

NEWTON-KRYLOV SOLVERS FOR TIME-STEPPERS *

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Abstract.

We study how the Newton-GMRES iteration can enable dynamic simulators (time-steppers) to perform fixed-point and path-following computations. For a class of dissipative problems, whose dynamics are characterized by a slow manifold, the Jacobian matrices in such computations are compact perturbations of the identity. We examine the number of GMRES iterations required for each nonlinear iteration as a function of the dimension of the slow subspace and the time-stepper reporting horizon. In a path-following computation, only a small number (one or two) of additional GMRES iterations is required.

Key words. Coarse time-steppers, GMRES, Newton-GMRES iteration

AMS subject classifications. 65F10, 65H10, 65H17, 65H20, 65L05,

1. Introduction. In studying the dynamic behavior of evolution equations,

$$(1.1) \quad du/dt = f(u; \lambda),$$

a computational modeler typically chooses between two paths: the first is developing a dynamic simulator for the process; the second is developing algorithms to locate particular features of the long-term dynamics of the process, such as steady states or limit cycles. The first path typically gives rise to initial value problems, and the corresponding codes are dynamic simulators - we will call them “time-steppers” since, given the state of the system at a moment in time they produce (an approximation of) the state of the system at a later moment. The second path typically gives rise to fixed point algorithms for solving coupled nonlinear algebraic equations; these may be the steady state equations themselves, or an augmented set arising in a continuation/bifurcation context. The Recursive Projection Method of Shroff and Keller [23] (see also the Adaptive Condensation of Jarausch and Mackens [12, 13] for symmetric problems) is an example of an algorithm that, in some sense, connects the two paths. The main idea is to construct a computational superstructure that designs and combines several calls to an existing (“legacy”) time-stepper, effectively turning it into a fixed point solver for

$$u - \Phi_T(u; \lambda) = 0,$$

where Φ_T is the result of integration of (1.1) with initial condition u for time T (see the review of Tuckerman and Barkley [29]). Here the action of the linearization of the time-stepper is estimated in a matrix-free fashion by the integration of appropriately chosen nearby initial conditions.

Over the last few years, this matrix-free computational enabling technology has found new applications in the field of multiscale computations. In current modelling

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practice, dynamic models are often constructed at a microscopic/stochastic level of description (e.g. molecular dynamics, kinetic Monte Carlo or Lattice Boltzmann codes); the closure required to obtain explicit, macroscopic “effective” equations is not available in closed form. Algorithms like RPM can then be “wrapped around” appropriately initialized ensembles of short bursts of microscopic simulations, and solve the effective equation without ever obtaining it in closed form. Several examples of such “coarse equation-free” computation have now been explored, and the mathematical underpinnings of the approach are being extensively studied [9, 19, 25, 27].

In this paper we study the Newton-GMRES iteration as a computational “wrapper” around a legacy time-stepper. This wrapper enables the computation and continuation of fixed points of the time- T map of the time-stepper (*i.e.* steady states of the corresponding dynamical equations). It is useful, for purposes of discussion, to consider that the time-stepper is available as an input-output black box (an executable) which cannot be modified.

The paper is organized as follows: We first review certain properties of GMRES in the context of problems whose linearization is a compact perturbation of the identity. We argue that time-steppers for a class of dissipative problems, whose long-term dynamics lie on a low-dimensional, slow manifold, may fit this description; we then proceed to examine Newton-GMRES convergence and number of iterations for fixed point computation of such time-steppers in a continuation context. Our numerical examples are the Chandrasekhar H-equation [5] and the time-stepper of a discretization of a reaction-diffusion problem known to possess a low-dimensional inertial manifold [8, 26]. We illustrate the effect, on the GMRES iterations, of the time-stepper reporting horizon both for fixed point and for pseudo-arclength continuation computations. We conclude with a brief discussion and thoughts about extensions of this approach.

2. Convergence Analysis.

2.1. GMRES Preliminaries. We will use Newton-GMRES to solve the nonlinear fixed point equation

$$(2.1) \quad u - \Phi_T(u; \lambda) \equiv F(u) = 0.$$

In what follows we will work in R^N and use the usual Euclidean norm; the idea is that equation (2.1) arises from integrating a set of ODEs, possibly from the discretization of a partial differential equation on a given mesh. We will also assume (and the consequences of this will become apparent below) that the long-term dynamics of the discretized PDE occur on an attracting “slow manifold” of low dimension $p \ll N$; p will be assumed independent of mesh refinement (*i.e.* it will remain constant as N increases.)

