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A FREQUENCY DECOMPOSITION WAVEFORM RELAXATION ALGORITHM FOR SEMILINEAR EVOLUTION EQUATIONS*

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Abstract. Semilinear evolution equations arise in many applications ranging from mathematical biology to chemical reactions (e.g., combustion). The significant difficulty in these equations is the nonlinearity, which combined with the discretized diffusion operator leads to large systems of nonlinear equations. To solve these equations, Newton's method or a variant thereof is often used, and to achieve convergence can require individual fine tuning for each case. This can be especially difficult if nothing is known about the solution behavior. In addition, one observes in many cases that not all frequency components are equally important for the solution; the frequency interaction is determined by the nonlinearity. It is therefore of interest to work in frequency space when analyzing the unknown behavior of such problems numerically.

We propose in this paper an algorithm which reduces the dimensionality of the nonlinear problems to be solved to a size chosen by the user. The algorithm performs a decomposition in frequency space into subspaces, and an iteration is used to obtain the solution of the original problem from the solutions on the frequency subspaces. We prove linear convergence of the algorithm on unbounded time intervals, a result which is also valid for the stationary case. On bounded time intervals, we show that the new algorithm converges superlinearly, a rate faster than any linear rate. We obtain this result by relating the algorithm to an algorithm of waveform relaxation type. By using time windows, one can thus achieve any linear contraction rate desired. An additional advantage of this algorithm is its inherent parallelism.

Key words. waveform relaxation, frequency decomposition, sequential spectral method, iterative approximation of evolution problems.

AMS subject classifications. 65M70, 65M55, 65H10.

1. Introduction.

Semilinear evolution equations are an important class of equations for modeling natural phenomena. In many of these applications, the spatial operator is rather simple, often just representing a diffusion, whereas the major effort of the modeling goes into the non-linear reaction terms. This often leads to infinite dimensional problems (due to the diffusion), whose difficulty lies in the nonlinearity of the reaction terms and not in the spatial operator. In addition, the behavior of a new nonlinear model is in general not known and questions of existence and uniqueness of solutions arise. In such situations it is desirable to have numerical methods available which are able to track multiple solutions and are robust in the sense that they do not fail because the Newton method inherently necessary due to the nonlinearity fails to converge. Applying a standard numerical method, it often requires considerable fine tuning of the various variants of Newton's method to obtain a solution, and then it is difficult to detect if it is the only one. In addition, one often observes in semilinear evolution equations that not all frequency components are of equal importance in the solution. The important activity of the solution is often confined to a relatively small subspace.

We propose in this paper a method which is suitable to explore semilinear evolution problems whose solution properties are not yet fully understood. Tam and coworkers investigated in [22] an algorithm which worked on frequency components of the solution individually, one at a time. This approach reduced the dimensionality of the nonlinear systems to be solved to one, and one dimensional nonlinear problems are much easier to handle than higher dimensional ones, since solutions can be confined to intervals and multiple solutions can be detected relatively easily. This algorithm also revealed the importance of certain frequency subspaces in the solution in several applications, including systems of non-linear partial differential equations, see [1]. The algorithm working on one frequency at a time is a special case of the

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frequency decomposition waveform relaxation algorithm we present in this paper. The algorithm was developed independently, and a preliminary analysis of it can be found in [12]. The algorithm uses the eigensystem of the differential operator in the semilinear evolution equation to define subspaces in frequency space. It then evolves the solution in one subspace while keeping it frozen in the other subspaces. A subspace iteration similar to the Schwarz iteration for steady problems, but now in frequency space, is used to obtain a sequence of approximate solutions, which is proved to converge to the solution of the original problem. The frequency decomposition presented here is related to a frequency decomposition and multi-grid method analyzed in [13] for steady state problems, but here we are interested in the coupling through the nonlinearity and we use the eigenfunctions of the linear differential operator to decouple the contributions of the linear part of the equation.

Decomposition and subspace iteration has been a field of high activity during the last decades, see for example the survey papers by Xu [25], Xu and Zou [26] and the references therein. Most of the analysis however involves steady problems and this paper's focus is on evolution equations. The classical approach in that case is to discretize the time component uniformly over the whole domain by an implicit scheme, and then to apply the decomposition and subspace iteration at each time step to solve the steady problems obtained by the time discretization. For an analysis of this approach in the parabolic case see [16, 4], and for hyperbolic problems see [2, 24]. Another, more recent approach for evolution problems is the following: one still decomposes the spatial domain, but solves time dependent subproblems during the subspace iteration. This approach has been known for ordinary differential equations under the name waveform relaxation, and the first link with domain decomposition was made by Bjørhus in [3] for first order hyperbolic problems. For the heat equation and an overlapping Schwarz decomposition, this approach was analyzed in [11, 10], and for more general parabolic problems in [8, 6]. This analysis has led to the class of overlapping Schwarz waveform relaxation algorithms. The application of such algorithms to the second order wave equation has been studied in [7]. A different type of splitting is used in the multigrid waveform relaxation algorithm, which was motivated by the multigrid techniques for steady problems, see for example [23], [21], [14], [15] and references therein. All algorithms in the class of waveform relaxation algorithms have the advantage that one does not need to impose a uniform time discretization for all subspaces, and also that one does not need to communicate information at each time step. The frequency decomposition waveform relaxation algorithm presented in this paper is an algorithm in this class, but with a new type of splitting, namely in frequency space.

