A Unified Framework Based on Operational Calculus for the Convergence Analysis of Waveform Relaxation Methods

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Report TW 421, March 2005

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Abstract

Waveform relaxation methods are iterative methods for the solution of systems of ordinary differential equations. The convergence analysis of waveform relaxation methods traditionally uses the theory of Volterra convolution equations. More specifically, the convergence theory is typically based on a theorem of Paley and Wiener that gives a condition for the solution of a linear Volterra convolution equation to be bounded. Extensions of this theorem to discrete convolution equations and vector-valued problems have been described in the literature. In this note, it is shown that the same results can be derived by an alternative approach based on operational calculus. An operational calculus defines what is meant by a function of an operator. A spectral mapping theorem then relates the spectrum of the resulting operator to the spectrum of the original operator. In this paper, the Dunford-Taylor operational calculus for scalar analytic functions is extended to matrix-valued analytic functions. Using the corresponding spectral mapping theorem, it is then straightforward to analyze the convergence of a large number of waveform relaxation algorithms. The theory is applied to the analysis of continuous waveform relaxation and to the analysis of discrete waveform relaxation based on general linear methods, both for initial value and time-periodic systems of ordinary differential equations.

Keywords : ordinary differential equations, waveform relaxation, operational calculus, spectral mapping theorem.
AMS(MOS) Classification : Primary : 65J10, Secondary : 47N40.

A UNIFIED FRAMEWORK BASED ON OPERATIONAL CALCULUS FOR THE CONVERGENCE ANALYSIS OF WAVEFORM RELAXATION METHODS

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Abstract.

Waveform relaxation methods are iterative methods for the solution of systems of ordinary differential equations. The convergence analysis of waveform relaxation methods traditionally uses the theory of Volterra convolution equations. More specifically, the convergence theory is typically based on a theorem of Paley and Wiener that gives a condition for the solution of a linear Volterra convolution equation to be bounded. Extensions of this theorem to discrete convolution equations and vector-valued problems have been described in the literature. In this note, it is shown that the same results can be derived by an alternative approach based on operational calculus. An operational calculus defines what is meant by a function of an operator. A spectral mapping theorem then relates the spectrum of the resulting operator to the spectrum of the original operator. In this paper, the Dunford-Taylor operational calculus for scalar analytic functions is extended to matrix-valued analytic functions. Using the corresponding spectral mapping theorem, it is then straightforward to analyze the convergence of a large number of waveform relaxation algorithms. The theory is applied to the analysis of continuous waveform relaxation and to the analysis of discrete waveform relaxation based on general linear methods, both for initial value and time-periodic systems of ordinary differential equations.

AMS subject classification (2000): 47N40, 65J10.

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1 Introduction.

Waveform relaxation is an iterative method for the solution of systems of ordinary differential equations (ODEs). Like classical iterations for systems of algebraic equations, such as the Jacobi and Gauss-Seidel methods, waveform relaxation proceeds by repeatedly solving a sequence of simpler systems. Consider the linear system

$$\dot{u} = Lu + f,$$

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with $u(t)$, $f(t) \in \mathbb{R}^m$ and $L \in \mathbb{R}^{m\times m}$. A matrix splitting $L = L^+ + L^-$ results in the iteration

$$\dot{u}^{(\nu)} = L^+ u^{(\nu)} + L^- u^{(\nu-1)} + f.$$

If L^+ is taken to be the diagonal (Jacobi) or the lower triangular part (Gauss-Seidel) of L, the simpler systems are scalar ODEs. For a given system and splitting, several waveform relaxation variants are possible depending on the way the time dimension is treated. From a theoretical point of view, it is interesting to study continuous waveform relaxation, where the simpler ODEs are solved exactly, on either a finite or an infinite time interval. In a practical implementation the ODEs have to be discretized and solved numerically. Different time discretization schemes lead to different discrete waveform relaxation methods. An Implicit Euler discretization, for example, results in the following method

$$\frac{u_i^{(\nu)} - u_{i-1}^{(\nu)}}{\Delta t} = L^+ u_i^{(\nu)} + L^- u_i^{(\nu-1)} + f_i.$$

For linear initial value problems, a convergence analysis based on the theory of Volterra integral equations was introduced in the seminal paper [20]. There, it is shown that continuous waveform relaxation can be described by a linear Volterra convolution operator $\mathcal{K}$ whose spectral radius $\rho(\mathcal{K})$ determines the convergence of the method. The spectral radius is characterized by the following theorem. It can be proven using the Paley-Wiener theorem that gives a necessary and sufficient condition for the boundedness of the solution of a linear Volterra convolution equation [20, 17, 14].

Theorem 1.1 (Th. 2.2, [20]). *Consider $\mathcal{K}$ as an operator in $L^p([0,\infty],\mathbb{C}^m)$ with $1 \le p \le \infty$, and assume $\sigma(L^+) \cap \mathbb{C}^+ = \phi$. Then, $\mathcal{K}$ is a bounded linear operator and*

$$\rho(\mathcal{K}) = \sup_{z\in\mathbb{C}^+} \rho((zI_m - L^+)^{-1}L^-). \tag{1.1}$$

A framework for the analysis of discrete waveform relaxation was provided in [21]. The following theorem is based on a discrete equivalent of the Paley-Wiener theorem [21, 17, 15].