GMRES is an iterative method for solving linear systems $Ax = b$ in R^N . The k th GMRES iteration minimizes the residual r over $x_0 + \mathcal{K}_k$, where x_0 is the initial iterate and \mathcal{K}_k is the k th Krylov subspace

$$\mathcal{K}_k = \text{span}\{r_0, Ar_0, \dots, A^{k-1}r_0\}.$$

A consequence [15, 22] of the minimization is that

$$(2.2) \quad \|r_k\| = \min_{p \in \mathcal{P}_k} \|p(A)r_0\|$$

where \mathcal{P}_k is the space of k th degree residual polynomials, *i.e.* polynomials of degree k such that $p(0) = 1$.

We will apply (2.2) to a special class of problems where

$$(2.3) \quad A = I - K + E.$$

In (2.3)

- $I - K$ is nonsingular,
- $K = P_D K P_D$, where P_D is an orthogonal projection onto a space D of dimension $p \ll N$, and
- E is a matrix with small norm.

We will analyze the performance of GMRES in a way different from the eigenvalue-based approach used for diagonalizable matrices [10, 15, 18, 28]. For the class of problems of interest here, we can prove a convergence result directly using methods similar to those in [3, 4, 7, 17]. The result in this paper has stronger and sharper convergence rates. This result carries through in the infinite-dimensional case also, using the L^2 norm for the corresponding function spaces.

THEOREM 2.1. *Let A be given by (2.3). Then there exists C such that for all $m \geq 1$,*

$$(2.4) \quad \|r_{m(p+1)}\| \leq C^m \|E\|^m.$$

Proof. Let p_C be the characteristic polynomial of $I - K$. Since D has dimension p , p_C has degree $p + 1$. Clearly

$$p_C(A) = p_C(I - K) + \Delta = \Delta.$$

by the Cayley-Hamilton theorem. Moreover, there is $C > 0$ such that

$$\|\Delta\| \leq C\|E\|.$$

In fact, if

$$p(z) = 1 + \sum_{k=1}^{p+1} \gamma_k z^k$$

then we may use

$$C = \sum_{k=1}^{p+1} k |\gamma_k| \|I - P_D K P_D\|^{k-1} + O(\|E\|^2).$$

Hence

$$\|p(A)\| \leq C\|E\|.$$

This is (2.4) for $m = 1$.

Define

$$p(z) = p_C(z)/p_C(0).$$

Clearly $p \in \mathcal{P}_{p+1}$. Hence, by (2.2)

$$(2.5) \quad \|r_{m(p+1)}\| \leq \|p^m(A)r_0\| \leq C^m \|E\|^m \|r_0\|,$$

as asserted. \square

The estimate in (2.5) does not depend on the eigenvalues of A , nor is there any requirement that A be normal or even diagonalizable.

As is standard, a GMRES iteration is terminated when

$$\|r_k\| \leq \eta \|r_0\|,$$

where η is an user-defined parameter. In the context of this paper $\|E\|$ is well below the termination tolerance τ , so we conclude that the iteration will terminate in at most $p + 1$ iterations. In the general case, of course, more cycles could be required.

2.2. Time-Steppers and Steady State Solutions. Let $\Phi(u)$ denote the output of the time-stepper with time step T and initial data u ; we have dropped the subscript T of Φ for convenience. We seek to solve

$$(2.6) \quad F(u) \equiv u - \Phi(u) = 0,$$

to find a steady state solution. Consider the structure of the eigenvalues $\mu_i = \exp(\sigma_i T)$ of Φ_u given the structure of the eigenvalues σ_i of the linearization of the original problem. We assume that there exists a significant gap between a few σ_i close to zero (p of them, to be exact) and the remaining large negative σ_j . The p small norm σ_i do not have to be stable - they can also be slightly unstable, so that the corresponding μ_i are close to the unit circle.

We then assume that T is large enough so that there is a space D of low dimension p , so that

$$\Phi(u) = P_D \Phi(P_D u) + E(u)$$

and E and its Jacobian E_u are small. For a problem where some of the p small σ_i are unstable, this large time T should not be so large that the unstable modes will cause the trajectory to move significantly away from the fixed point. In such cases the proper choice of T is a somewhat delicate matter [19, 23].

The equation for the Newton step from a current iterate u_c is

$$(2.7) \quad F_u(u_c)s = s - \Phi_u(u_c)s = -F(u_c),$$

here F_u and Φ_u are the Jacobians of F and Φ .