In Section 2, we introduce the semilinear parabolic equation for which we study the frequency decomposition waveform relaxation algorithm, and we give basic existence results on which our analysis later is based. In Section 3, we introduce the frequency subspace decomposition. The formulation is kept general and the frequency subspaces are characterized by invariant subspaces of the spatial operator. In Section 4, we analyze the frequency decomposition waveform relaxation algorithm for both bounded and unbounded time intervals. The convergence results obtained differ considerably. On unbounded time intervals, we prove linear convergence of the algorithm under a strong Lipschitz condition on the nonlinear term. This case is of importance, since it also proves convergence of the algorithm for the steady state case, which is often significantly harder to handle numerically. On bounded time intervals, the convergence behavior is even better: we prove superlinear convergence of the algorithm, assuming that the nonlinear function is Lipschitz for an arbitrary constant. In all the analysis, we provide complete estimates for the contraction rates and constants involved. Section 5 shows the performance of the frequency decomposition waveform relaxation algorithm on two model problems, a double well potential in one dimension and a combustion

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problem in two dimensions.

2. Problem Formulation. We present the frequency decomposition waveform relaxation algorithm for a general evolution problem using the theory of semigroups of linear operators. This has the advantage that the results are valid both at the continuous level and for various types of discretizations. We start by recalling results from [18], which we need later in the analysis of the algorithm. We consider the initial value problem

$$\begin{aligned} \frac{du(t)}{dt} + Au(t) &= f(t, u(t)), \qquad t > t_0, \\ u(t_0) &= u_0, \end{aligned} \tag{2.1}$$

where $-A$ is the infinitesimal generator of an analytic semigroup on a Banach space X with the norm $||\cdot||$. A is a sectorial operator, and by the assumptions on A, fractional powers A^α of A can be defined for $0 \leq \alpha \leq 1$, and A^α is a closed, linear, invertible operator with domain $D(A^\alpha)$. The closedness of A^α implies that $D(A^\alpha)$ endowed with the graph norm of A^α, i.e., the norm $|||x||| := ||x|| + ||A^\alpha x||$, is a Banach space. Since A^α is invertible, its graph norm $|||\cdot|||$ is equivalent to the norm $||\cdot||_\alpha := ||A^\alpha \cdot||$. Thus $D(A^\alpha)$ equipped with the norm $||\cdot||_\alpha$ is a Banach space, which we denote by X_α. The main assumption on the nonlinear function f for existence and uniqueness of a solution is

ASSUMPTION 2.1. *Let U be an open subset of $\mathbb{R}^+ \times X_\alpha$. The function $f : U \longrightarrow X$ satisfies Assumption 2.1, if, for every $(t, u) \in U$, there is a neighborhood $V \subset U$ and constants $L \geq 0$, $0 < \delta \leq 1$, such that*

$$||f(t_1, u_1) - f(t_2, u_2)|| \leq L(|t_1 - t_2|^\delta + ||u_1 - u_2||_\alpha) \tag{2.2}$$

for all $(t_i, u_i) \in V$.

THEOREM 2.2. *Let $-A$ be the infinitesimal generator of an analytic semigroup $G(t)$ satisfying $||G(t)|| \leq M$, and assume further that $0 \in \rho(-A)$, the resolvent set of A. If f satisfies Assumption 2.1, then, for every initial data $(t_0, x_0) \in U$, the initial value problem (2.1) has a unique local solution $u \in C([t_0, t_1[: X) \cap C^1(]t_0, t_1[: X)$, where $t_1 = t_1(t_0, u_0) > t_0$.*

Proof. The proof can be found in [18, page 196]. □

Under a stronger Lipschitz condition of similar type, global existence and uniqueness can also be established, see [18].

Since we have applications in mind with diffusion, differential operators are of interest. Let Ω be a bounded domain in $\mathbb{R}^n$ with smooth boundary $\partial\Omega$. Consider the differential operator

$$A(x, D) := \sum_{|\sigma| \leq 2m} a_\sigma(x) D^\sigma,$$

where σ is a multi index and D denotes the derivative. The following theorem from [18] is of key importance:

THEOREM 2.3. *If $A(x, D)$ is a strongly elliptic operator of order $2m$, then the operator $-A$ defined by $Au = A(x, D)u$ is the infinitesimal generator of an analytic semigroup of operators on $L^2(\Omega)$.*

3. Subspace Decomposition. To simplify notation, we consider in the sequel only nonlinear functions f in (2.1) which do not depend explicitly on time, $f = f(u)$, and we consider the fixed bounded time interval $[0, T]$, $T < \infty$. We also restrict the formulation of our algorithm to the special case where the Banach space X is a Hilbert space, equipped with the inner product (x, y) for $x, y \in X$, and with it the associated norm $||x|| := \sqrt{(x, x)}$ for $x \in X$. Suppose we have a decomposition of the Hilbert space X into n subspaces X_i, which might be disjoint or overlapping, $X = \text{span}\{X_1, X_2 \dots X_n\}$. For the frequency decomposition we have in mind, we use the normalized eigenfunctions $A\phi_j = \lambda_j \phi_j$ to define the subspaces, and we assume that the eigenpairs are ordered, $|\lambda_1| \leq |\lambda_2| \leq \dots$. For example, two subspaces could be defined by

$$X_1 := \text{span}\{\phi_1, \phi_2, \dots, \phi_{m_1}\}, \quad X_2 := \text{span}\{\phi_{m_2}, \phi_{m_2+1}, \dots, \phi_m\},$$

where $m_2 \leq m_1 + 1$. Note that the subspaces are overlapping if this inequality is strict. Also the second subspace might be infinite dimensional, $m = \infty$. We could also select subspaces which do not separate low and high frequencies, and thus both could be infinite dimensional. In applications however truncations are common. We define the orthogonal projector $\mathbb{P}_i : X \longrightarrow X_i$ to be the unique linear self-adjoint operator with range X_i such that $\mathbb{P}_i^2 = \mathbb{P}_i$. For the frequency decomposition introduced above, we would have, for a given $u \in X$,

$$\mathbb{P}_1 u = \sum_{j=1}^{m_1} u_j \phi_j, \quad \mathbb{P}_2 u = \sum_{j=m_2}^{m} u_j \phi_j, \quad u_j = (u, \phi_j).$$