Theorem 1.2 (Th. 3.1, [21]). *Consider $\mathcal{K}$ as an operator in $l^p(\infty,\mathbb{C}^m)$ with $1 \le p \le \infty$, and suppose $\sigma(L^+) \cap \Sigma = \phi$. Then, $\mathcal{K}$ is a bounded linear operator and*

$$\rho(\mathcal{K}) = \sup_{z\in\Sigma} \rho((zI_m - L^+)^{-1}L^-), \tag{1.2}$$

where Σ is the complement of the interior of the stability region of the time discretization scheme scaled by $\frac{1}{\Delta t}$.

Extensions to time-periodic problems, to large scale iterative methods such as multigrid and domain decomposition, to finite element discretizations of PDEs and to different time discretization schemes such as implicit Runge-Kutta, boundary value and general linear methods can be found in [17, 29, 3, 14, 15, 28, 27].

The formulae for the spectral radii of continuous and discrete waveform relaxation operators are clearly very similar. This note suggests an approach, based on operational calculus, that unifies the convergence analyses of the different waveform relaxation methods. The approach can be summarized by the general formula

$$\rho(F(T)) = \sup_{z\in\sigma(T)} \rho(F(z)), \tag{1.3}$$

where T is any closed linear operator (with non-empty resolvent set) and F is a matrix-valued function analytic in a neighborhood of $\sigma(T)$, the spectrum of T. Taking $T = \frac{d}{dt}$ and $F(z) = (zI_m - L^+)^{-1}L^-$, for example, gives the formula for continuous waveform relaxation. The operational calculus for scalar functions is well known. It is shown here that the convergence of waveform relaxation methods can be analyzed by using a straightforward extension to matrix-valued functions. The approach based on operator theory can be interpreted as a generalization of the analysis of iterative methods for matrices to the analysis of the corresponding methods for matrices of operators (or equivalently matrix-valued operators). In §2 the operator calculus is first introduced for matrices, then for bounded linear operators and finally for closed linear operators. Section 3 shows how continuous and discrete waveform relaxation for initial value problems on finite and infinite time intervals and for time-periodic problems fit into the general framework. For the discrete case, time discretization based on general linear methods is considered. Linear multistep, implicit Runge-Kutta and block boundary value methods can be derived as special cases. Section 4 provides some concluding remarks.

2 Spectral Mapping Theorems for Matrix-Valued Functions of Operators.

The theory of this section is introduced first for matrices, then for bounded linear operators and finally for closed (possibly unbounded) linear operators. Each class of operators is a generalization of the next. In principle, it would suffice to consider only closed linear operators. However, for ease of understanding and clarity of exposition the step by step approach is preferred. For each of the three cases, a definition is given for what is meant by $f(T)$, a function of an operator. A set of rules is provided for calculating with such functions. Using this so called operational calculus, the spectrum of $f(T)$ is characterized. The theory for scalar functions is well developed. Detailed descriptions of the Dunford-Taylor operational calculus for scalar functions can be found in functional analysis monographs such as [5, 25, 9, 23] and textbooks such as [24, 16]. See [7] for a recent state of the art. Here, extensions to matrix-valued functions are given. These results will be applied in §3 to characterize the convergence of waveform relaxation methods.

2.1 Operational Calculus for Functions of Matrices

The operational calculus for functions of matrices is a special case of the general theory since matrices can be considered as representations of linear operators in finite dimensional vector spaces. Considering this case separately is nevertheless useful because the results can be obtained using only standard linear algebra.

2.1.1 Scalar Functions of Matrices

There are many ways to define a function of a matrix. Most definitions turn out to be equivalent in practice ([22] cited in [6]). The following definitions are used here. A similar formulation will be used as the starting point for defining functions of more general operators.

DEFINITION 2.1. *The family of scalar functions $f : \mathbb{C} \to \mathbb{C}$, analytic in some neighborhood of $\sigma(T)$ is denoted by $\mathcal{F}(T)$.*

DEFINITION 2.2. *Given a matrix $T \in \mathbb{C}^{n\times n}$ and a function $f \in \mathcal{F}(T)$, the matrix $f(T) \in \mathbb{C}^{n\times n}$ is defined by*

$$f(T) = \frac{1}{2\pi i}\oint f(z)(zI_X - T)^{-1}dz. \tag{2.1}$$

All line integration is over a contour that is appropriately chosen in relation to the spectrum $\sigma(T)$ (for more details see [5, 25]). A characterization of $f(T)$ derived from this definition is given by the following theorem [6, Th. 11.1.1].

THEOREM 2.1. *Let $T = X\,\mathrm{diag}(J_1, \ldots, J_q)X^{-1}$ be the Jordan decomposition of $T \in \mathbb{C}^{n\times n}$ with Jordan blocks $J_i \in \mathbb{C}^{n_i\times n_i}$,*

$$J_i = \begin{bmatrix} \lambda_i & 1 & \cdots & 0 \\ 0 & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & 1 \\ 0 & \ldots & 0 & \lambda_i \end{bmatrix}.$$

If $f \in \mathcal{F}(T)$, then

$$f(T) = X\,\mathrm{diag}(f(J_1), \ldots, f(J_q))X^{-1}$$

with

$$f(J_i) = \begin{bmatrix} f(\lambda_i) & f^{(1)}(\lambda_i) & \cdots & \frac{f^{(n_i-1)}(\lambda_i)}{(n_i-1)!} \\ 0 & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & f^{(1)}(\lambda_i) \\ 0 & \ldots & 0 & f(\lambda_i) \end{bmatrix}.$$

The following rules constitute a so called operational calculus for functions of matrices. They can be proven using Definition 2.2 or Theorem 2.1. These rules are also a special case of the rules for bounded linear operators.