A Newton-GMRES [1, 2, 15] method solves (2.7) with GMRES, terminating the linear (or inner) iteration when

$$\|F_u(u_c)s\| \leq \eta_c \|F(u_c)\|$$

where η_c may be changed as the outer (or nonlinear) iteration progresses [6, 15, 16]. For the application here, we assume that $\|E'(u)\|$ is much less than any choice of η we make during the iteration.

The linear system (2.7) fits exactly in to the paradigm of § 2.1 with $K = P_D \Phi_u(P_D u) P_D$ and $E = E_u(u)$. Hence we conclude that a GMRES iteration for (2.7) will take at most $p + 1$ iterations to drive the residual to $O(\|E\|)$.

2.3. Time-Steppers and Continuation. In a continuation context Φ depends on a parameter λ . As is standard [14] we add an additional arclength parameter s to obtain the augmented system

$$(2.8) \quad G(u, \lambda, s) = \begin{pmatrix} F(u(s), \lambda(s)) \\ \dot{u}^T(u - u_0) + \dot{\lambda}(\lambda - \lambda_0) - (s - s_0) \end{pmatrix}.$$

In (2.8), \dot{u} and $\dot{\lambda}$ are approximations to du/ds and $d\lambda/ds$, which can be obtained in several ways [14]. In the calculations reported in § 3 we used the estimate of the slope given by the last two points, (u_0, λ_0) and (u_{-1}, λ_{-1}) computed on the branch.

G is defined on R^{N+1} and

$$G_{u,\lambda}(u, \lambda) = \begin{pmatrix} F_u & F_\lambda \\ \dot{u}^T & \dot{\lambda} \end{pmatrix},$$

We seek to show that G' also fits into our paradigm, with p replaced by at most $p+2$. Hence, at most two additional linear iterations will be needed for each Newton iteration of the augmented system.

We use (2.6) to obtain

$$G_{u,\lambda} = \begin{pmatrix} I - P_D \Phi_u(P_D u; \lambda) P_D & -P_D \Phi_\lambda \\ \dot{u}^T & \dot{\lambda} \end{pmatrix} + \begin{pmatrix} -E_u & -E_\lambda \\ 0 & 0 \end{pmatrix}.$$

Let

$$\mathcal{A} = \begin{pmatrix} I & 0 \\ 0 & 1 \end{pmatrix} - \mathcal{K} + \mathcal{E}$$

where,

$$\mathcal{K} = \begin{pmatrix} P_D \Phi_u P_D & P_D \Phi_\lambda \\ -\dot{u}^T & 1 - \dot{\lambda} \end{pmatrix},$$

and

$$\mathcal{E} = \begin{pmatrix} -E_u & -E_\lambda \\ 0 & 0 \end{pmatrix}.$$

This fits the paradigm of § 2.1. To see that, let

$$\mathcal{D} = \text{span} \left(\begin{pmatrix} D \\ 0 \end{pmatrix}, \begin{pmatrix} \dot{u} \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 1 \end{pmatrix} \right) \subset R^{N+1},$$

Clearly the range of \mathcal{K}

$$R(\mathcal{K}) = \text{span} \left(\begin{pmatrix} D \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 1 \end{pmatrix} \right) \subset \mathcal{D}.$$

To apply the results from the previous section, however, we need $\mathcal{K} = P_{\mathcal{D}} \mathcal{K} P_{\mathcal{D}}$, where $P_{\mathcal{D}}$ is the orthogonal projector onto \mathcal{D} . This is why the extra dimension $(\dot{u}, 0)^T$ is required.

To see this, let $y = (u, \mu) \in R^{N+1}$ be orthogonal to \mathcal{D} . This means that $y = (\omega, 0)$, where ω is orthogonal to both D and \dot{u} . Clearly

$$\mathcal{K}y = \begin{pmatrix} P_D \Phi_u P_D \omega \\ -\dot{u}^T \omega \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix},$$

so $\mathcal{K}(I - P_{\mathcal{D}}) = 0$. Since $R(\mathcal{K}) \subset \mathcal{D}$, we have $P_{\mathcal{D}} \mathcal{K} = \mathcal{K}$. Summarizing

$$\mathcal{K} = P_{\mathcal{D}} \mathcal{K} P_{\mathcal{D}}$$

and

$$\dim(\mathcal{D}) \leq p + 2.$$

The dimension of \mathcal{D} can be taken $p + 1$ if \dot{u} is nearly in the range of P_D , *i. e.*

$$(2.9) \quad \|(I - P_D)\dot{u}\| = O(\|E_u\| + \|E_\lambda\|).$$

In this case, we can let

$$\mathcal{D} = \text{span} \left(\left(\begin{array}{c} D \\ 0 \end{array} \right), \left(\begin{array}{c} 0 \\ 1 \end{array} \right) \right) \subset R^{N+1},$$

$$\mathcal{K} = \left(\begin{array}{cc} P_D \Phi_u P_D & P_D \Phi_\lambda \\ -(P_D \dot{u})^T & 1 - \dot{\lambda} \end{array} \right),$$

and

$$\mathcal{E} = \left(\begin{array}{cc} -E_u & -E_\lambda \\ ((I - P_D)\dot{u})^T & 0 \end{array} \right).$$