Our interest here is in subproblems coupled through the non-linearity and not through A, therefore we require the decomposition to be such that A and $\mathbb{P}_i$ commute, which is the case for the frequency decomposition. Applying the projection operators $\mathbb{P}_i$ to the evolution equation (2.1), we get a sequence of n subproblems,

$$\begin{aligned} \frac{dv_i}{dt} + Av_i &= \mathbb{P}_i f(u), \qquad 0 < t < T, \\ v_i(0) &= \mathbb{P}_i u_0, \end{aligned} \tag{3.1}$$

$i = 1, 2, \dots, n$, where $v_i := \mathbb{P}_i u$. We also select operators $\mathbb{R}_i : X_i \longrightarrow X$, such that

$$u = \sum_{i=1}^{n} \mathbb{R}_i v_i, \tag{3.2}$$

and we assume that they commute with A as well. In the case of the frequency decomposition, we have

$$\begin{aligned} \mathbb{R}_1 v_1 = \mathbb{R}_1 \sum_{j=1}^{m_1} u_j \phi_j &= \sum_{j=1}^{m_2-1} u_j \phi_j + \sum_{j=m_2}^{m_1} \alpha_j u_j \phi_j, \\ \mathbb{R}_2 v_2 = \mathbb{R}_2 \sum_{j=m_2}^{m} u_j \phi_j &= \sum_{j=m_2}^{m_1} \beta_j u_j \phi_j + \sum_{j=m_1+1}^{m} u_j \phi_j, \end{aligned}$$

for some weights $\alpha_j + \beta_j = 1$, $j = m_2, \dots, m_1$. Using the operators $\mathbb{R}_i$, we can define the new function

$$\hat{f}(v_1, v_2, \dots, v_n) := f(\sum_{i=1}^{n} \mathbb{R}_i v_i),$$

and write the sequence of subproblems of the evolution equation as

$$\begin{aligned} \frac{dv_i}{dt} + Av_i &= \mathbb{P}_i \hat{f}(v_1, v_2, \dots, v_n), \qquad 0 < t < T, \\ v_i(0) &= \mathbb{P}_i u_0. \end{aligned} \tag{3.3}$$

Now evolving the solution in some subspaces X_i, $i \in S$, where S denotes a subset of indices in $\{1, 2, \ldots, n\}$, while fixing the solution in the remaining subspaces X_j, $j \notin S$, is equivalent to relaxing some of the arguments of $\hat{f}$. Doing this, we obtain an algorithm of waveform relaxation type [17]. For example, a Picard iteration, where all the arguments are relaxed, would read

$$\begin{aligned} \frac{dv_i^{k+1}}{dt} + Av_i^{k+1} &= \mathbb{P}_i \hat{f}(v_1^k, \ldots, v_n^k), \qquad 0 < t < T, \\ v_i^{k+1}(0) &= \mathbb{P}_i u_0, \end{aligned} \tag{3.4}$$

and thus all the subproblems in the corresponding subspaces X_i would be linear and decoupled. A Jacobi relaxation would lead to the subproblems

$$\begin{aligned} \frac{dv_i^{k+1}}{dt} + Av_i^{k+1} &= \mathbb{P}_i \hat{f}(v_1^k, \ldots, v_{i-1}^k, v_i^{k+1}, v_{i+1}^k, \ldots, v_n^k), \qquad 0 < t < T, \\ v_i^{k+1}(0) &= \mathbb{P}_i u_0, \end{aligned} \tag{3.5}$$

and thus all the nonlinear subproblems in the corresponding subspaces X_i are decoupled and their dimension is the dimension of the corresponding subspace. If the dimension is chosen to be one, we obtain the algorithm proposed in [22], which analyzes the solution one eigenmode at a time. Applying $\mathbb{R}_i$ to equation (3.5) and summing over i, we obtain

$$\begin{aligned} \frac{du^{k+1}}{dt} + Au^{k+1} &= \tilde{f}(u^{k+1}, u^k), \qquad 0 < t < T, \\ u^{k+1}(0) &= u_0, \end{aligned} \tag{3.6}$$

where we used the identity $u = \sum_{i=1}^m \mathbb{R}_i \mathbb{P}_i u$ that follows from (3.2), and we have defined the new function

$$\tilde{f}(u^{k+1}, u^k) := \sum_{i=1}^m \mathbb{R}_i \mathbb{P}_i \hat{f}(\mathbb{P}_1 u^k, \ldots, \mathbb{P}_{i-1} u^k, \mathbb{P}_i u^{k+1}, \mathbb{P}_{i+1} u^k, \ldots, \mathbb{P}_n u^k).$$

The resulting algorithm (3.6) is now a waveform relaxation algorithm in classical notation. Note that any other relaxation scheme in frequency space would lead to a system of the form (3.6) as well. It thus suffices in the analysis of the frequency decomposition and subspace iteration algorithm to investigate iterations of the form (3.6). This is accomplished in the next section.

