

Preface

This book summarizes and highlights progress in our understanding of Dynamical Systems during six years of the German Priority Research Program “Ergodic Theory, Analysis, and Efficient Simulation of Dynamical Systems”. The program was funded by the Deutsche Forschungsgemeinschaft (DFG) and aimed at combining, focussing, and enhancing research efforts of active groups in the field by cooperation on a federal level. The surveys in the book are addressed to experts and non-experts in the mathematical community alike. In addition they intend to convey the significance of the results for applications far into the neighboring disciplines of Science.

Three fundamental topics in Dynamical Systems are at the core of our research effort:

- behavior for large time
- dimension
- measure, and chaos

Each of these topics is, of course, a highly complex problem area in itself and does not fit naturally into the deplorably traditional confines of any of the disciplines of ergodic theory, analysis, or numerical analysis alone. The necessity of mathematical cooperation between these three disciplines is quite obvious when facing the formidable task of establishing a bidirectional transfer which bridges the gap between deep, detailed theoretical insight and relevant, specific applications. Both analysis and numerical analysis play a key role when it comes to building that bridge. Some steps of our joint bridging efforts are collected in this volume.

Neither our approach nor the presentations in this volume are monolithic. Rather, like composite materials, the contributions are gaining strength and versatility through the broad variety of interwoven concepts and mathematical methodologies which they span.

Fundamental concepts which are present in this volume include bifurcation, homoclinicity, invariant sets and attractors, both in the autonomous and nonautonomous situation. These concepts, at first sight, seem to mostly address *large time behavior*, most amenable to methodologies of analysis. Their intimate relation to concepts like (nonstrict) hyperbolicity, ergodicity, entropy, stochasticity and control should become quite apparent, however, when browsing through this volume.

The fundamental topic of *dimension* is similarly ubiquitous throughout our articles. In analysis it figures, for example, as a rigorous reduction from

infinite-dimensional settings like partial differential equations, to simpler infinite-, finite- or even low-dimensional model equations, still bearing full relevance to the original equations. But in numerical analysis – including and transcending mere discretization – specific computational realization of such reductions still poses challenges which are addressed here.

Another source of inspiration comes from very refined *measure*-theoretic and dimensional concepts of ergodic theory which found their way into algorithmic realizations presented here.

By no means do these few hints exhaust the conceptual span of the articles. It would be even more demanding to discuss the rich circle of methods, by which the three fundamental topics of large time behavior, dimension, and measure are tackled. In addition to SBR-measures, Perron-Frobenius type transfer operators, Markov decompositions, Pesin theory, entropy, and Oseledec's theorems, we address kneading invariants, fractal geometry and self-similarity, complex analytic structure, the links between billiards and spectral theory, Lyapunov exponents, and dimension estimates. Including Lyapunov-Schmidt and center manifold reductions together with their Shilnikov and Lin variants and their efficient numerical realizations, symmetry and orbit space reductions together with closely related averaging methods, we may continue, numerically, with invariant subspaces, Godunov type discretization schemes for conservation laws with source terms, (compressed) visualization of complicated and complex patterns of dynamics, and present an algorithm, GAIO, which enables us to approximately compute, in low dimensions, objects like SBR-measures and Perron-Frobenius type transfer operators. At which point our cursory excursion through methodologies employed here closes up the circle.

So much for the mathematical aspects. The range of applied issues, mostly from physics but including some topics from the life sciences, can also be summarized at most superficially, at this point. This range comprises such diverse areas as crystallization and dendrite growth, the dynamo effect, and efficient simulation of biomolecules. Fluid dynamics and reacting flows are addressed, including the much studied contexts of Rayleigh-Bénard and Taylor-Couette systems as well as the stability question of three-dimensional surface waves. The Ginzburg-Landau and Swift-Hohenberg equations appear, for example, as do mechanical problems involving friction, population biology, the spread of infectious diseases, and quantum chaos. It is the diversity of these applied fields which well reflects both the diversity and the power of the underlying mathematical approach. Only composite materials enable a bridge to span that far.

The broad scope of our program has manifested itself in many meetings, conferences, and workshops. Suffice it to mention the workshop on “Entropy” which was coorganized by Andreas Greven, Gerhard Keller, and Gerald Warnecke at Dresden in June 2000, jointly with the two neighboring DFG Priority Research Programs “Analysis and Numerics for Conservation Laws” and “Interacting Stochastic Systems of High Complexity”. For further information

concerning program and participants of the DFG Priority Research Program “Ergodic Theory, Analysis, and Efficient Simulation of Dynamical Systems”, including a preprint server, see