If F_u is well conditioned and $|\dot{\lambda}|$ and $\|F_\lambda\|$ are not too large, then (2.9) holds. To see this we differentiate $F = 0$ and obtain

$$F_u \dot{u} + F_\lambda \dot{\lambda} = 0,$$

which implies, if F_u is nonsingular, that

$$(2.10) \quad \dot{u} = -F_u^{-1} F_\lambda \dot{\lambda}.$$

Our assumptions are that $\|E_u\|$ and $\|E_\lambda\|$ are much smaller than $\|F_u\|$ and $\|F_\lambda\|$. Hence, if F_u is well conditioned, the Banach lemma implies that

$$F_u^{-1} = (I - P_D \Phi_u P_D)^{-1} + O(\|E_u\|).$$

Moreover,

$$F_\lambda = -P_D \Phi_\lambda + O(\|E_\lambda\|).$$

We incorporate this into (2.10) to obtain

$$(2.11) \quad \dot{u} = (I - P_D \Phi_u P_D)^{-1} P_D \Phi_\lambda \dot{\lambda} + O\left(|\dot{\lambda}|(\|E_u\| \|F_\lambda\| + \|E_\lambda\|)\right),$$

which implies (2.9) if $|\dot{\lambda}|$ and $\|F_\lambda\|$ are $O(1)$.

Summarizing, if $\|E_u\|$ and $\|E_\lambda\|$ are much smaller than $\|F_u\|$ and $\|F_\lambda\|$ respectively, $|\dot{\lambda}|$ and $\|F_\lambda\|$ are $O(1)$, and if F_u is well conditioned, then (2.9) holds. Near folds and bifurcations, F_u is singular, and in those cases we may need to require that the dimension of \mathcal{D} be $p + 2$.

3. Numerical Results. All the computations were done using MATLAB version 6.0 Release 12 on a PC with a Pentium4 2.53GHz CPU.

3.1. The H-equation. As a first example, we solved a problem which does not arise in a time-stepper context, but for which the Jacobian fits our paradigm [21]. The solution and continuation problem for a 100-node midpoint rule discretization of the Chandrasekhar H-equation

$$F(x)_i = x_i - \left(1 - \frac{c}{2N} \sum_{j=1}^N \frac{\mu_i x_j}{\mu_i + \mu_j} \right)^{-1}$$

were obtained with a Newton-GMRES solver `nsoli` from [16]. We set the relative and absolute tolerances in the solver to 10^{-12} .

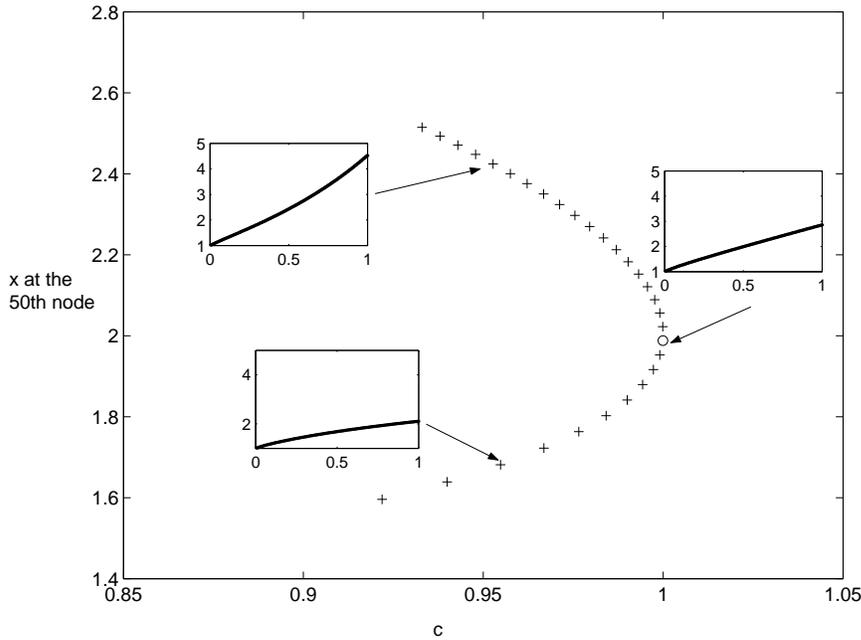


FIG. 3.1. *Bifurcation diagram of the H-equation for c close to 1. The parameter c is equal to 0.9999179 at the point marked by a circle.*