REMARK 3.1. *The analysis presented in the sequel applies to any splitting leading to a system of the form (3.6). In particular, one could also choose a decomposition of the nonlinear function $f(u)$ directly into a function $\tilde{f}(u, v)$ such that $\tilde{f}(u, u) = f(u)$, which would be motivated by different means than the frequency decomposition.*

4. Convergence Analysis.

We derive linear and superlinear bounds on the convergence rates of the frequency decomposition and subspace iteration algorithm for solving the evolution equation (2.1). We will need

LEMMA 4.1. *If A is a sectorial operator and Re$(\lambda_1) > \delta > 0$, then for any $\alpha \geq 0$, there exists a constant $K = K(\alpha)$, such that*

$$||e^{-At}||_\alpha \leq K t^{-\alpha} e^{-\delta t}, \quad \forall t > 0.$$

Proof. The proof can be found in [19]. ☐

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4.1. Gronwall Type Estimates. We also need an estimate for a particular kernel, which is recursively applied in the analysis of the waveform relaxation algorithm. This estimate is established in this section. Denoting by $\Gamma(x)$ the Gamma function,

$$\Gamma(x) = \int_0^\infty z^{x-1}e^{-z}dz,$$

and the infinity norm of a bounded function $f(x)$ by

$$||f(\cdot)||_T := \sup_{0<t<T} |f(t)|,$$

where T can be infinite, we have the following results:

LEMMA 4.2. *Suppose for some $0 \le \alpha < 1$ and $T < \infty$ we have a sequence of functions $p^k : [0,T] \mapsto I\!R$ with $p^k(0) = 0$ for $k = 0, 1, \ldots$ satisfying the inequality*

$$p^{k+1}(t) \le \int_0^t \frac{1}{(t-\tau)^\alpha}(C_1 p^{k+1}(\tau) + C_2 p^k(\tau))d\tau$$

for some constants $C_1 \ge 0$ and $C_2 > 0$. Then we have

$$p^k(t) \le \frac{(C\Gamma(1-\alpha))^k}{\Gamma(k(1-\alpha)+1)} t^{k(1-\alpha)} ||p^0(\cdot)||_T,$$

where the constant $C = C(C_1, C_2, T, \alpha)$ is given by

$$C = C_2 e^{\frac{(C_1\Gamma(1-\alpha))^{n+1}}{\Gamma((n+1)(1-\alpha))}T^{(n+1)(1-\alpha)}} \left(2\sum_{j=1}^{n}(C_1\Gamma(1-\alpha))^j T^{j(1-\alpha)} + 1\right), \tag{4.1}$$

and $n = \left\lceil \frac{\alpha}{1-\alpha} \right\rceil$.

Proof. The proof is obtained by induction. The result clearly holds for $k = 0$. So suppose it holds for k. Then we have

$$p^{k+1}(t) \le C_1 \int_0^t \frac{1}{(t-\tau)^\alpha} p^{k+1}(\tau)d\tau + C_2 \int_0^t \frac{(C\Gamma(1-\alpha))^k}{\Gamma(k(1-\alpha)+1)} \frac{\tau^{k(1-\alpha)}}{(t-\tau)^\alpha} d\tau ||p^0(\cdot)||_T.$$

To be able to estimate the term containing p^{k+1} on the right, we follow an idea used in [5]. We iterate the inequality n times using each time the identity

$$\int_\tau^t (t-s)^{x-1}(s-\tau)^{y-1}ds = (t-\tau)^{x+y-1}B(x,y), \quad x, y > 0,$$

where $B(x,y)$ denotes the Beta function, Euler's integral of the first kind [9],

$$B(x,y) = \int_0^1 (1-s)^{x-1}s^{y-1}ds.$$

We obtain now a bounded kernel, namely

$$p^{k+1}(t) \le E\int_0^t \frac{1}{(t-s)^{(n+1)\alpha-n}} p^{k+1}(s)ds + D(k,t)t^{(k+1)(1-\alpha)}, \tag{4.2}$$

with E and $D(k,t)$ given by

$$E = C_1^{n+1} \prod_{j=1}^{n} B(j(1-\alpha), 1-\alpha),$$

$$D(k,t) = C_2 ||p^0(\cdot)||_T \frac{(C\Gamma(1-\alpha))^k}{\Gamma(k(1-\alpha)+1)} B(1-\alpha, k(1-\alpha)+1)$$
$$\times \left(\sum_{j=1}^{n} C_1^j B(j(1-\alpha), (k+1)(1-\alpha)+1) \prod_{l=1}^{j-1} B(l(1-\alpha), 1-\alpha) t^{j(1-\alpha)} + 1 \right).$$

Now we use the fact that the Beta function can be written in terms of the Gamma function [9],

$$B(x,y) = \frac{\Gamma(x)\Gamma(y)}{\Gamma(x+y)}.$$

Substituting this expression into the products in E and $D(t,k)$ reveals that the products are telescopic. We obtain

$$E = \frac{(C_1\Gamma(1-\alpha))^{n+1}}{\Gamma((n+1)(1-\alpha))},$$

$$D(k,t) = C_2 ||p^0(\cdot)||_T \frac{C^k \left(\Gamma(1-\alpha)\right)^{k+1}}{\Gamma((k+1)(1-\alpha)+1)}$$
$$\times \left(\sum_{j=1}^{n} \frac{\Gamma((k+1)(1-\alpha)+1) \left(C_1\Gamma(1-\alpha)\right)^j}{\Gamma((k+j+1)(1-\alpha)+1)} t^{j(1-\alpha)} + 1 \right).$$

