)}{\tilde{\Omega}(z)} D_B + U_B \right) + \left(\frac{1 - \tilde{\Omega}(z)}{\tilde{\Omega}(z)} D_A + U_A \right) \right).$$

i.e., it equals the SOR iteration matrix for (2.1) with complex overrelaxation parameter $\tilde{\Omega}(z)$, [8]. If the matrices B and A are such that $zB + A$ is consistently ordered, Hu et al. showed that there exists an optimal ellipse $E(0, p(z), q(z), \phi(z))$ (centred around the origin, i.e., with $d(z) = 0$ and surrounding $\sigma(\mathbf{K}^{\text{JAC}}(z))$) such that $\tilde{\Omega}_{\text{opt}}(z)$, the value of the overrelaxation parameter minimising the spectral radius of (5.18), is given by $2/(1 + \sqrt{1 - c^2(z)})$, while

$$(5.19) \quad \rho(\mathbf{K}^{\text{CSOR}, \text{opt}}(z)) = \left(\frac{p(z) + q(z)}{1 + \sqrt{1 - c^2(z)}} \right)^2,$$

see [4, 5]. In addition, if the spectrum of the latter matrix is not collinear, this ellipse contains an eigenvalue of $\mathbf{K}^{\text{JAC}}(z)$, while in the collinear case, this ellipse equals the line segment between the extremal eigenvalues of $\mathbf{K}^{\text{JAC}}(z)$. Hence, if the ellipse of the CSOR method is used also for the Chebyshev acceleration of the Jacobi relaxation method for (2.1), Theorem 4.1 and Corollary 4.4 yield

$$(5.20) \quad \varrho(P_n^R(z, \mathbf{K}^{\text{JAC}}(z))) = \bar{\varrho}(P_n^R(z, \mathbf{K}^{\text{JAC}}(z))) = \frac{p(z) + q(z)}{|1 + \sqrt{1 - c^2(z)}|}.$$

As such, the optimal SOR method for (2.1) turns out to be twice as fast as the resulting Chebyshev–Jacobi iteration for this problem. Finally, we remark that - under the right assumptions - the above conclusions remain valid after taking the suprema of (5.19) and (5.20) over the right half complex plane/imaginary axis.

5.3. The Chebyshev–Gauss–Seidel WR method.

5.3.1. The $B = I$ -case. The Gauss–Seidel WR method for ODE systems $\dot{u}(t) + Au(t) = f(t)$ is given by (2.2) with $M_B = I$, $N_B = 0$, $M_A = D_A - L_A$ and $N_A = U_A$. The following lemma is the Gauss–Seidel equivalent of Lemma 5.3.

LEMMA 5.7. *Consider an ODE system $\dot{u}(t) + Au(t) = f(t)$. Assume A is consistently ordered with constant positive diagonal $D_A = d_a I$ ($d_a > 0$) and the eigenvalues*

of $\mathbf{K}^{\mathbf{JAC}}(0)$ are real with $\mu_1 = \rho(\mathbf{K}^{\mathbf{JAC}}(0)) < 1$. Then, if we consider $\mathcal{K}^{CH-GS,opt}$ as an operator in $L_p(0, \infty)$, we have

$$(5.21) \quad \varrho(\mathcal{K}^{CH-GS,opt}) = \varrho(P_n^{R,opt}(0, \mathbf{K}^{\mathbf{GS}}(0))) = \frac{\mu_1^2}{(1 + \sqrt{1 - \mu_1^2})^2}.$$