Figure. 3.1 is a bifurcation diagram with respect to the parameter c , showing a turning point at $c = 1$. For all values of c shown in this continuation, the eigenvalues of the linearization of the solution are close to 1; only a single one of them changes in marked way, ranging from -0.9 on the upper branch through zero at the turning point to 0.5 on the lower branch.

Figure. 3.2 shows the GMRES performance for a representative value of c (0.9999179), close to the turning point, marked by a circle in Figure 3.1. We report on computations from the continuation itself, where the initial iterate was the standard linear predictor, and from a second stand-alone computation where the initial iterate was the solution plus a perturbation function $0.05 \sin(x)$. In Figure 3.2 we plot the convergence history for Newton-GMRES in the two cases. The convergence rates and the costs of the solves are roughly the same.

The first column of Table. 3.1 shows the ten eigenvalues farthest from 1 for the linearization of each of the two problems. In the continuation case, there is one more

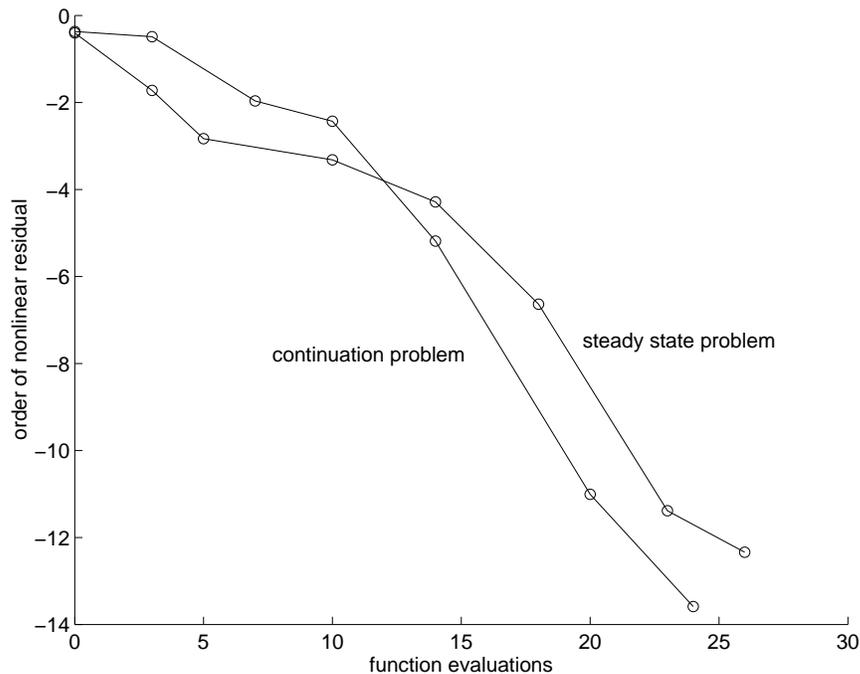


FIG. 3.2. Convergence plot for the steady state and continuation problem of H -equation

eigenvalue far away from 1 than in the stand-alone case. In both cases the linearization clearly fits the pattern of a compact perturbation of the identity.

Eigenvalues of steady state problem	Eigenvalues of continuation problem
0.0207265	-5.2022448
0.9424114	5.2008250
0.9900391	0.9746094
0.9974043	0.9828252
0.9992541	0.9977360
0.9998164	0.9991859
0.9999612	0.9998098
0.9999926	0.9999577
0.9999987	0.9999919
0.9999998	0.9999985

TABLE 3.1

Eigenvalues for the linearized steady state and continuation problems of the H -equation at $c = 0.9999179$

3.2. The Chafee-Infante reaction diffusion problem. We then solved the steady state and continuation problems for a discretization of a dissipative reaction-diffusion PDE in one dimension, the so-called Chafee-Infante problem,

$$u_t - \frac{1}{\lambda} u_{xx} + u^3 - u = 0, x \in [0, \pi]$$

with boundary conditions $u(0, t) = 0, u(\pi, t) = 0$. We used 201 finite difference discretization points.