Now we need to estimate $D(k,t)$ by a constant independent of t to apply the standard Gronwall Lemma, and we want to have the sum independent of k. We estimate in $D(k,t)$ the terms

$$t^{j(1-\alpha)} \leq T^{j(1-\alpha)} \quad \text{and} \quad \frac{\Gamma((k+1)(1-\alpha)+1)}{\Gamma((k+j+1)(1-\alpha)+1)} \leq 2,$$

and the kernel in the integral of (4.2) by

$$\frac{1}{(t-s)^{(n+1)\alpha-n}} \leq T^{n-(n+1)\alpha},$$

where the exponent on the right is positive with the condition on n, to obtain

$$p^{k+1}(t) \leq E T^{n-(n+1)\alpha} \int_0^t p^{k+1}(s) ds + \tilde{D}(k) t^{(k+1)(1-\alpha)},$$

with

$$\tilde{D}(k) = C_2 ||p^0(\cdot)||_T \frac{C^k \left(\Gamma(1-\alpha)\right)^{k+1}}{\Gamma((k+1)(1-\alpha)+1)} \left(2 \sum_{j=1}^{n} \left(C_1\Gamma(1-\alpha)\right)^j T^{j(1-\alpha)} + 1 \right).$$

Now we apply the standard Gronwall Lemma and obtain

$$p^{k+1}(t) \leq \tilde{D}(k) e^{ET^{(n+1)(1-\alpha)}} t^{(n+1)(1-\alpha)}.$$

Using the definition of the constant C leads to the desired result. □

LEMMA 4.3. *Suppose we have for some* $0 \leq \alpha < 1$

$$p^{k+1}(t) \leq \int_0^t \frac{e^{-\delta(t-\tau)}}{(t-\tau)^\alpha}(C_1 p^{k+1}(\tau) + C_2 p^k(\tau))d\tau$$

for some constants $C_1 \geq 0$, $C_2 > 0$, $\delta > 0$ *such that*

$$\delta^{1-\alpha} > C_1 \Gamma(1-\alpha).$$

Then

$$||p^k(\cdot)||_\infty \leq \left(\frac{C_2\Gamma(1-\alpha)}{\delta^{1-\alpha} - C_1\Gamma(1-\alpha)}\right)^k ||p^0(\cdot)||_\infty.$$

Proof. We have

$$|p^{k+1}(t)| \leq \int_0^t \frac{e^{-\delta(t-\tau)}}{(t-\tau)^\alpha} d\tau (C_1||p^{k+1}(\cdot)||_\infty + C_2||p^k(\cdot)||_\infty).$$

Applying the variable transform $z = \delta t(1 - \tau/t)$ leads to

$$\begin{aligned} |p^{k+1}(t)| &\leq \frac{1}{\delta^{1-\alpha}} \int_0^{\delta t} \frac{e^{-z}}{z^\alpha} dz (C_1||p^{k+1}(\cdot)||_\infty + C_2||p^k(\cdot)||_\infty) \\ &= \frac{1}{\delta^{1-\alpha}} \Gamma_{\delta t}(1-\alpha)(C_1||p^{k+1}(\cdot)||_\infty + C_2||p^k(\cdot)||_\infty), \end{aligned}$$

where $\Gamma_y(x)$ denotes the incomplete Gamma function,

$$\Gamma_y(x) = \int_0^y z^{x-1}e^{-z}dz.$$

Taking the limit as t goes to infinity, we obtain

$$||p^{k+1}(\cdot)||_\infty \leq \frac{\Gamma(1-\alpha)}{\delta^{1-\alpha}}(C_1||p^{k+1}(\cdot)||_\infty + C_2||p^k(\cdot)||_\infty).$$

Now using $\delta^{1-\alpha} > C_1\Gamma(1-\alpha)$, the result follows. □

4.2. Convergence Results. We consider now solution algorithms of the form (3.6) for the evolution equation (2.1). The equations for the error e^{k+1} are given by

$$\begin{aligned} \frac{de^{k+1}}{dt} + Ae^{k+1} &= \tilde{f}(u,u) - \tilde{f}(u^{k+1}, u^k), \qquad 0 < t < T, \\ e^{k+1}(0) &= 0. \end{aligned} \tag{4.3}$$

THEOREM 4.4 (Linear Convergence). *If* $\tilde{f}$ *is Lipschitz from* X_α *to* X $(0 \leq \alpha < 1)$ *in both arguments,*

$$\begin{aligned} ||\tilde{f}(u_2,v) - \tilde{f}(u_1,v)|| &\leq L_1||u_2 - u_1||_\alpha, \quad \forall u_1, u_2, v \in X_\alpha, \\ ||\tilde{f}(u,v_2) - \tilde{f}(u,v_1)|| &\leq L_2||v_2 - v_1||_\alpha, \quad \forall u, v_1, v_2 \in X_\alpha, \end{aligned} \tag{4.4}$$

for some Lipschitz constants L_1 and L_2 satisfying

$$L_1 < \frac{\delta^{1-\alpha}}{K\Gamma(1-\alpha)}, \quad L_2 < \frac{\delta^{1-\alpha}}{K\Gamma(1-\alpha)} - L_1,$$

with $K = K(\alpha)$ and δ the constants given in Lemma 4.1, then iteration (3.6) converges at least linearly on unbounded time intervals,

$$\sup_{t>0} ||e^k(t)||_\alpha \leq \gamma^k \sup_{t>0} ||e^0(t)||_\alpha,$$

with

$$\gamma = \frac{L_2 K\Gamma(1-\alpha)}{\delta^{1-\alpha} - L_1 K\Gamma(1-\alpha)} < 1.$$