- www.math.fu-berlin.de/~danse/

For other DFG programs we refer to

- www.dfg.de
- www.dfg.de/aufgaben/Schwerpunktprogramme.html

At the end of this preface, I would like to thank at least some of the many friends and colleagues who have helped on so many occasions to make this program work. First of all, I would like to mention the members of the scientific committee who have helped initiate the entire program and who have accompanied and shaped the scientific program throughout its funding period: Ludwig Arnold, Hans-Günther Bothe, Peter Deuffhard, Klaus Kirchgässner, and Stefan Müller. The precarious conflict between great expectations and finite funding was expertly balanced by our all-understanding referees Hans Wilhelm Alt, Jürgen Gärtner, François Ledrappier, Wilhelm Niethammer, Albrecht Pietsch, Gerhard Wanner, Harry Yserentant, Eberhard Zeidler, and Eduard Zehnder. The hardships of finite funding as well as any remaining administrative constraints were further alleviated as much as possible, and beyond, by Robert Paul Königs and Bernhard Nunner, representing DFG at its best. The www-services were designed, constantly expanded and improved with unrivalled expertise and independence by Stefan Liebscher. And Regina Löhr, as an aside to her numerous other secretarial activities and with ever-lasting patience and friendliness, efficiently reduced the administrative burden of the coordinator to occasional emails which consisted of no more than “OK. BF”. Martin Peters and his team at Springer-Verlag ensured a very smooth cooperation, including efficient assistance with all \TeX nicities. But last, and above all, my thanks as a coordinator of this program go to the authors of this volume and to all participants – principal investigators, PostDocs and students alike – who have realized this program with their contributions, their knowledge, their dedication, and their imagination.

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Bernold Fiedler

On Dynamics and Bifurcations of Nonlinear Evolution Equations Under Numerical Discretization

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Abstract. This article reviews recent results on long-time behaviour, invariant sets and bifurcations of evolution equations under discretization by numerical methods. The emphasis is on time discretization. Finite-time error bounds of low order for non-smooth data, of high order for smooth data, and attractive invariant manifolds are tools that pervade large parts of the article. To illustrate the mechanisms, the following combinations of dynamics/equations have been selected for a detailed discussion:

1. Shadowing near hyperbolic equilibria of singularly perturbed ODEs
2. Hyperbolic periodic orbits of delay differential equations
3. Hopf bifurcation of semilinear parabolic equations
4. Inertial manifolds of semilinear parabolic equations
5. Attractors of damped wave equations.

Introduction

This article was written under the premise that it should

- (a) survey the subject area,
- (b) review work by the author in the DANSE project,
- (c) give one or the other new result.

These goals are not necessarily compatible. Clearly, (b) inflicts a strong bias on (a). With (a) and/or (b) achieved, (c) can only be rudimentary within the assigned pages. This caveat notwithstanding, may the reader find this article useful!

What are the mechanisms that make a numerical discretization capture the long-time dynamics of the differential equation? How good can the approximation be? These are the questions underlying the present article. Answers are different for different classes of equations:

- (i) ordinary differential equations for which the Jacobian of the right-hand side has a bound that is much smaller than the inverse of the step size needed to approximate solutions over some finite time (“nonstiff” ODEs);

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- (ii) evolution equations for which the linearization involves unbounded operators or operators of arbitrarily large norm, e.g., partial differential equations, singularly perturbed ODEs, and (less obviously) delay differential equations.

The present paper is concerned with class (ii). Reference to the more developed subject of dynamics of discretized nonstiff ODEs is made only for a comparison of the arguments. A further distinction needs to be made between “dissipative” and “conservative” problems, e.g., damped wave equations versus Hamiltonian wave equations. The dynamic properties considered here will be for the “dissipative” type.

Inhomogeneous and far-spread as the class of equations is, it nevertheless turns out that there are a few tools which go a long way with many different evolution equations and dynamic phenomena. Of these tools, I would like to single out the roles played by low-order nonsmooth-data error bounds and high-order smooth-data error bounds over finite times, and the reduction of the dynamics to the nonstiff case via attractive invariant manifolds. It is a strange fact that two of the papers that have influenced me most in this area, have never been published: Larsson’s report [35] which highlights the importance of error bounds for general initial data that do not admit a smooth solution; and Nipp and Stoffer’s report [47] on an extremely useful version of an invariant manifold theorem. That theorem is recapitulated in Appendix A.

The sampling in the three-dimensional lattice of Dynamics \times Equations \times Numerical Methods, as listed in the abstract, has been guided by the objective of showing relationships as well as differences among a wide variety of problems, and admittedly by (b) above. Section 5 was chosen to comply with (c). Each section presents the analytical framework and the numerical method, and states just one theorem. The result and its background are explained, and related results are indicated. The sections can be read independently, but they share common ground.

Stuart [55] gives a good survey of the field as of ~ 1995 . That article concerns sectorial evolution equations, which is where most of the work has been done. Stuart and Humphries [56] is a basic reference on the dynamics of nonstiff ODE discretizations, Hairer, Nørsett and Wanner [19,20] on time discretization methods.