THEOREM 2.2. *If f, $g \in \mathcal{F}(T)$ and α, $\beta \in \mathbb{C}$, then*

- *$\alpha f + \beta g \in \mathcal{F}(T)$ and $\alpha f(T) + \beta g(T) = (\alpha f + \beta f)(T)$ (linearity),*
- *$f \cdot g \in \mathcal{F}(T)$ and $f(T) \cdot g(T) = (f \cdot g)(T)$ (multiplication),*
- *if f has a power series expansion $f(z) = \sum_{k=0}^{\infty} \alpha_k z^k$, valid in a neighborhood of $\sigma(T)$, then $f(T) = \sum_{k=0}^{\infty} \alpha_k T^k$ (power series),*

If $f \in \mathcal{F}(T)$, $g \in \mathcal{F}(f(T))$ and $h(z) = g(f(z))$, then

- *$h \in \mathcal{F}(T)$ and $h(T) = g(f(T))$ (function composition).*

The following spectral mapping theorem is a direct consequence of Theorem 2.1.

THEOREM 2.3. *Let T be a complex square matrix. If $f \in \mathcal{F}(T)$, then*

$$\sigma(f(T)) = \{f(z),\, z \in \sigma(T)\} =: f(\sigma(T)).$$

2.1.2 Matrix-Valued Functions of Matrices

DEFINITION 2.3. *The family of all matrix-valued functions $F : \mathbb{C} \to \mathbb{C}^{m\times m}$, analytic in some neighborhood of $\sigma(T)$ is denoted by $\mathcal{F}^{m\times m}(T)$.*

Note that a matrix-valued analytic function is equivalent to a matrix of analytic functions. Matrix-valued functions of matrices can be defined by applying Definition 2.2 componentwise.

DEFINITION 2.4. *Given a matrix $T \in \mathbb{C}^{n\times n}$ and a function $F \in \mathcal{F}^{m\times m}(T)$, the matrix $F(T) \in \mathbb{C}^{mn\times mn}$ is defined by*

$$F(T) = \frac{1}{2\pi i} \oint F(z) \otimes (zI_X - T)^{-1} dz.$$

The expression $A \otimes B$ denotes the Kronecker or tensor product. The matrix $A \otimes B$ is obtained by replacing each element a_{ij} in A with the matrix $a_{ij}B$. If $A \in \mathbb{C}^{m\times m}$ and $B \in \mathbb{C}^{n\times n}$ then $A \otimes B \in \mathbb{C}^{mn\times mn}$.

From the operational calculus for scalar functions, an operational calculus for matrix-valued functions can be derived. For example, if $F, G \in \mathcal{F}^{m\times m}(T)$, then $F \cdot G \in \mathcal{F}^{m\times m}(T)$ and $F(T) \cdot G(T) = (F \cdot G)(T)$.

By applying Theorem 2.1 componentwise, it can be found that

$$F(T) = (I_m \otimes X)\, \mathrm{diag}(F(J_1), \ldots, F(J_q))(I_m \otimes X^{-1}) \tag{2.2}$$

Since $\mathrm{diag}(F(J_1), \ldots, F(J_q))$ is block diagonal, the spectrum of $F(T)$ is given by the union of the spectra of the diagonal blocks $F(J_i)$. These blocks themselves contain triangular blocks with constant diagonals (or, equivalently, they are block triangular with a constant block diagonal if all the tensor products are reversed). This observation leads to the following generalization of the spectral mapping theorem.

THEOREM 2.4. *Let T be a complex square matrix. If $F \in \mathcal{F}^{m\times m}(T)$, then*

$$\sigma(F(T)) = \bigcup_{z\in\sigma(T)} \sigma(F(z)) =: \sigma(F(\sigma(T))).$$

The following corollary follows immediately.
COROLLARY 2.5. *Let T be a complex square matrix. If $F \in \mathcal{F}^{m\times m}(T)$, then*

$$\rho(F(T)) = \max_{z\in\sigma(T)} \rho(F(z))$$

2.2 Operational Calculus for Functions of Bounded Linear Operators

The following terminology and notations are used in this section. A linear operator T in a Banach space X is bounded if $\exists M : \forall x \in X : \|Tx\| < M\|x\|$. The norm of a bounded linear operator is given by $\|T\| = \sup_{\|x\|=1} \|Tx\|$. The resolvent set of a linear operator T in X is the set of complex numbers λ for which $(\lambda I_X - T)^{-1}$ is an everywhere defined bounded linear operator. The spectrum $\sigma(T)$ of T is the complement of the resolvent set in $\mathbb{C}$. The spectral radius of a linear operator is given by $\rho(T) = \sup_{\lambda\in\sigma(T)} |\lambda| = \lim_{n\to\infty} \|T^n\|^{1/n}$. The spectrum of a bounded linear operator is a closed and bounded set.

2.2.1 Scalar Functions of Bounded Linear Operators

The definitions from the section 2.1 can still be used when T is a bounded linear operator. The formulation of the theorems is analogous as well. Proofs for the operational calculus and spectral mapping theorems for scalar functions of bounded linear operators can be found in [5, 25]. Only the spectral mapping theorems are stated here.
THEOREM 2.6. *Let T be a bounded linear operator. If $f \in \mathcal{F}(T)$, then*

$$\sigma(f(T)) = f(\sigma(T)).$$

2.2.2 Matrix-Valued Functions of Bounded Linear Operators

It is straightforward to extend the operational calculus for scalar functions to matrix-valued functions. Using the resulting operational calculus, the following generalization of Theorem 2.4 to bounded linear operators can be given.
THEOREM 2.7. *Let T be a bounded linear operator. If $F \in \mathcal{F}^{m\times m}(T)$, then*

$$\sigma(F(T)) = \sigma(F(\sigma(T))). \tag{2.3}$$

PROOF. The proof is patterned after the proof of Theorem 2.6 [5, Th. 11, p. 569].