REMARK 4.5. *The Lipschitz condition (4.4) is similar to the Lipschitz condition (2.2) required for a unique solution. In the case of Theorem 4.4, there are however additional constraints on the size of the Lipschitz constants to obtain linear convergence. These constraints will be removed in Theorem 4.6 for superlinear convergence.*

Proof. The solution of the error equations can formally be written as

$$e^{k+1}(t) = \int_0^t e^{-A(t-\tau)}(\tilde{f}(u(\tau), u(\tau)) - \tilde{f}(u^{k+1}(\tau), u^k(\tau)))d\tau.$$

Applying A^α on both sides and taking norms, we obtain

$$||e^{k+1}(t)||_\alpha \leq \int_0^t ||e^{-A(t-\tau)}||_\alpha ||\tilde{f}(u(\tau), u(\tau)) - \tilde{f}(u^{k+1}(\tau), u^k(\tau))||d\tau.$$

Using the Lipschitz condition on $\tilde{f}$ and Lemma 4.1, we get

$$||e^{k+1}(t)||_\alpha \leq K \int_0^t \frac{e^{-\delta(t-\tau)}}{(t-\tau)^\alpha}(L_1||e^{k+1}(\tau)||_\alpha + L_2||e^k(\tau)||_\alpha)d\tau.$$

Now denoting by $p^{k+1}(t) := ||e^k(t)||_\alpha$ and applying Lemma 4.3, the result follows. □

THEOREM 4.6 (Superlinear Convergence). *If $\tilde{f}$ is Lipschitz from X_α to X $(0 \leq \alpha < 1)$ in both arguments (4.4) with arbitrary Lipschitz constants L_1 and L_2, then iteration (3.6) converges superlinearly on bounded time intervals, $0 < t < T$, with at least the rate*

$$\sup_{0<t<T} ||e^k(t)||_\alpha \leq \frac{(C\Gamma(1-\alpha))^k}{\Gamma(k(1-\alpha)+1)} T^{k(1-\alpha)} \sup_{0<t<T} ||e^0(t)||_\alpha,$$

where the constant C is given by

$$C = KL_2 e^{\frac{(KL_1\Gamma(1-\alpha))^{n+1}}{\Gamma((n+1)(1-\alpha))}T^{(n+1)(1-\alpha)}} \left(2\sum_{j=1}^{n}(KL_1\Gamma(1-\alpha))^j T^{j(1-\alpha)} + 1\right),$$

$n = \left\lceil \frac{\alpha}{1-\alpha} \right\rceil$, *and the constant $K = K(\alpha)$ is given in Lemma 4.1.*

Proof. Proceeding as in Theorem 4.4, we get

$$||e^{k+1}(t)||_\alpha \leq K \int_0^t \frac{e^{-\delta(t-\tau)}}{(t-\tau)^\alpha}(L_1||e^{k+1}(\tau)||_\alpha + L_2||e^k(\tau)||_\alpha)d\tau.$$

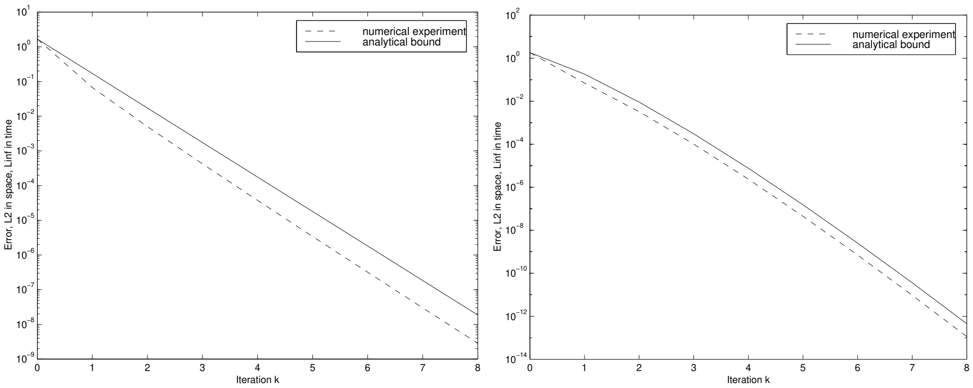

FIG. 5.1. *Linear convergence on a long time interval on the left, and superlinear convergence on a shorter time interval on the right.*

Now denoting by $p^{k+1}(t) := e^{\delta t}||e^k(t)||_\alpha$ and applying Lemma 4.2, the result follows. ☐

Note that the bound on the convergence rate is superlinear, since the Gamma function grows faster than any constant to the power k. It is also interesting to note that, while the linear convergence bound depends in an essential way on the dissipation represented by the parameter δ, the superlinear convergence bound is independent of this parameter.

5. Numerical Examples. We show two sets of numerical experiments, first a double well potential in one dimension, and then a combustion problem in two dimensions. The first problem illustrates the two different types of convergence rates the analysis predicts, and shows the dependence of the convergence rate on the splitting of the algorithm. The combustion experiment is motivated by [1], where the algorithm was used to investigate sub-critical and super-critical solutions.