1 Shadowing Near Hyperbolic Equilibria of Singularly Perturbed Ordinary Differential Equations

Following [41], we consider numerical solutions to singularly perturbed differential equations in the neighbourhood of a saddle point. We apply an implicit Runge-Kutta method with a step size larger than the small perturbation parameter. The main result is a shadowing property: After an initial transient, the numerical solution in a neighbourhood of the hyperbolic stationary point

remains for all times close to some exact solution of the differential equation. Conversely, after the elapse of a short time also every exact solution in the neighbourhood remains close to some numerical solution. In both cases, the approximation takes place with the order of approximation of smooth solutions on finite intervals. We will see that the main difficulty, as compared to the analogous problem for nonstiff ordinary differential equations, is that finite-time errors are not uniformly small for arbitrary initial data in an open set. This difficulty, which we will again encounter with all the other classes of evolution equations considered in this article, is here overcome by using strongly attractive invariant manifolds for both the continuous and the discrete problem.

1.1 Analytical Framework

We consider the singularly perturbed problem

$$\begin{aligned}\frac{dy}{dt} &= f(y, z) \\ \varepsilon \frac{dz}{dt} &= g(y, z), \quad 0 < \varepsilon \ll 1,\end{aligned}\tag{1}$$

in the neighbourhood of a stationary point at the origin. The functions f and g are arbitrarily differentiable. With subscripts denoting partial derivatives, we assume the following.

$$\text{All eigenvalues of } g_z(0, 0) \text{ have negative real part.}\tag{2}$$

$$(f_y - f_z g_z^{-1} g_y)(0, 0) \text{ has no eigenvalues on the imaginary axis.}\tag{3}$$

The first condition is familiar in the theory of singularly perturbed problems and yields the uniform well-posedness of the system as $\varepsilon \rightarrow 0$; see, e.g., [50]. The second assumption is equivalent to stating that for small ε the fixed point of (1) is *hyperbolic*, that is, the Jacobian of the system (1) at the stationary point has no eigenvalues on the imaginary axis.

1.2 Numerical Method

We consider an implicit Runge-Kutta method applied to (1) with step size $h \geq \varepsilon$:

$$y_{n+1} = y_n + h \sum_{j=1}^m b_j Y'_{nj}, \quad z_{n+1} = z_n + h \sum_{j=1}^m b_j Z'_{nj},$$

with internal stages ($i = 1, \dots, m$)

$$Y_{ni} = y_n + h \sum_{j=1}^m a_{ij} Y'_{nj}, \quad Z_{ni} = z_n + h \sum_{j=1}^m a_{ij} Z'_{nj}$$

satisfying relations of the form of (1):

$$\begin{aligned} Y'_{ni} &= f(Y_{ni}, Z_{ni}) \\ \varepsilon Z'_{ni} &= g(Y_{ni}, Z_{ni}) . \end{aligned}$$

The method is determined by its coefficients a_{ij} and b_j .

We assume that the Runge-Kutta method is *strongly A-stable*, that is, the stability function

$$R(w) = 1 + wb^T(I - w\mathcal{Q})^{-1}\mathbb{1} ,$$

(where $b^T = (b_1, \dots, b_m)$, $\mathcal{Q} = (a_{ij})_{i,j=1}^m$, $\mathbb{1} = (1, \dots, 1)^T$) satisfies

$$|R(w)| \leq 1 \quad \text{for } \operatorname{Re} w \leq 0 ,$$

all eigenvalues of the Runge-Kutta matrix $\mathcal{Q} = (a_{ij})_{i,j=1}^m$ have positive real part, and $R(\infty) = 1 - b^T \mathcal{Q}^{-1} \mathbb{1}$ satisfies

$$|R(\infty)| < 1 .$$

We require the following approximation properties: the method has *classical order* p , that is, the error of the method applied to nonstiff ordinary differential equations is $O(h^p)$ on bounded time intervals. The approximation properties for the singularly perturbed problem (1) depend in addition on the *stage order* q , which is determined by the condition

$$\sum_{j=1}^m a_{ij} c_j^{k-1} = \frac{c_i^k}{k} \quad \text{for } k = 1, \dots, q \text{ and all } i . \quad (4)$$

Here c_i is defined by (4) with $k = 1$.

A well-known and widely used class of Runge-Kutta methods satisfying the above assumptions are the Radau IIA methods [20], which for each stage number $m \geq 1$ have $p = 2m - 1$, $q = m$, and satisfy $a_{mj} = b_j$ ($j = 1, \dots, m$), which in particular implies $R(\infty) = 0$.

1.3 Statement of the Result

Theorem 1. [41] *Under the above assumptions, there are positive constants r and h_0 such that the following holds for $0 < \varepsilon \leq h \leq h_0$.*

(A) *For every Runge-Kutta solution with $\|(y_n, z_n)\| \leq r$ for $0 \leq n \leq N$, there exists a solution $(y(t), z(t))$ of (1) for $0 \leq t \leq T = Nh$, such that for $0 \leq n \leq N$*

$$\begin{aligned} \|y_n - y(nh)\| &\leq C \cdot (h^p + \varepsilon h^{q+1} + \varepsilon \rho^n) \\ \|z_n - z(nh)\| &\leq \begin{cases} C \cdot (h^p + \varepsilon h^q + \rho^n) & \text{if } a_{mj} = b_j \text{ for } j = 1, \dots, m , \\ C \cdot (h^{q+1} + \rho^n) & \text{else .} \end{cases} \end{aligned}$$

Here $\rho < 1$ and C depend only on f , g , r and h_0 , and in particular are independent of ε , h , and N . Moreover, for $\varepsilon \ll h$ we have $\rho = |R(\infty)| + O(\varepsilon/h)$.