Proof. Since $zI + A$ is consistently ordered for $\operatorname{Re}(z) \geq 0$, we have that $\lambda \in \sigma(\mathbf{K}^{\mathbf{GS}}(z))$ if and only if $\lambda = 0$ or $\sqrt{\lambda} \in \sigma(\mathbf{K}^{\mathbf{JAC}}(z))$, [6, Lemma 3.8]. Hence, the optimal ellipse $E_{opt}(z)$ surrounding $\sigma(\mathbf{K}^{\mathbf{GS}}(z))$ is given by $[0, \mu_1^2(z)]$ with $\mu_1(z) = \frac{d_a \mu_1}{z + d_a}$ as in the proof of Lemma 5.3. From this follows that $d_{opt}(z) = c_{opt}(z) = \frac{\mu_1^2(z)}{2}$ and $p_{opt}(z) = |\mu_1^2(z)|/2$. As this line segment does not contain the point 1 and the resulting $\tilde{\Gamma}_{opt}(z)$ and $(\tilde{\Lambda}_{opt})_n(z)$ are bounded and analytic for $\operatorname{Re}(z) \geq 0$, we may apply Lemma 4.5 and (4.17)–(4.18), i.e.,

$$\begin{aligned} \varrho(\mathcal{K}^{GS-CH,opt}) &= \sup_{z \in i\mathbb{R}} \varrho(P_n^{R,opt}(z, \mathbf{K}^{\mathbf{GS}}(z))) \\ &= \sup_{z \in i\mathbb{R}} \left| \frac{|\mu_1^2(z)|/2}{1 - \mu_1^2(z)/2 + \sqrt{(1 - \mu_1^2(z)/2)^2 - (\mu_1^2(z)/2)^2}} \right|. \end{aligned}$$

It can be checked that this function attains its supremum for $z = 0$, from which (5.21) follows. \square

If we apply this lemma to the heat equation, discretised using finite differences, we immediately see that the resulting WR method is as fast as the optimal CSOR variant.

COROLLARY 5.8. *Consider the heat equation (5.1), discretised using finite differences. Then, if we consider $\mathcal{K}^{CH-GS,opt}$ as an operator in $L_p(0, \infty)$, we have*

$$(5.22) \quad \varrho(\mathcal{K}^{CH-GS,opt}) = \frac{\cos^2(\pi h)}{(1 + \sqrt{1 - \cos^2(\pi h)})^2} \approx 1 - 2\pi h.$$

An illustration can be found in the left picture of Figure 5.3, where we plotted contourlines of $\varrho(P_n^{R,opt}(z, \mathbf{K}^{\mathbf{GS}}(z)))$ for the two-dimensional heat equation, discretised using finite differences and $h = 1/32$.

5.3.2. The $B \neq I$ -case. We can prove a similar result as in Corollary 5.8 for the one-dimensional heat equation, discretised using linear finite elements.

LEMMA 5.9. *Consider the one-dimensional heat equation (5.1), discretised using linear finite elements. Then, if we consider $\mathcal{K}^{CH-GS,opt}$ as an operator in $L_p(0, \infty)$, we have*

$$(5.23) \quad \varrho(\mathcal{K}^{CH-GS,opt}) = \frac{\cos^2(\pi h)}{(1 + \sqrt{1 - \cos^2(\pi h)})^2} \approx 1 - 2\pi h.$$

Proof. The proof is completely similar to the proof of Lemma 5.7 with $\mathbf{K}^{\mathbf{GS}}(z) = (z(D_B - L_B) + (D_A - L_A))^{-1}(zU_B + U_A)$ and $\mu_1(z) = \frac{2zh^2 - 12}{4zh^2 + 12} \cos(\pi h)$. \square

We provide contourlines of $\varrho(P_n^{R,opt}(z, \mathbf{K}^{\mathbf{GS}}(z)))$ for $h = 1/32$ in the right picture of Figure 5.3. Note that the optimal Chebyshev–Gauss–Seidel WR method is as fast as its static counterpart and the optimal CSOR WR method.