5.1. Double Well Potential Model Problem. The double well potential model problem we consider is

$$\frac{\partial u}{\partial t} - \frac{\partial^2 u}{\partial x^2} = C(u - u^3), \qquad 0 < x < 1,\ 0 < t < T,$$

with a given initial condition, and homogeneous boundary conditions. First we investigate the special case of the Picard iteration, where all the arguments of the nonlinear function are relaxed,

$$\frac{\partial u^{k+1}}{\partial t} - \frac{\partial^2 u^{k+1}}{\partial x^2} = C(u^k - (u^k)^3), \qquad 0 < x < 1,\ 0 < t < T,$$

and thus all the subproblems to be solved are linear and decoupled. This illustrates the two different convergence behaviors of the algorithm.

We solve the equation by discretizing in space by centered finite differences on a grid with 100 nodes, and integrate in time using backward Euler and 300 time steps. We set $C = 1$, and use as initial condition $u(x, 0) = x(1 - x)$. In a first experiment, we choose a long time interval, $T = 3$, where we expect the algorithm to be in the linear convergence regime. We start the iteration with a constant initial guess $u^0 = 0$. Figure 5.1 on the left shows how the algorithm converges linearly. The error is measured throughout this section in the discrete L^2 norm in space (including the mesh parameter and thus corresponding to the continuous L^2 norm), and in the L^∞ norm in time. By error we always denote the difference

	Error, L^2 in space and L^∞ in time			
k	$m_1 = 1$	$m_1 = 2$	$m_1 = 3$	$m_1 = 5$
0	1.7726e-02	1.7726e-02	1.7726e-02	1.7726e-02
1	1.7485e-06	1.7485e-06	4.5537e-08	3.8604e-09
2	1.7471e-09	1.7471e-09	1.2516e-11	4.4270e-13
3	4.0306e-13	4.0306e-13	1.7345e-15	4.0523e-17

TABLE 5.1

Dependence of the convergence of the frequency decomposition for the double well potential on the splitting parameter m_1.

between the converged solution and the iterates. The solid line depicts the convergence rate according to Theorem 4.4 with $K = 1$ and $\delta = \pi^2$, the first eigenvalue of the operator under consideration. The dashed line shows the measured convergence rate in the numerical simulation. Note how the convergence rate agrees quite well with the predicted rate.

To observe superlinear convergence, we reduce the time interval to $T = 1/10$ and use again the initial guess $u^0 = 0$ to start the iteration. Figure 5.1 shows on the right how the algorithm converges superlinearly. As before, the error is measured in the discrete L^2 norm in space and in the L^∞ norm in time, and the solid line depicts the convergence rate according to Theorem 4.6 and the dashed line the measured convergence rate in the numerical simulation. Note how the convergence rate becomes better as the iteration progresses. The superlinear rate is predicted quite well by the theoretical bound.

Next, we consider a frequency decomposition for the discretized spatial operator. We choose two subspaces, the first one span by the first m_1 eigenfunctions, and the second one by the remaining eigenfunctions, thus obtaining a splitting without overlap. Note that the fast Fourier transform is the ideal tool for the frequency decomposition on a discretized operator, where geometry permits. We use the same numerical method as for the first experiment with $T = 1$. Table 5.1 shows the dependence of the convergence rate on the splitting parameter m_1. First note that the first and the second column show the same convergence rate, it does not matter if the second frequency is in the first or second subspace. This is due to the symmetry in the problem: the second frequency is irrelevant for the solution and thus also for the algorithm. This is also the case for all the other even frequencies, and they are thus not considered in the computation in Table 5.1. Second note the fast convergence, which indicates a weak coupling through the nonlinearity $u - u^3$. The convergence rate increases when more of the low frequencies are included in the first subspace. Finally, we computed how much of the solution is contained in the low frequencies in the above experiment. The first subspace with one frequency only, $m_1 = 1$, contains after the first iteration 97% of the solution. With two frequencies, the first and the third one, $m_1 = 3$, the first subspace contains after one iteration 99.5% of the solution, and with three frequencies 99.9%. This motivates the qualitative study of the behavior of nonlinear problems using a low dimensional frequency subspace, as it was done in [22] and [1].

5.2. Combustion Model Problem. Combustion problems have the inherent property that a small change in a parameter or in the initial data can change the solution drastically: either it explodes or it does not [20]. It can be very difficult to trace such a sensitive path in the non-linear solution process with many variables arising from the spatial discretization. It was therefore proposed in [22] to analyze each frequency separately, one at a time. For one frequency at a time, the nonlinear problem is one dimensional and can always be solved safely, sometimes even analytically. An iteration of the type presented here then leads to the global solution, if desired.

	Error, L^2 in space and L^∞ in time			
k	$m_1 = 1$	$m_1 = 5$	$m_1 = 6$	$m_1 = 11$
0	1.7279e-01	1.7279e-01	1.7279e-01	1.7279e-01
1	5.0731e-03	1.0854e-03	1.0854e-03	5.3048e-04
2	9.2856e-04	7.4087e-05	7.4082e-05	1.5452e-05
3	8.7745e-05	3.7472e-06	3.7471e-06	8.6243e-07
4	1.6778e-05	2.4962e-07	2.4961e-07	2.8455e-08
5	1.5979e-06	1.3166e-08	1.3165e-08	1.5902e-09

TABLE 5.2

Dependence of the convergence of the frequency decomposition for the combustion problem on the splitting parameter m_1 in the sub-critical case.