(B) Conversely, for every solution of (1) with $\|(y(t), z(t))\| \leq r$ for $0 \leq t \leq T = Nh$, there exists a Runge-Kutta solution (y_n, z_n) , $0 \leq n \leq N$, such that the difference to $(y(nh), z(nh))$ satisfies the above bounds with $\rho = e^{-\kappa h/\varepsilon}$, with C and $\kappa > 0$ independent of ε , h , and N .

1.4 Discussion and Comparison with the Nonstiff ODE Case

Theorem 1 is an analogue of a shadowing result of Beyn [4] for numerical solutions near a hyperbolic stationary point of the ordinary differential equation

$$\frac{dx}{dt} = f(x), \quad (5)$$

where sufficiently many derivatives of the nonlinearity f are assumed to be bounded. The following is shown in [4, Theorem 3.1] for p th order methods applied with step size h :

For every numerical solution (x_n) , $0 \leq n \leq N$, which stays in a sufficiently small neighborhood U of the stationary point, there is a solution $x(t)$ of (5) satisfying $\|x_n - x(nh)\| \leq Ch^p$. Conversely, for every solution $x(t)$ in U , $0 \leq t \leq T = Nh$, there is a Runge-Kutta solution (x_n) with $\|x_n - x(nh)\| \leq Ch^p$. The constant C is independent of h and N .

As in Theorem 1, it is essential that the estimates remain uniform on time intervals that can become arbitrarily large. We review briefly the considerations that lead to Beyn's result.

Let R^h denote the Runge-Kutta map, so that $R^h(x)$ is the result of one step of the method applied with step size h , starting from the point x . A numerical solution sequence (x_n) thus satisfies

$$x_{n+1} = R^h(x_n).$$

Further, let S^h denote the flow map of the differential equation (5) over time h , so that for a solution $x(t)$ of (5) we have

$$x(t+h) = S^h(x(t)).$$

The local error $R^h(x) - S^h(x)$ then satisfies

$$R^h(x) - S^h(x) = O(h^{p+1}), \quad \frac{\partial R^h}{\partial x}(x) - \frac{\partial S^h}{\partial x}(x) = O(h^{p+1}) \quad (6)$$

uniformly for x in an arbitrary compact set.

The first estimate is obtained by comparing the Taylor expansions of the exact and the numerical solution, the second estimate follows by interpreting the two error expressions combined as the local error of the Runge-Kutta

method applied to the system composed of (5) and its variational equation $dv/dt = \partial f/\partial x(x)v$.

By the variation-of-constants formula, a sequence of exact solution values $\tilde{x}_n = x(nh)$ satisfies a recurrence relation

$$\tilde{x}_{n+1} = e^{hA}\tilde{x}_n + h\phi(\tilde{x}_n), \quad (7)$$

where A is the Jacobian of (5) at the stationary point $x^* = 0$, and where ϕ is an h -dependent function with $\phi(0) = 0$ and Lipschitz constant of size $O(r)$ in an r -neighbourhood $B(r)$ of the stationary point. Similarly, by (6), every numerical solution sequence satisfies a recursion of the form

$$x_{n+1} = e^{hA}x_n + h\psi(x_n), \quad (8)$$

where ψ has a Lipschitz constant of size $O(r) + O(h^p)$ in $B(r)$, and

$$\psi(x) - \phi(x) = O(h^p) \quad \text{uniformly in } B(r).$$

By the assumption of hyperbolicity, A has the form (up to a similarity transform)

$$A = \begin{pmatrix} A^- & 0 \\ 0 & A^+ \end{pmatrix}$$

where all eigenvalues of A^- have negative real part and those of A^+ have positive real part. We now apply the discrete variation-of-constants formula to the stable components in (7) and (8) in the forward direction, and to the unstable components in the backward direction:

$$\begin{aligned} x_n^- &= \exp(nhA^-)x_0^- + h \sum_{j=0}^{n-1} \exp((n-j-1)hA^-)\psi^-(x_j), \\ x_n^+ &= \exp((n-N)hA^+)x_N^+ - h \sum_{j=n}^{N-1} \exp((n-j-1)hA^+)\psi^+(x_j). \end{aligned}$$

As the Lipschitz constants of ϕ and ψ can be made arbitrarily small by reducing the radius r of the neighbourhood, the Banach contraction principle yields the following: *Let (x_n) be a solution of (8) with $\|x_n\| \leq r$ ($n = 0, \dots, N$). If r is sufficiently small, there is a unique solution of (7) with boundary values $\tilde{x}_0^- = x_0^-$, $\tilde{x}_N^+ = x_N^+$. This solution satisfies*

$$x_n - \tilde{x}_n = O(h^p) \quad \text{uniformly for } n = 0, \dots, N.$$

Evidently, the same holds with the roles of x_n and \tilde{x}_n interchanged. This yields Beyn's shadowing result as stated above. We emphasize that this construction depends crucially on the uniform approximation estimate (6).