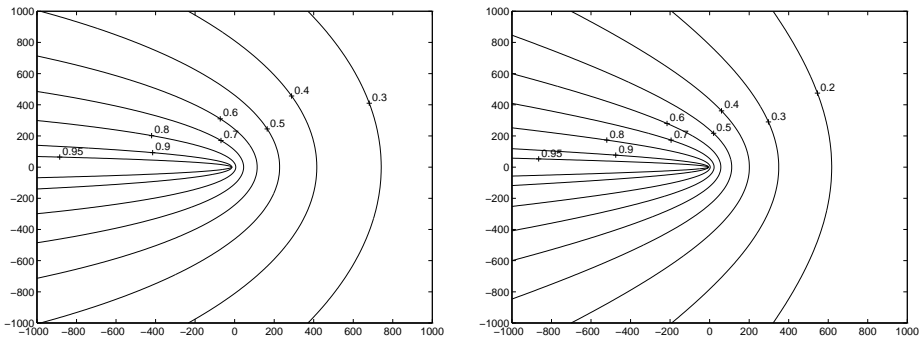


FIG. 5.3. Contourlines of $q(P_n^{Ropt}(z, \mathbf{K}^{GS}(z)))$ for (5.1) with $m = 2$, discretised using finite differences - left picture - and $m = 1$, discretised using linear finite elements - right picture - with $h = 1/32$.

Finally, we notice that the results of Lemmas 5.7 and 5.9 and Corollary 5.8 remain valid if we use a red/black ordering of the unknowns, as the spectra of the resulting Gauss–Seidel symbols equal those of the symbols $\mathbf{K}^{GS}(z)$, obtained with lexicographic ordering. Moreover, in analogy with the static iteration case, see e.g. [18] or [19, p. 374 and p. 386], we recommend the use of the coloured ordering in order to obtain the best convergence behaviour in practice.

6. Numerical results. In this section we will present the results of some numerical experiments, and we will show that the observed convergence behaviour agrees very well with the continuous-time theory for small enough time steps. We do not comment here on the particular influence of the time discretisation method, but refer to [7] and [8, §4] for a discrete-time analysis of WR methods.

In Table 6.1 we report the observed averaged spectral radii of the Chebyshev–Picard method for the one-dimensional heat equation, discretised in space using finite differences. The n -th iteration convergence factor is determined by calculating the l_2 -norm of the discrete error of the n -th approximation, and by dividing the result for successive iterates. As this factor takes a nearly constant value after a sufficiently large number of iterations, the averaged convergence factor is defined as the geometric average of these iteration convergence factors in the stable regime. We used the Crank–Nicolson (CN) method with time step $\tau = 1/100$ for time discretisation. The discrete approximations of the kernels $\Gamma_{opt}(t)$ and $(\Lambda_{opt})_n(t)$ are calculated from their transformed expressions $\tilde{\Gamma}_{opt}(z)$ and $(\tilde{\Lambda}_{opt})_n(z)$ by the Fourier-transform method developed in [8, §5.4]. (In the Picard case, the latter expressions have a pole at $z = 0$. Yet, these singularities are removable and they do not cause any problems.) Observe that the experimental results correspond very well with the theoretical spectral radii.

Similar results can be found for the convolution-based Chebyshev acceleration of Jacobi and red/black Gauss–Seidel WR. In particular, we report the observed averaged convergence factors of the latter methods for the two-dimensional heat equation with finite differences and the one-dimensional heat equation with linear finite elements in Tables 6.2 and 6.3, respectively. Again, the observed convergence factors are very close to their predicted theoretical values derived in §5.

TABLE 6.1

Averaged convergence factors of the Chebyshev-Picard method for (5.1) with CN time discretisation with time step $\tau = 1/100$.

h	1/8	1/16	1/32	1/64
$m = 1$, finite differences	0.648	0.811	0.900	0.949
$\cos(\pi h)/(1 + \sqrt{1 - \cos^2(\pi h)})$	0.668	0.821	0.906	0.952
$1 - \pi h$	0.607	0.804	0.902	0.951

TABLE 6.2

Averaged convergence factors of the Chebyshev-Jacobi WR method for (5.1) with CN time discretisation with time step $\tau = 1/100$.

h	1/8	1/16	1/32	1/64
$m = 2$, finite differences	0.656	0.814	0.903	0.951
$m = 1$, linear finite elements	0.648	0.811	0.901	0.951
$\cos(\pi h)/(1 + \sqrt{1 - \cos^2(\pi h)})$	0.668	0.821	0.906	0.952
$1 - \pi h$	0.607	0.804	0.902	0.951