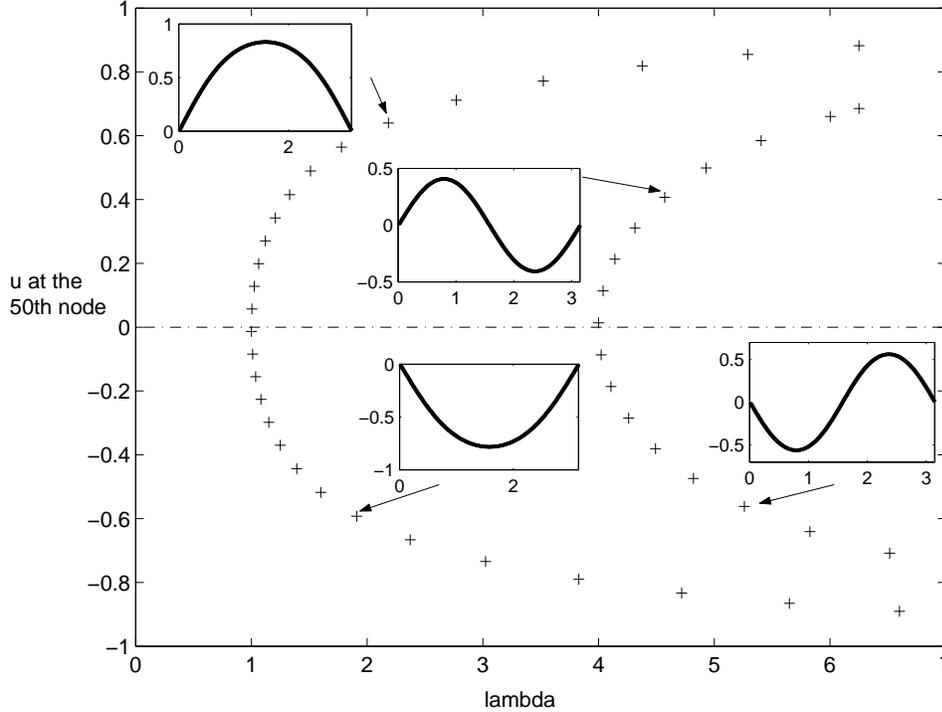


FIG. 3.3. *Bifurcation diagram for the Chafee-Infante reaction diffusion problem.*

Figure. 3.3 shows the bifurcation diagram for this problem for a range of parameter values ($0 < \lambda < 7$) where up to five different spatially structured steady states exist. Our computational tests were performed on the upper stable solution branch close to $\lambda = 2$. In this example we studied both the steady state problem (setting the right-hand-side of the finite difference equations equal to zero) and the time-stepper formulation (our integration routine was ode15s). The steady state (equations) / fixed point (time-stepper) and continuation problems were solved with Newton-GMRES solver *nsoli* for various time reporting horizons. The results for $\lambda = 2.1386697$ are shown in Fig. 3.4. Relative and absolute tolerances were chosen to be 10^{-12} . The initial guess for the direct solution was chosen to be the true solution plus a perturbation function $0.1 \sin(x)$.

One thing should be made clear at this point. Using several time steps of an implicit integrator, with the concomitant nonlinear solves, is clearly not an efficient way of solving a fixed point problem (a single nonlinear solve). The integrator is used here as a “legacy code”, a code that one cannot modify. It is in the context of such legacy codes that our approach becomes useful, as well as in the case of multiscale computations, where the time evolution is performed by a simulator at a different level of description (e.g. Lattice-Boltzmann or kinetic Monte Carlo).

3.3. Clustering of Eigenvalues. Using the Finite Difference Method, the ODE system from discretizing the original PDE has a form of $\dot{u}(t) = f(u), u \in R^n$. At a steady state u^* , the matrix f_u has n eigenvalues: $\sigma_i, i = 1, \dots, n$. If we solve for u^*