Let us now return to the singularly perturbed problem (1) and its Runge-Kutta discretization. Here we face the difficulty that an approximation estimate (6) does not hold when $\varepsilon \leq h$. Since general solutions of (1) undergo

rapid initial changes, the best possible local error estimate valid in a neighbourhood of the stationary point is only $R^h(x) - S^h(x) = O(1)!$

More favourable error bounds exist only for initial values (y_0, z_0) which are such that the corresponding solution $(y(t), z(t))$ of (1) is “smooth” in the sense that arbitrarily many derivatives are bounded independently of ε . For such initial data, the following sharp finite-time error bounds were shown in [18] to hold for numerical solutions obtained by strongly A -stable Runge-Kutta methods of classical order p and stage order q :

$$\begin{aligned} \|y_n - y(nh)\| &\leq C(h^p + \varepsilon h^{q+1}) \\ \|z_n - z(nh)\| &\leq \begin{cases} C(h^p + \varepsilon h^q) & \text{if } a_{mj} = b_j \text{ for } j = 1, \dots, m, \\ Ch^{q+1} & \text{else.} \end{cases} \end{aligned}$$

The constants depend on bounds for the derivatives of the solution and on the length T of the time interval, but are independent of ε , h and n with $nh \leq T$. We note that these orders of approximation are the same as stated in Theorem 1.

The way to circumvent the missing uniformity in the error bounds, is to make use of *attractive invariant manifolds*. As is known from the geometric theory of singular perturbation problems [14], [46], there is a manifold $\mathcal{M}_\varepsilon = \{(y, z) : z = s_\varepsilon(y)\}$ (locally near the stationary point, which itself is on \mathcal{M}_ε), such that solutions of (1) starting on \mathcal{M}_ε remain on \mathcal{M}_ε and are smooth in the above sense. Also the function s_ε defining the manifold has arbitrarily many derivatives bounded independently of ε . An arbitrary solution $(y(t), z(t))$ of (1) near $(0, 0)$ rapidly approaches a solution on \mathcal{M}_ε : There is a solution $(\tilde{y}(t), \tilde{z}(t))$ on \mathcal{M}_ε such that

$$\|y(t) - \tilde{y}(t)\| + \varepsilon \cdot \|z(t) - \tilde{z}(t)\| \leq C\varepsilon e^{-\kappa t/\varepsilon}, \quad 0 \leq t \leq T,$$

with some constants C and $\kappa > 0$ which do not depend on ε and T (“property of asymptotic phase”). If $(y(t), z(t)) = (y(t), s_\varepsilon(y(t)))$ is a solution of (1) on \mathcal{M}_ε , then $y(t)$ is a solution of the differential equation with smooth right-hand side

$$\frac{dy}{dt} = f(y, s_\varepsilon(y)), \quad (9)$$

which has $y = 0$ as a stationary point. There, the Jacobian is of the form $(f_y - f_z g_z^{-1} g_y)(0, 0) + O(\varepsilon)$. By condition (3), this matrix has no eigenvalues on the imaginary axis for small ε .

Not only the continuous system (1), but also its Runge-Kutta discretization admits an invariant manifold. A combination of results and techniques of [47] and [18] yields the following result; cf. Nipp and Stoffer [48].

For $0 < \varepsilon \leq h \leq h_0$, there is a local attractive invariant manifold $\mathcal{M}_{\varepsilon, h} = \{(y, z) | z = s_{\varepsilon, h}(y)\}$ for the Runge-Kutta discretization. $\mathcal{M}_{\varepsilon, h}$ is close to \mathcal{M}_ε :

$$\|s_{\varepsilon, h}(y) - s_\varepsilon(y)\| \leq \begin{cases} C\varepsilon h^q & \text{if } b_i = a_{si} \text{ for all } i, \\ Ch^{q+1} & \text{else.} \end{cases}$$

There is a property of asymptotic phase: for every (y_0, z_0) in an h - and ε -independent open set that contains $\mathcal{M}_{\varepsilon, h}$, there exists $(\tilde{y}_0, \tilde{z}_0) \in \mathcal{M}_{\varepsilon, h}$ such that the corresponding Runge-Kutta solutions satisfy

$$\|y_n - \tilde{y}_n\| + \varepsilon \cdot \|z_n - \tilde{z}_n\| \leq C \varepsilon \rho^n, \quad 0 \leq n \leq N,$$

where $\rho < 1$ and C do not depend on ε , h , and N . For $\varepsilon \ll h$ we have $\rho = |R(\infty)| + O(\varepsilon/h)$.

With these results at hand, the construction of the shadowing solution in [41] proceeds in several steps. Starting from a given Runge-Kutta solution (y_n, z_n) , $0 \leq n \leq N$, of (1) staying in an r -neighborhood of $(0, 0)$, with r sufficiently small (but independent of ε), a solution $(y(t), z(t))$ of (1) shadowing the numerical solution is constructed as follows.