First, it is shown that $\sigma(F(T)) \supset \sigma(F(\sigma(T)))$. Let $\lambda \in \sigma(T)$ and $\mu \in \sigma(F(\lambda))$. Take v a normalized eigenvector of the matrix $F(\lambda)$ for the eigenvalue μ, i.e., $F(\lambda)v = \mu v$ and $v^*v = 1$. Define the matrix-valued function G in the domain of definition of F by

$$G(\xi) = (F(\lambda) - F(\xi))/(\lambda - \xi).$$

By the matrix-valued operational calculus it follows that

$$\begin{aligned} G(T)(I_m \otimes (\lambda I_X - T)) &= F(\lambda) \otimes I_X - F(T) \\ &= -(\mu I_m - F(\lambda)) \otimes I_X + \mu I_m \otimes I_X - F(T). \end{aligned}$$

Multiplying from the right by $v \otimes I_X$ and using $(\mu I_m - F(\lambda))v = 0$ results in

$$G(T)(v \otimes I_X)(\lambda I_X - T) = (\mu I_m \otimes I_X - F(T))(v \otimes I_X). \tag{2.4}$$

Assume $\mu \notin \sigma(F(T))$, then $\mu I_m \otimes I_X - F(T)$ has a bounded everywhere defined inverse, denoted by A. Multiplying (2.4) from the left by $(v^* \otimes I_X)A$ shows that $(v^* \otimes I_X)AG(T)(v \otimes I_X)$ would be a bounded everywhere defined inverse of $\lambda I_X - T$. This contradicts the assumption that $\lambda \in \sigma(T)$ and therefore $\mu \in \sigma(F(T))$.

Next, it is shown that $\sigma(F(T)) \subset \sigma(F(\sigma(T)))$. Let $\mu \in \sigma(F(T))$ and suppose that $\mu \notin \sigma(F(\sigma(T)))$. Then the function

$$H(\xi) = (F(\xi) - \mu I)^{-1}$$

is analytic in the same neighborhood of $\sigma(T)$ as F. By the matrix-valued operational calculus it follows that

$$H(T)(F(T) - \mu I_m \otimes I_X) = I_m \otimes I_X.$$

Hence $H(T)$ is a bounded everywhere defined inverse of $F(T) - \mu I_m \otimes I_X$ which contradicts the assumption that $\mu \in \sigma(F(T))$. □

The following analogue of Corollary 2.5 holds.

COROLLARY 2.8. *Let T be a bounded linear operator. If $F \in \mathcal{F}^{m\times m}(T)$, then*

$$\rho(F(T)) = \max_{z \in \sigma(T)} \rho(F(z))$$

2.3 Operational Calculus for Functions of Closed Linear Operators

A linear operator T with domain $\mathcal{D}(T) \subset X$ is closed if its graph, i.e., the set of all points (x, Tx), is closed. This is equivalent to the following implication: if $\lim_{n\to\infty} x_n = x$ and $\lim_{n\to\infty} Tx_n = y$ for $x_n \in \mathcal{D}(T)$ then $x \in \mathcal{D}(T)$ and $y = Tx$. A closed linear operator T with $\mathcal{D}(T) = X$ is bounded. The definitions for resolvent set, spectrum and spectral radius are those of §2.2. The spectrum of a closed linear operator is closed, but not necessarily bounded. A definition of a function of an unbounded closed operator can be given by taking into account the behavior of the function at infinity. Operators whose spectrum is the whole complex plane have to be explicitly excluded.

2.3.1 Scalar Functions of Closed Linear Operators

Definition 2.5. *The family of all scalar functions $f : \mathbb{C} \to \mathbb{C}$, analytic in some neighborhood of $\sigma(T)$ and at infinity is denoted by $\mathcal{F}_\infty(T)$.*

The definition of a scalar function of a closed (possibly unbounded) linear operator can be based on the definition for bounded linear operators (see [5]). Let Φ be the homeomorphism of the Riemann sphere to itself defined by

$$\Phi(\lambda) = (\lambda - \alpha)^{-1}, \quad \Phi(\infty) = 0, \quad \Phi(\alpha) = \infty. \tag{2.5}$$

Definition 2.6. *Given a closed linear operator T with a non-empty resolvent set, let α be an element of the resolvent set and $A = (T - \alpha I)^{-1}$ a bounded linear operator. For a function $f \in \mathcal{F}_\infty(T)$, the linear operator $f(T)$ is defined by $f(T) = \phi(A)$ where the function $\phi \in \mathcal{F}(A)$ is given by $\phi(z) = f(\Phi^{-1}(z))$.*
The following theorem is derived in [5].

Theorem 2.9. *Given a closed linear operator T and a function $f \in \mathcal{F}_\infty(T)$, the linear operator $f(T)$, defined in Definition 2.6, is given by*

$$f(T) = f(\infty) I_X + \frac{1}{2\pi i} \oint f(z)(zI_X - T)^{-1} dz. \tag{2.6}$$

It is therefore independent of the choice of α from the resolvent set of T. In [25] the equality (2.6) is taken as the definition for $f(T)$.

The operational calculus is again analogous to the case for matrices and not repeated here.

Definition 2.7. *The extended spectrum is defined as $\sigma_\infty(T) = \sigma(T) \cup \{\infty\}$*

The following spectral mapping theorem for scalar functions of closed linear operators follows from Theorem 2.6 by Definition 2.6 and the fact that Φ is a one-to-one mapping between $\sigma_\infty(T)$ and $\sigma(A)$ [5]. For a different proof see [25].