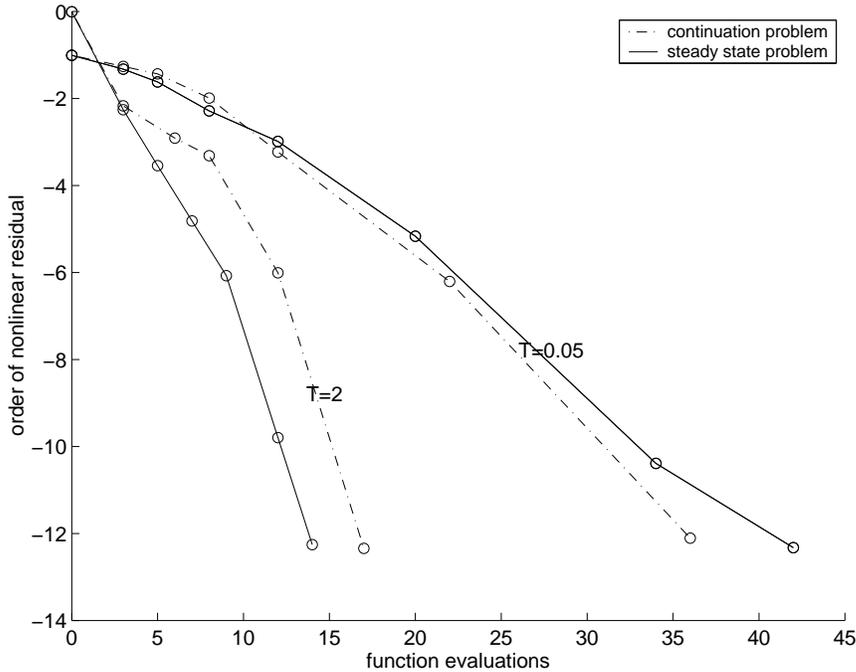


FIG. 3.4. Convergence of time-stepper based fixed point computation for the steady state and the continuation of the discretized RD problem. Every circle corresponds to a Newton step. A single “function evaluation” consists of integration over one time reporting horizon.

with a time-stepper, the system to be solved is $u(0) - \Phi_T(u; \lambda) = 0$, which also has n eigenvalues: $1 - e^{\sigma_i T}$, $i = 1, \dots, n$.

We have used the forward in time time-stepper to compute both stable and unstable steady states. We have marked the unstable steady state we computed using a reporting horizon of $T = 0.1$ for $\lambda = 4.5710239$ using forward in time time-stepping. When the parameter λ is equal to 2.183867, u^* is a stable steady state and all the eigenvalues are negative. When we increase T , all the eigenvalues $1 - e^{\sigma_i T}$ are approaching (“clustering at”) 1. Clustering of eigenvalues is known to be beneficial for GMRES performance. Conversely, when we decrease T , eigenvalues start leaving the cluster. This results in additional GMRES iterations.

To quantify the dependence of the performance of the iteration on T we use the number of GMRES iterations at the final step in Figure 3.5. When T is large, we consistently see 2 linear iterations. As T is reduced, we see an increase in GMRES iterations, as expected. In this particular example, when $T = 1.78$, the number of GMRES iterations increases to 3.

In an attempt to quantify this further we identify a “cluster” of eigenvalues that seems to be correlated with the performance of the GMRES iteration. In Fig. 3.6, we treat those eigenvalues in the interval $[0.84, 1]$ as “in the cluster”. The number of eigenvalues outside the cluster (or smaller than 0.84) and the number of function evaluations needed to finish the last Newton step are compared in Tab. 3.2 below. A clear, strong correlation emerges.

3.4. Conclusion. We have extended and sharpened results for the performance of GMRES for discretizations of compact fixed point problems to the special class

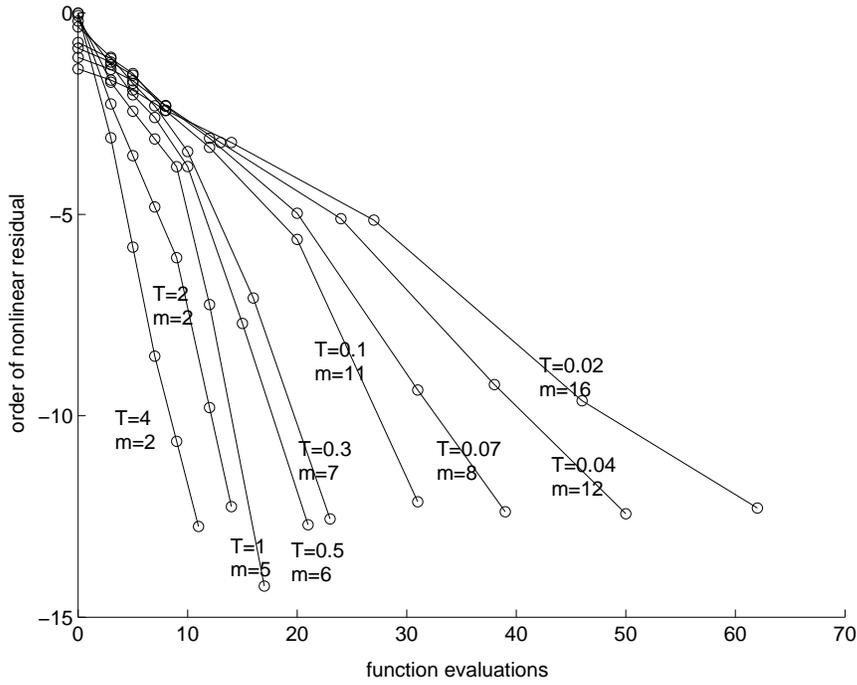


FIG. 3.5. Convergence of time-stepper based fixed point Newton-GMRES computation for different time reporting horizons. Every circle corresponds to a Newton step, and m is the number of function evaluations for the last Newton step.