1. Take the Runge-Kutta solution $(\tilde{y}_n, \tilde{z}_n)$ on $\mathcal{M}_{\varepsilon, h}$ with the same asymptotic phase, so that $y_n - \tilde{y}_n = O(\varepsilon \rho^n)$ for $0 \leq n \leq N$.
2. Construct a Runge-Kutta solution (η_n) of (9) shadowing (\tilde{y}_n) : $\tilde{y}_n - \eta_n = O(\varepsilon h^{q+1})$ for $0 \leq n \leq N$.
3. Apply Beyn's result to (9) to obtain a shadowing solution $y(t)$ with $\eta_n - y(nh) = O(h^p)$ for $0 \leq n \leq N$. Take $z(t) = s_\varepsilon(y(t))$.

This yields part (A) of Theorem 1. For part (B), one proceeds similarly from a given solution $(y(t), z(t))$, $0 \leq t \leq T = Nh$, of (1).

- 1'. Take the solution $(\tilde{y}(t), \tilde{z}(t))$ on \mathcal{M}_ε with the same asymptotic phase, so that $y(t) - \tilde{y}(t) = O(\varepsilon e^{-\kappa t/\varepsilon})$ for $0 \leq t \leq T$.
- 2'. Apply the converse direction of Beyn's result to (9) to obtain a Runge-Kutta solution (η_n) of (9) shadowing $(\tilde{y}(nh))$: $\tilde{y}(nh) - \eta_n = O(h^p)$ for $0 \leq n \leq N$.
- 3'. Construct a Runge-Kutta solution (y_n, z_n) of (1) on $\mathcal{M}_{\varepsilon, h}$ shadowing $(\eta_n, s_\varepsilon(\eta_n))$: $\eta_n - y_n = O(\varepsilon h^{q+1})$ for $0 \leq n \leq N$, and $z_n = s_{\varepsilon, h}(y_n)$.

Steps 2 and 3' are the technically demanding steps in these constructions; see [41] for the details.

1.5 Related Results

In the nonstiff ODE case, Beyn [4] further shows that the local stable and unstable manifolds near the hyperbolic stationary point are approximated with the order of the method. For the Runge-Kutta discretization of the singularly perturbed problem (1), the techniques of [41, 47] yield also that there are local stable and unstable submanifolds of the attractive invariant manifold $\mathcal{M}_{\varepsilon, h}$ of the discretization which approximate the stable and unstable manifolds of the reduced equation (9), again with the order of the finite-time smooth-data error bounds.

The results of [41] permit to relate the dynamics of Runge-Kutta discretizations of the singularly perturbed problem (1) to those of the discretization of the nonstiff differential equation (9). This reduction makes it possible

to transfer many of the known results on the long-time behaviour of discretizations of nonstiff ODEs to singularly perturbed problems — at least as long as trajectories stay away from regions where some eigenvalue of g_z has non-negative real part. This restriction excludes, for example, relaxation oscillations.

For BDF-like multistep methods applied to singularly perturbed problems, optimal-order finite-time smooth-data error bounds were derived in [40,49], and their attractive invariant manifolds were studied by Nipp and Stoffer [49]. A combination of [49] and [41] extends Theorem 1 to multistep discretizations.

There is a rich literature on “numerical shadowing”, mainly for nonstiff ordinary differential equations. (Zentralblatt lists over 40 articles, e.g., by Chow, Coomes/Koçak/Palmer, Corless, Eirola, Haderer, Kloeden, Pilyugin, Sauer/Yorke, Van Vleck.) Less has been done for stiff differential equations or partial differential equations, and apparently nothing for delay differential equations.

Alouges and Debussche [1] extend Beyn’s shadowing result near hyperbolic equilibria to implicit Euler time discretizations of semilinear parabolic problems, Larsson and Sanz-Serna [37,38] to finite element space discretizations and full discretizations. Ostermann and Palencia [51] derive a shadowing result for an implicit Euler time discretization of non-autonomous parabolic problems.

The shadowing lemma of Chow, Lin and Palmer [9] combined with non-smooth-data error bounds for finite element and Runge-Kutta discretizations of semilinear parabolic equations [35,43] yields numerical shadowing near general hyperbolic invariant sets of such equations.

Larsson and Pilyugin [36] investigate numerical shadowing near the attractor for finite element/implicit Euler discretizations of reaction-diffusion equations in one space dimension, using a reduction to known finite-dimensional results on Morse-Smale systems via inertial manifolds. It is shown that every numerical trajectory shadows some exact solution of the problem after the elapse of a finite time.

Long-time error bounds of numerical discretizations of semilinear parabolic problems near asymptotically stable stationary points were obtained earlier [25,34,53].

2 Hyperbolic Periodic Orbits of Delay Differential Equations

Following [29], we study the persistence of stable hyperbolic periodic orbits of delay differential equations under numerical discretization. We show the existence of attractive closed curves for Runge-Kutta discretizations, which approximate the periodic orbit with the full order of the method. The proof requires an infinite-dimensional analytical/numerical framework and com-

bines finite-time error bounds for both smooth and non-smooth data with an invariant manifold theorem.