Theorem 2.10. *Let T be a closed linear operator. If $f \in \mathcal{F}_\infty(T)$, then*

$$\sigma(f(T)) = f(\sigma_\infty(T)).$$

2.3.2 Matrix-Valued Functions of Closed Linear Operators

Definition 2.8. *The family of all matrix-valued functions $F : \mathbb{C} \to \mathbb{C}^{m \times m}$, analytic in some neighborhood of $\sigma(T)$ and at infinity is denoted by $\mathcal{F}_\infty^{m \times m}(T)$.*

The construction used to derive scalar functions of closed linear operators from the case of bounded linear operators can also be used for matrix-valued functions. Alternatively Theorem 2.9 can be applied componentwise.

Definition 2.9. *Given a closed linear operator T and a function $F \in \mathcal{F}_\infty^{m \times m}(T)$, the linear operator $F(T)$ is defined by*

$$F(T) = F(\infty) \otimes I_X + \frac{1}{2\pi i} \oint F(z) \otimes (zI_X - T)^{-1} dz.$$

A spectral mapping theorem for matrix-valued functions of closed linear operators can be derived from the one for bounded linear operators in the same way as for scalar functions.

THEOREM 2.11. *Let T be a closed linear operator. If $F \in \mathcal{F}_\infty^{m\times m}(T)$, then*

$$\sigma(F(T)) = \sigma(F(\sigma_\infty(T))). \tag{2.7}$$

The following analogue of Corollaries 2.5 and 2.8 holds.

COROLLARY 2.12. *Let T be a closed linear operator. If $F \in \mathcal{F}_\infty^{m\times m}(T)$, then*

$$\rho(F(T)) = \max_{z\in\sigma_\infty(T)} \rho(F(z))$$

This formula is equivalent to (1.3).

3 Waveform Relaxation.

In this section several waveform relaxation methods are described and their convergence is analyzed using the operational calculi of §2. As expected, the results derived with the theory based on Volterra equations [20, 17, 29, 14, 15, 27] can be reproduced in a much more general setting.

3.1 An Abstract Setting for the Analysis of Waveform Relaxation

The following general set of equations is considered

$$(I_m \otimes T)u = (L \otimes I_X)u + f, \tag{3.1}$$

with $u, f \in X^m$, X a Banach space, T an operator in X, $L \in \mathbb{C}^{m\times m}$ and I_X and I_m identity operators in X and $\mathbb{C}^m$. Typically, the operator T will be the time derivative operator $\frac{d}{dt}$ or a discrete equivalent, although the results will continue to hold for any closed linear operator. A splitting of the form $L = L^+ + L^-$ results in the waveform relaxation method

$$(I_m \otimes T)u^{(\nu)} = (L^+ \otimes I_X)u^{(\nu)} + (L^- \otimes I_X)u^{(\nu-1)} + f, \tag{3.2}$$

For the classical Jacobi (L^+: diagonal of L) or Gauss-Seidel (L^+: lower triangular part of L) splittings, one iteration requires the solution of m decoupled equations. By considering the iteration for the errors $e^{(\nu)} = u^{(\nu)} - u$

$$(I_m \otimes T)e^{(\nu)} = (L^+ \otimes I_X)e^{(\nu)} + (L^- \otimes I_X)e^{(\nu-1)}, \tag{3.3}$$

it is clear that the convergence of the waveform relaxation method can be studied using the spectrum of the iteration operator

$$F(T) = (I_m \otimes T - L^+ \otimes I_X)^{-1}(L^- \otimes I_X). \tag{3.4}$$

The matrix-valued function F, defined by

$$F(z) = (zI - L^+)^{-1}L^- \tag{3.5}$$

is analytic in $\mathbb{C}\backslash\sigma(L^+)$ and at infinity. It is therefore always assumed that

$$\sigma(L^+) \cap \sigma(T) = \phi. \tag{3.6}$$

Equation (3.1) is considered for simplicity. The more general results from [14, 15] where I_m is replaced by a non-singular matrix M can be obtained by taking

$$F(z) = (M^+ + zL^+)^{-1}(M^- + zL^-) \quad \text{where} \quad M = M^+ + M^-.$$

A whole range of waveform relaxation methods can now be analyzed by defining an appropriate 'time derivative' operator T. For each waveform relaxation method discussed in the following sections the Banach space X, the operator T, its domain $\mathcal{D}(T)$ and spectrum $\sigma(T)$ or extended spectrum $\sigma_\infty(T)$ are specified. The spectrum and spectral radius of the waveform relaxation operator $F(T)$ can then be derived by using the theory of §2 as summarized by the formulae

$$\sigma(F(T)) = \sigma(F(\sigma_\infty(T))) \quad \text{and} \quad \rho(F(T)) = \max_{z\in\sigma_\infty(T)} \rho(F(z)). \tag{3.7}$$

In some cases T itself can be obtained as a function of an even simpler operator.

3.2 Continuous Waveform Relaxation

Continuous waveform relaxation is obtained by defining $Tx := \dot{x}$, in which case (3.1) is just the system of ordinary differential equations

$$\dot{u} = Lu + f,$$

for functions u and f defined on $[0, t_F]$. For initial value problems the extra condition $u(0) = u_0$ is added and t_F can be infinite. For periodic problems the extra condition is $u(0) = u(t_F)$.