We analyze here the combustion problem

$$\frac{\partial u}{\partial t} - \Delta u = Ce^{\frac{\alpha u}{\alpha + u}}, \qquad 0 < x, y < 1,\ 0 < t < T,$$

with homogeneous boundary conditions and a given initial condition $u(x, y, 0)$. It is well known that for large values of α solutions grow to order e^α; they are called super-critical. For small values of α, solutions stay order one and are called sub-critical. In between at some point, a sudden change takes place. A similar dependence can also be shown for the initial data.

An experiment working directly with the continuous, normalized eigenfunctions associated with the linear spatial part,

$$\phi_{i,j} = 2\sin(i\pi x)\sin(j\pi y), \quad i, j = 1, 2, \ldots$$

is performed in the thesis [1], to trace the evolution of each mode separately. A clear separation between sub-critical and super-critical solutions depending on the initial data was obtained considering the first eigenmode only.

Here, we work with the discretized spatial operator and the associated eigenfunctions. We use as initial condition $u(x, y, 0) = 100xy(1-x)(1-y)$, and set the constant $C = 1$. We discretize uniformly in space using finite differences on an 11×11 spatial grid, and integrate in time using Backward Euler with 20 time steps. We use again a spectral decomposition with the first m_1 modes in the first subspace and with the remaining ones in the second subspace. Table 5.2 shows the convergence for various sizes of the first spectral subspace for $\alpha = 34$ in the sub-critical case, where again we denote by error the difference between the converged solution and the iterates. Note again that not all frequencies contribute to the solution. By symmetry we can exclude all the eigenmodes with an even component in either the x or the y direction or both. Therefore, the table only shows convergence rates for $m_1 = 1$, where the mode 1-1 is the only mode in the first subspace, then for $m_1 = 5$, where the mode 1-3 is added to the first subspace, for $m_1 = 6$, where the mode 3-1 is added, and finally $m_1 = 11$, when the mode 3-3 is added. Note that splitting the two modes 1-3 and 3-1 between the two subspaces leaves the convergence rate practically like having both modes in the first subspace.

Similarly to the case of the double well potential, adding more and more of the low modes to the first subspace enhances the performance of the frequency decomposition algorithm. Again the solution is dominated by the low modes. After one iteration with only the lowest mode in the first subspace, the approximation in that subspace contains already 98% of the solution, while when keeping the three lowest modes, after one iteration 99.2% of the solution are confined to the first subspace. Note however that the convergence is slower than

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Error, L^2 in space and L^∞ in time						
	lower resolution			higher resolution		
k	$m_1 = 1$	$m_1 = 6$	$m_1 = 11$	$m_1 = 1$	$m_1 = 6$	$m_1 = 11$
0	3.2515e-01	3.2515e-01	3.2515e-01	1.5395e-01	1.5395e-01	1.5395e-01
1	3.2095e-02	1.0777e-02	6.6680e-03	1.4512e-02	4.7042e-03	2.8117e-03
2	9.9649e-03	3.7754e-03	2.0804e-03	4.3384e-03	1.5362e-03	7.9829e-04
3	2.3353e-03	6.9933e-04	3.3455e-04	9.2008e-04	2.6130e-04	1.1908e-04
4	4.6069e-04	1.4275e-04	6.1936e-05	1.6445e-04	4.7106e-05	1.9287e-05
5	7.1504e-05	1.9062e-05	7.4141e-06	2.2138e-05	5.5585e-06	2.0696e-06

TABLE 5.3

Dependence of the convergence of the frequency decomposition for the combustion problem on the splitting parameter m_1 in the super-critical case, for two different resolutions in the discretization.

for the double well potential, which indicates a stronger coupling of the frequencies by this nonlinearity.

Finally, Table 5.3 shows the convergence of the algorithm in the super-critical case $\alpha = 35$. Here we were required to shorten the time interval to $T = 0.01$ in accordance with Theorem 4.6 to achieve convergence. Note that higher frequencies are becoming more important in the super-critical case: if the first subspace contains one frequency only, $m_1 = 1$, after the first iteration only 92% of the solution is contained in this subspace, compared to 98% in the sub-critical case. In Table 5.3, we also show a second numerical experiment on a refined grid, both in space and in time the number of grid points were doubled. The numerical results show that this has only little influence on the convergence behavior of the method.

6. Conclusion. We have analyzed a generalized version of the nonlinear eigenfunction expansion algorithm proposed in [22] to explore the behavior of solutions of nonlinear evolution equations. This algorithm has two main interests: the first one is that the solution of a large system of nonlinear equations at each time step is reduced to solutions of many independent scalar nonlinear problems, for which fail-safe algorithms are available. Second, the algorithm permits to explore individual frequency subspaces separately to investigate in a numerically sound way rapid changes occurring typically in nonlinear problems of combustion type. A third advantage, which should not be neglected, is the parallelism of this algorithm, when a full solution of the problem is desired.

We showed that the generalized version of the frequency decomposition algorithm converges under a strong Lipschitz condition on unbounded time intervals and therefore also for the steady state. On bounded time intervals, convergence was proved under a Lipschitz condition controled by the length of the time interval. Hence by shortening the time interval, the algorithm can always be made to converge. In this case, the technique of time windowing often used in waveform relaxation can be useful: one decomposes the time interval of interest $[0, T]$ into smaller time windows, and uses the algorithm sequentially on the small time windows where rapid convergence occurs.

More needs to be understood for the frequency decomposition algorithm, in particular the question of how to choose the subspaces. The present convergence analysis does not reveal this dependence because of the general Lipschitz conditions used. But the numerical experiments suggest that if there is a way of a priory knowing which frequencies are relevant as the solution evolves, those should be put into one subspace.

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