2.1 Analytical Framework

We consider a delay differential equation with fixed delay $\tau > 0$,

$$\frac{dx}{dt}(t) = f(x(t), x(t - \tau)) \quad (10)$$

where f is bounded and sufficiently often differentiable with bounded derivatives. With d denoting the dimension of the system (10), we let

$$\mathcal{C} = \mathcal{C}([-\tau, 0], \mathbf{R}^d)$$

be the Banach space of \mathbf{R}^d -valued continuous functions on $[-\tau, 0]$ equipped with the maximum norm, which we denote by $\|\cdot\|$. For a given initial function $x^0 \in \mathcal{C}$, Eq. (10) has a unique solution $x : [-\tau, \infty) \rightarrow \mathbf{R}^d$. For $t \geq 0$, we define

$$x^t \in \mathcal{C} \quad \text{via} \quad x^t(\theta) = x(t + \theta) \quad \text{for} \quad \theta \in [-\tau, 0] .$$

To indicate the dependence of the solution section x^t on the initial function x^0 , we write

$$x^t = S^t(x^0) .$$

This gives a semigroup on \mathcal{C} . Further, $S^t : \mathcal{C} \rightarrow \mathcal{C}$ is a Fréchet differentiable map. We denote its derivative at $x^0 \in \mathcal{C}$ by $DS^t(x^0)$.

We assume that (10) has a *stable hyperbolic periodic orbit*, that is, (10) has a nonconstant periodic solution

$$\bar{x} : \mathbf{R} \rightarrow \mathbf{R}^d \quad \text{of period} \quad \omega > 0 ,$$

and the derivative of the period map, $DS^\omega(\bar{x}^0)$, has 1 as a simple eigenvalue, whereas the remaining part of the spectrum of $DS^\omega(\bar{x}^0)$ is bounded in modulus by a number strictly smaller than 1. Let

$$\Gamma = \{\bar{x}^t : t \in \mathbf{R}\}$$

denote the periodic orbit of (10) in \mathcal{C} .

2.2 Numerical Method

We restrict our attention to step sizes $h > 0$ for which the delay τ is an integer multiple:

$$\tau = \nu h , \quad \text{with integer } \nu .$$

A Runge-Kutta discretization of (10) reads as follows [19]: Given an initial function $x^0 \in \mathcal{C}$, we define starting values (for $i = 1, \dots, m$)

$$\begin{aligned} X_{ni} &= x^0(nh + c_i h) , & n &= -\nu, \dots, -1 \\ x_0 &= x^0(0) \end{aligned}$$

and set recursively for $n = 0, 1, 2, \dots$

$$x_{n+1} = x_n + h \sum_{i=1}^m b_i X'_{ni}$$

with internal stage relations ($i = 1, \dots, m$)

$$X_{ni} = x_n + h \sum_{j=1}^m a_{ij} X'_{nj}$$

and

$$X'_{ni} = f(X_{ni}, X_{n-\nu, i}) .$$

The method is determined by the real coefficients a_{ij} , b_j , c_i ($i, j = 1, \dots, m$), where $c_i \in [0, 1]$. It is explicit if $a_{ij} = 0$ for $i \leq j$. We assume that the Runge-Kutta method has classical order p .

For a formulation of the result on the persistence of the periodic orbit under the discretization, we need to interpolate the discrete solution values to functions in \mathcal{C} . For $t = nh$ with integer $n \geq 0$, we construct

$$R_h^t(x^0) = x_h^t \in \mathcal{C}$$

by setting $x_h^0 = x^0$ and defining $x_h^t(\theta)$ for $-h \leq \theta \leq 0$ by polynomial interpolation through $x_n, x_{n-1}, \dots, x_{n-p}$ (with $x_k = x^0(kh)$ for negative k), and we set recursively $x_h^t(\theta) = x_h^{t-h}(\theta+h)$ for $-\tau \leq \theta \leq -h$, for $t = h, 2h, 3h, \dots$.

2.3 Statement of the Result

Theorem 2. [29] *In the above situation, for any given $L > 0$, there are positive constants r , c , C , C_0 and h_0 such that the following holds for $0 < h \leq h_0$. There is a closed curve $\Gamma_h \subset \mathcal{C}$ which attracts numerical solutions at an exponential rate,*

$$\text{dist}(R_h^t(x^0), \Gamma_h) \leq C e^{-ct} , \quad t = nh > 0 ,$$

whenever the initial function x^0 is in an r -neighbourhood of the periodic orbit, viz. $\text{dist}(x^0, \Gamma) \leq r$, and x^0 has a Lipschitz constant not exceeding L . The Hausdorff distance to the periodic orbit Γ is bounded by

$$\text{dist}_H(\Gamma_h, \Gamma) \leq C_0 h^p .$$

2.4 Discussion and Comparison with the ODE Case

Theorem 2 is related to results by Braun and Hershenvov [7], Beyn [6], and Eirola [12] on invariant curves of numerical discretizations of (nonstiff) smooth

ordinary differential equations with a hyperbolic periodic orbit. Theorem 2 considers only the stable case, but similar to ODEs, the result could be extended to general hyperbolic periodic orbits. In the stable case, the result for p th-order Runge-Kutta discretizations of smooth ordinary differential equations with sufficiently small step size h reads as follows.