The abstract iteration (3.2) takes the form

$$\dot{u}^{(\nu)} = L^+u^{(\nu)} + L^-u^{(\nu-1)} + f,$$

together with $u^{(\nu)}(0) = u_0$ or $u^{(\nu)}(0) = u^{(\nu)}(t_F)$. The error iteration (3.3) becomes

$$\dot{e}^{(\nu)} = L^+e^{(\nu)} + L^-e^{(\nu-1)},$$

together with $e^{(\nu)}(0) = 0$ or $e^{(\nu)}(0) = e^{(\nu)}(t_F)$.

3.2.1 Functions on Finite Time Intervals

Consider the Banach space $X = C[0, t_F]$ of continuous functions on the interval $[0, t_F]$ with norm $\|x\| = \max_{t\in[0,t_F]} \|x(t)\|$. Let T be the operator defined by $(Tx)(t) = \dot{x}(t)$ with domain

$$\mathcal{D}(T) = \{x : \dot{x} \in C[0, t_F], x(0) = 0\}.$$

T is a closed unbounded linear operator and its spectrum is empty ($\sigma(T) = \phi$). Its extended spectrum is therefore given by

$$\sigma_\infty(T) = \{\infty\},$$

see, for example, [5, p. 604], [25, p. 297] and [25, p. 291]. Together with (3.4)-(3.7) the classical result $\rho(F(T)) = 0$ is recovered [20].

3.2.2 Functions on Infinite Time Intervals

Consider the Banach space $X = L^p([0,\infty],\mathbb{C})$, $1 \le p \le \infty$ and let T be the operator defined by $(Tx)(t) = \dot{x}(t)$ with domain

$$\mathcal{D}(T) = \{x : x \,\text{is absolutely continuous on}\, [0,a], a > 0, \dot{x} \in X, x(0) = 0\}.$$

T is a closed unbounded linear operator. The equation $\lambda x(t) - \dot{x}(t) = y(t)$, together with $x(0) = 0$, has a bounded solution $x(t) = -\int_0^t e^{\lambda(t-s)} y(s)ds$ for every $y \in X$ whenever $\Re(\lambda) < 0$. Therefore the operator $(\lambda I_X - T)^{-1}$ is bounded and everywhere defined when $\Re(\lambda) < 0$ and, since the spectrum is closed, this gives

$$\sigma(T) = \mathbb{C}^+, \qquad \sigma_\infty(T) = \mathbb{C}^+ \cup \{\infty\}.$$

Together with (3.4)-(3.7) this leads to the classical result for the convergence of waveform relaxation on infinite time intervals given in Theorem 1.1.

3.2.3 Periodic Functions

Consider the Banach space $X = C[0,1]$ and let T be the operator defined by $(Tx)(t) = \dot{x}(t)$ with domain

$$\mathcal{D}(T) = \{x : \dot{x} \in C[0,1], x(0) = x(1)\}.$$

T is a closed unbounded linear operator. The equation $\lambda x(t) - \dot{x}(t) = y(t)$, together with $x(0) = x(1)$, has a bounded solution $x(t) = -\int_0^t e^{\lambda(t-s)} y(s)ds + \frac{e^\lambda}{e^\lambda - 1}\int_0^1 e^{\lambda(t-s)} y(s)ds$ for every $y \in X$ whenever $\lambda \notin 2\pi i\mathbb{Z}$ and thus

$$\sigma(T) = 2\pi i\mathbb{Z}, \qquad \sigma_\infty(T) = 2\pi i\mathbb{Z} \cup \{\infty\},$$

from which the convergence results for time-periodic waveform relaxation in [29] follow. For this case see [5, p. 604]. Similar results can be obtained for the Banach spaces $X = L^p(-\pi,\pi)$, $1 \le p \le \infty$ on the unit circle [5, p. 605], [25, p. 176].

3.3 Discrete Waveform Relaxation using General Linear Methods

For discrete waveform relaxation, the operator T can be defined by discretizing the equation $\dot{x} = Tx$. In this section the theory is applied for time discretization based on general linear methods (GLMs) [4, 8]. The well known linear multistep and implicit Runge-Kutta methods [3, 4, 8] and also the block boundary value methods [2, 10, 11] belong to this class of methods. The results for discrete waveform relaxation using linear multistep and implicit Runge-Kutta methods [21, 17, 27] can therefore be derived as special cases. Boundary value methods [2] are another generalization of linear multistep methods. The spectral properties of discrete waveform relaxation using boundary value methods [27] can be derived in the same way as for GLMs by using the results in [2, 12, 1].

There are several ways to formulate GLMs for an ODE of the form $\dot{x}(t) = f(t, x(t))$ (see [4]). We choose to use the equations

$$\tilde{x}_i = Cx_{i-1} + \Delta t A \tilde{f}(\tilde{t}_i, \tilde{x}_i), \tag{3.8}$$

$$x_i = Dx_{i-1} + \Delta t B \tilde{f}(\tilde{t}_i, \tilde{x}_i), \tag{3.9}$$

with $A \in \mathbb{R}^{s\times s}$, $B \in \mathbb{R}^{r\times s}$, $C \in \mathbb{R}^{s\times r}$, $D \in \mathbb{R}^{r\times r}$, $\tilde{t}_i \in \mathbb{R}^s$, $\tilde{x}_i \in \mathbb{R}^s$ and $x_i \in \mathbb{R}^r$ and where $\tilde{f}$ denotes componentwise application of f. This formulation highlights the analogy with IRK methods for which $r = 1$. The s stage values $\tilde{x}_i$ are typically approximations of $x(t)$ for some t within the current time step. The r values x_i can contain, for example, approximations of $x(t)$, brought forward from previous time steps or scaled approximations of derivatives of $x(t)$. In order to have a stable method, the matrix D has to be power bounded. Further conditions are needed to ensure that the method is consistent. The matrices C and D are typically chosen such that all rows sum to one and D is of rank one.