TABLE 6.3

Averaged convergence factors of the red/black Chebyshev-Gauss-Seidel WR method for (5.1) with CN time discretisation with time step $\tau = 1/100$.

h	1/8	1/16	1/32	1/64
$m = 2$, finite differences	0.430	0.661	0.816	0.904
$m = 1$, linear finite elements	0.410	0.650	0.807	0.899
$\cos^2(\pi h)/(1 + \sqrt{1 - \cos^2(\pi h)})^2$	0.447	0.674	0.822	0.907
$1 - 2\pi h$	0.215	0.607	0.804	0.902

REFERENCES

- [1] K. Burrage. *Parallel and Sequential Methods for Ordinary Differential Equations*. Oxford University Press, Oxford, 1995.
- [2] M. Eiermann. On semiiterative methods generated by Faber polynomials. *Numer. Math.*, 56:139–156, 1989.
- [3] L. A. Hageman and D. M. Young. *Applied Iterative Methods*. Computer Science and Applied Mathematics. Academic Press, New York, 1981.
- [4] M. Hu, K. Jackson, J. Janssen, and S. Vandewalle. Remarks on the optimal convolution kernel for CSOR waveform relaxation. *Adv. in Comput. Math.*, 7(1–2):135–156, 1997.
- [5] M. Hu, K. Jackson, and B. Zhu. Complex optimal SOR parameters and convergence regions. Department of Computer Science, University of Toronto, Canada, Working Notes, 1995.
- [6] J. Janssen and S. Vandewalle. Multigrid waveform relaxation on spatial finite-element meshes: The continuous-time case. *SIAM J. Numer. Anal.*, 33(2):456–474, April 1996.
- [7] J. Janssen and S. Vandewalle. Multigrid waveform relaxation on spatial finite-element meshes: The discrete-time case. *SIAM J. Sci. Comput.*, 17(1):133–155, January 1996.
- [8] J. Janssen and S. Vandewalle. On SOR waveform relaxation methods. *SIAM J. Numer. Anal.*, 34(6), December 1997. (to appear).
- [9] B. Leimkuhler. Estimating waveform relaxation convergence. *SIAM J. Sci. Comput.*, 14(4):872–889, July 1993.
- [10] E. Lelarmee, A. E. Ruehli, and A. L. Sangiovanni-Vincentelli. The waveform relaxation method for time-domain analysis of large scale integrated circuits. *IEEE Trans. CAD*, 1(3):131–145, July 1982.
- [11] C. Lubich. Chebyshev acceleration of Picard-Lindelöf iteration. *BIT*, 32:535–538, 1992.
- [12] T. A. Manteuffel. The Tchebychev iteration for nonsymmetric linear systems. *Numer. Math.*, 28:307–327, 1977.
- [13] U. Miekkala and O. Nevanlinna. Convergence of dynamic iteration methods for initial value problems. *SIAM J. Sci. Statist. Comput.*, 8(4):459–482, July 1987.
- [14] O. Nevanlinna. Linear acceleration of Picard-Lindelöf iteration. *Numerische Mathematik*,

- 57:147–156, 1990.
- [15] A. R. Newton and A. L. Sangiovanni-Vincentelli. Relaxation-based electrical simulation. *SIAM J. Sci. Statist. Comput.*, 4(3):485–524, September 1983.
 - [16] M. W. Reichelt, J. K. White, and J. Allen. Optimal convolution SOR acceleration of waveform relaxation with application to parallel simulation of semiconductor devices. *SIAM J. Sci. Comput.*, 16(5):1137–1158, September 1995.
 - [17] R. Skeel. Waveform iteration and the shifted Picard splitting. *SIAM J. Sci. Stat. Comput.*, 10(4):756–776, July 1989.
 - [18] G. J. Tee. Eigenvectors of the successive overrelaxation process, and its combination with chebyshev semi-iteration. *Comput. J.*, 6:250–263, 1963.
 - [19] D. M. Young. *Iterative Solution of Large Linear Systems*. Academic Press, New York, 1971.