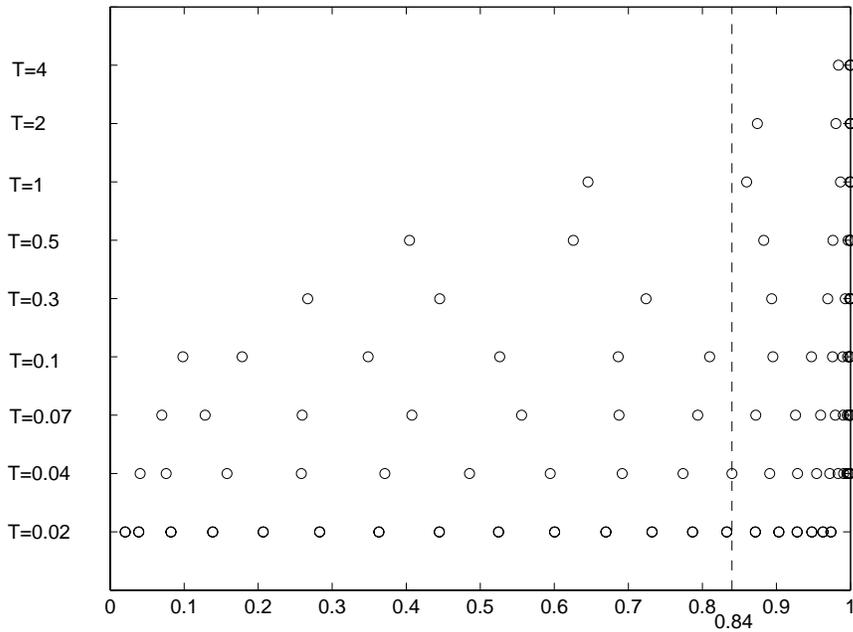


FIG. 3.6. Twenty smallest eigenvalues of the linearized time-stepper at the steady state for different time reporting horizons; the dashed line corresponds to the eigenvalue that first leaves the cluster when $T = 1.78$.

T	4	2	1	0.5	0.3	0.1	0.07	0.04	0.02
Number of eigenvalues outside the cluster	0	0	1(2)*	2	3	6	7	10	14
Function evaluations needed for clustering eigenvalues	2	2	2	2	2	2	2	2	2
Actual total function evaluations	2	2	5	6	7	11	8	12	16

TABLE 3.2

of problems that arise in a time-stepper context. The key feature leading to the enhancement of GMRES performance is the compactification of the spectrum. In previous work, a Green’s function based reformulation of the steady state problem for elliptic PDEs [7] led to a linearization that was a compact perturbation of the identity, and an efficient solution via Newton-GMRES. Time-steppers compactify the spectrum of the linearization in a natural way, and their properties can be exploited to obtain accurate bounds on the convergence rates of the linear iterations in a Newton-GMRES continuation. We show that the additional equation in a pseudo-arclength formulation of a parameter-dependent family of nonlinear equations adds at most two GMRES iterations when the eigenvalues are well separated, and obtain a bound on the convergence in terms of the separation of the spectrum and the dimension of the slow subspace (associated with a slow/inertial manifold for the dynamics).

We reported on numerical results that support the theory, first with an integral equation, for which we can numerically demonstrate that all but two of the eigenvalues of the linearization lie in a tight cluster about 1. The second example was a parametric study of the steady state of a discretized parabolic partial differential equation implemented through time-steppers.

The “natural” compactification of the spectrum using time-steppers provides a natural connection with the performance of matrix-free iterative methods. This compactification may prove useful in writing computational wrappers, that will accelerate the convergence of legacy dynamic simulators to stationary states. We also expect this compactification to assist in writing computational wrappers that will assist dynamic simulators at a different level of model description (e.g. kinetic Monte Carlo, Brownian Dynamics or Molecular Dynamics codes [11, 20, 24]) to locate stationary states and perform continuation/bifurcation analysis of macroscopic system observables in the so-called equation-free framework [19].

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