3.3.1 Finite Sequences

The discrete equivalent of $\dot{x} = Tx$ is found by using (3.8)-(3.9) which results in

$$\tilde{x}_i = Cx_{i-1} + \Delta t A (T\tilde{x})_i, \tag{3.10}$$

$$x_i = Dx_{i-1} + \Delta t B (T\tilde{x})_i. \tag{3.11}$$

These equations define T as an operator in the space of sequences of stage values $\mathbb{C}^{ns}$. Using the backward shift operator $S \in \mathbb{C}^{n\times n}$, given by $(Sx)_1 = 0$, $(Sx)_i = x_{i-1}$, $1 < i \leq n$ or

$$S = \begin{bmatrix} 0 & & & \\ 1 & \ddots & & \\ & \ddots & \ddots & \\ & & 1 & 0 \end{bmatrix} \tag{3.12}$$

and taking into account the initial condition $x_0 = 0$ this can also be written as

$$\tilde{x} = (C \otimes S)x + \Delta t (A \otimes I_X) T\tilde{x}, \tag{3.13}$$

$$x = (D \otimes S)x + \Delta t (B \otimes I_X) T\tilde{x}. \tag{3.14}$$

By eliminating x and using the matrix-valued operational calculus, it can be seen that $T = G(S)$ with

$$G(z) = \frac{1}{\Delta t}(A + zC(I_r - zD)^{-1}B)^{-1}. \tag{3.15}$$

Since the spectrum of S is $\{0\}$, it follows from the spectral mapping theorem for matrix-valued functions of matrices that

$$\sigma(T) = \sigma\left(\frac{1}{\Delta t}A^{-1}\right).$$

Together with (3.4)-(3.7) the results in [27] for the convergence analysis of discrete waveform relaxation on finite intervals are recovered.

3.3.2 Infinite Sequences

The same approach as for finite sequences allows T to be defined as an operator in the space of infinite sequences of stage values $l^p(\infty, \mathbb{C}^s)$. The backward shift operator in $l^p(\infty, \mathbb{C}^s)$ is defined by $(Sx)_1 = 0$, $(Sx)_i = x_{i-1}$, $i > 1$ or

$$S = \begin{bmatrix} 0 & & \\ 1 & \ddots & \\ & \ddots & \end{bmatrix}. \tag{3.16}$$

The spectrum of S is derived by considering the recurrence relation $\lambda x_i - x_{i-1} = y_i$ with $x_0 = 0$. Its solution is $x_i = \sum_{j=1}^{i} \lambda^{j-i-1} y_j$, $i \geq 1$. If $y \in l^p(\infty, \mathbb{C}^s)$, then $x \in l^p(\infty, \mathbb{C}^s)$ for $|\lambda| > 1$. Since the spectrum is closed this gives

$$\sigma(S) = \{\lambda \in \mathbb{C} : |\lambda| \leq 1\}.$$

(See also [25, p. 266]). For more information about the spectral properties of Toeplitz operators such as S see [1, 2]. Using the spectral mapping theorem for matrix-valued functions of bounded linear operators, one arrives at

$$\sigma(T) = \frac{1}{\Delta t} \bigcup_{|z|\leq 1} \sigma\left((A + zC(I_r - zD)^{-1}B)^{-1}\right).$$

It is shown in [27] that this is the complement of the interior of the stability domain of the GLM as defined in [4, 8] scaled by $\frac{1}{\Delta t}$. A similar result was originally derived for the special case of linear multistep methods in [21]. In general, the interior of the stability region of a time discretization method corresponds to the resolvent set of the discrete time derivative operator in $l^p(\infty)$. Combining the expression for $\sigma(T)$ with (3.4)-(3.7) recovers the results in [27] for the convergence analysis of discrete waveform relaxation on infinite intervals.

REMARK 3.1. Certain GLMs lead to a function G that has poles on the unit circle. The time derivative operator T for such methods is unbounded. Its spectrum can be derived directly or by using an extended operational calculus [7]. Alternatively, the expression for $\rho(F(T))$ can be obtained as

$$\sup_{z\in\sigma(S)} \rho(F(G(z))),$$

i.e., by considering the function $F(G(z))$ which is again analytic on the closed unit disc.

3.3.3 Periodic Sequences

For time-periodic problems discretized by GLMs the time derivative operator T in C^{sn} can be formulated as a function of the circulant backward shift matrix

$$P = \begin{bmatrix} 0 & \cdots & 0 & 1 \\ 1 & \ddots & & 0 \\ & \ddots & \ddots & \vdots \\ & & 1 & 0 \end{bmatrix}, \tag{3.17}$$

with spectrum $\sigma(P) = \{e^{\frac{2\pi ij}{n}}, j = 0, \ldots, n-1\}$. Using the matrix-valued function (3.15) the operator T is given by $T = G(P)$. The corresponding spectrum is

$$\sigma(T) = \frac{1}{\Delta t} \bigcup_{\sigma(P)} \sigma\left((A + zC(I_r - zD)^{-1}B)^{-1}\right).$$

Together with (3.4)-(3.7) this results in an expression for the convergence rate of discrete waveform relaxation for time-periodic problems (for the case of linear multistep methods see [29]).

4 Concluding Remarks.

A general framework for the analysis of waveform relaxation methods based on the Dunford-Taylor operational calculus was described. To do this, the theory of scalar functions of operators had to be extended to matrix-valued functions of operators. When applied to waveform relaxation for initial value problems, the results from the theory based on Volterra convolution operators are recovered. The theory presented here, however, is more general. For a given matrix splitting, a waveform relaxation method can be defined and analyzed for every closed linear operator.

Finally, we would like to point out some possible generalizations and ideas for further research. The theory developed in this paper covers most classical waveform relaxation results for linear systems of ODEs. It does not immediately cover waveform relaxation for linear systems of delay differential equations [26]. For this case, an operational calculus is needed for a larger class of functions that are not necessarily analytic at infinity. An extended operational calculus [7] such as the Hille-Phillips calculus, based on the theory of semigroups of operators [9], would be appropriate. It is also possible to study pseudospectra of waveform relaxation operators [13, 19] using functions of operators. For a spectral mapping theorem for the pseudospectra of scalar functions of matrices and bounded linear operators see [18].

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REFERENCES

1. A. Böttcher and B. Silbermann, *Introduction to Large Truncated Toeplitz Matrices*, Springer-Verlag, New York, 1999.
2. L. Brugnano and D. Trigiante, *Solving Differential Problems by Multistep Initial and Boundary Value Methods*, Gordon and Breach Science Publishers, Amsterdam, 1998.
3. K. Burrage, *Parallel and Sequential Methods for Ordinary Differential Equations*, The Clarendon Press Oxford University Press, New York, 1995.

4. J. C. Butcher, *Numerical Methods for Ordinary Differential Equations*, John Wiley & Sons Ltd., Chichester, 2003.
5. N. Dunford and J. T. Schwartz, *Linear Operators. Part I*, Interscience Publishers, Inc., New York, 1957.
6. G. H. Golub and C. F. Van Loan, *Matrix Computations*, Johns Hopkins University Press, Baltimore, MD, third ed., 1996.
7. M. Haase, *The functional calculus for sectorial operators*. `http://www.mathematik.uni-ulm.de/m5/haase/`, 2004. book manuscript; to appear in: Operator Theory: Advances and Applications, Birkhäuser Verlag, Basel 2005.
8. E. Hairer and G. Wanner, *Solving Ordinary Differential Equations. II*, Springer-Verlag, Berlin, second ed., 1996.
9. E. Hille and R. S. Phillips, *Functional Analysis and Semi-Groups*, American Mathematical Society, Providence, R. I., 1974.
10. F. Iavernaro and F. Mazzia, *Solving ordinary differential equations by generalized Adams methods: properties and implementation techniques*, Appl. Numer. Math., 28 (1998), pp. 107–126.
11. ——, *Block-boundary value methods for the solution of ordinary differential equations*, SIAM J. Sci. Comput., 21 (1999), pp. 323–339.
12. F. Iavernaro, F. Mazzia, and D. Trigiante, *Eigenvalues and quasi-eigenvalues of banded Toeplitz matrices: some properties and applications*, Numer. Algorithms, 31 (2002), pp. 157–170.
13. Z. Jackiewicz, B. Owren, and B. Welfert, *Pseudospectra of waveform relaxation operators*, Comput. Math. Appl., 36 (1998), pp. 67–85.
14. J. Janssen and S. Vandewalle, *Multigrid waveform relaxation of spatial finite element meshes: The continuous-time case*, SIAM J. Numer. Anal., 33 (1996), pp. 456–474.
15. ——, *Multigrid waveform relaxation on spatial finite element meshes: The discrete-time case*, SIAM J. Sci. Comput., 17 (1996), pp. 133–155.
16. P. D. Lax, *Functional Analysis*, Wiley-Interscience [John Wiley & Sons], New York, 2002.
17. C. Lubich and A. Ostermann, *Multigrid dynamic iteration for parabolic equations*, BIT, 27 (1987), pp. 216–234.
18. S.-H. Lui, *A pseudospectral mapping theorem*, Math. Comp., 72 (2003), pp. 1841–1854.
19. A. Lumsdaine and D. Wu, *Spectra and pseudospectra of waveform relaxation operators*, SIAM J. Sci. Comput., 18 (1997), pp. 286–304. Dedicated to C. William Gear on the occasion of his 60th birthday.
20. U. Miekkala and O. Nevanlinna, *Convergence of dynamic iteration methods for initial value problem*, SIAM J. Sci. Statist. Comput., 8 (1987), pp. 459–482.

21. ———, *Sets of convergence and stability regions*, BIT, 27 (1987), pp. 554–584.

22. R. F. Rinehart, *The equivalence of definitions of a matric function*, Amer. Math. Monthly, 62 (1955), pp. 395–414.

23. W. Rudin, *Functional Analysis*, McGraw-Hill Book Co., New York, 1973.

24. M. Schechter, *Principles of Functional Analysis*, Academic Press, New York, 1971.

25. A. E. Taylor, *Introduction to Functional Analysis*, John Wiley & Sons Inc., New York, 1958.

26. J. Van lent, J. Janssen, and S. Vandewalle, *Multigrid waveform relaxation for delay partial differential equations*, in Proceedings of the 5th IFAC International Workshop on Time Delay Systems, Elsevier, 2004. to appear.

27. J. Van lent and S. Vandewalle, *Multigrid methods for implicit Runge-Kutta and boundary value method discretizations of parabolic PDEs*, SIAM Journal on Scientific Computing. to appear.

28. ———, *Multigrid waveform relaxation for anisotropic partial differential equations*, Numer. Algorithms, 31 (2002), pp. 361–380.

29. S. Vandewalle and R. Piessens, *On dynamic iteration methods for solving time-periodic differential equations*, SIAM J. Numer. Anal., 30 (1993), pp. 286–303.