There is a closed curve which is invariant under the numerical method and $O(h^p)$ close to the stable hyperbolic orbit of the ordinary differential equation. Locally, it attracts numerical solutions exponentially with an h -independent rate.

We now indicate how this result for ordinary differential equations follows directly from the attractive invariant manifold theorem of Kirchgraber, Nipp and Stoffer [32,47] restated here in the appendix. Consider the differential equation (5) and denote its flow by $S^t(x_0) = x(t)$. Let the equation have the periodic orbit $\bar{x}(t)$ with period ω . By definition, the orbit is stable hyperbolic if the derivative of the period map, $\partial S^\omega(\bar{x}(0))/\partial x$, has 1 as a simple eigenvalue, and all other eigenvalues are strictly smaller than 1 in modulus. We now use normal coordinates, in terms of which every point in a neighbourhood of the periodic orbit is written as $x = \bar{x}(\alpha) + \beta$, where $\alpha \in \mathbf{R}$ is unique up to integer multiples of the period ω , and β is unique in the maximal invariant subspace of $\partial S^\omega(\bar{x}(\alpha))/\partial x$ that does not contain the eigenvector to the eigenvalue 1. Written in these coordinates, the flow map S^t satisfies, for sufficiently large t , the conditions of Theorem A.1 on a strip $\mathbf{R} \times B$, with B a ball. The estimate (6) for the local error implies that, on finite time intervals, there is a uniform error estimate between the Runge-Kutta solution $R_h^t(x) = x_n$ at $t = nh$ and the exact solution $S^t(x)$,

$$R_h^t(x) - S^t(x) = O(h^p), \quad \frac{\partial R_h^t}{\partial x}(x) - \frac{\partial S^t}{\partial x}(x) = O(h^p) \quad (11)$$

uniformly for x in an arbitrary compact set.

Hence, the Runge-Kutta map R_h^t is a small Lipschitz perturbation of the flow map. R_h^t thus still satisfies the assumptions of Theorem A.1 for sufficiently small h , and the existence of an attractive invariant closed curve of the numerical discretization follows. Corollary A.2 provides the $O(h^p)$ bound for the distance to the periodic orbit.

We return to the delay differential equation (10). As in the previous section, a principal difficulty in extending the ODE result is that the uniform error bounds (6) or (11) are no longer valid. For the above Runge-Kutta discretization, the following finite-time *nonsmooth-data error bound* is known [29]: If $x^0, v \in \mathcal{C}$ are Lipschitz bounded by L , and $\|v\| \leq 1$, then the difference between the Runge-Kutta solution $x_h^t = R_h^t(x^0)$ and the exact solution $x^t = S^t(x^0)$ corresponding to the initial function x^0 , is bounded by

$$\|R_h^t(x^0) - S^t(x^0)\| \leq CLh, \quad \|DR_h^t(x^0)v - DS^t(x^0)v\| \leq CLh$$

with a constant C which depends on t , but is independent of x^0 and v with the stated properties. Without assuming additional regularity of $x^0, v \in \mathcal{C}$, such as Lipschitz continuity, there is no uniform convergence on bounded sets of \mathcal{C} as $h \rightarrow 0$. On the other hand, for sufficiently differentiable initial data x^0 , there is the full-order *smooth-data error bound* [19, Sec. II.17]

$$\|R_h^t(x^0) - S^t(x^0)\| \leq C h^p ,$$

where C depends on bounds of the first p derivatives of x^0 , and on t .

A further difficulty not present in the ODE case results from the fact that the numerical method incorporates the delay via past internal stages, not via past solution values. As a consequence, a Runge-Kutta step must be viewed as a mapping

$$(x_{n+k}, X_{n+k,1}, \dots, X_{n+k,m})_{k=-\nu}^0 \mapsto (x_{n+1+k}, X_{n+1+k,1}, \dots, X_{n+1+k,m})_{k=-\nu}^0$$

or, extending to continuous functions via polynomial interpolation, as a mapping $\mathcal{C} \times \mathcal{C}^m \rightarrow \mathcal{C} \times \mathcal{C}^m$. The attractive curve Γ_h in \mathcal{C} of Theorem 2 is in general *not* an invariant curve of the numerical method, but instead it consists of the projection to the first component of an attractive invariant curve in $\mathcal{C} \times \mathcal{C}^m$ of the Runge-Kutta map. This leads to additional problems in bringing the invariant manifold theorem into play; see [29] for details. Here, for simplicity, we continue the discussion with a Runge-Kutta method for which all internal stages are linear combinations of numerical solution values, such as the explicit or implicit Euler method or the trapezoidal rule or the implicit midpoint rule. In this case, the numerical one-step map R^h can indeed be viewed as a map on \mathcal{C} , and for $t = nh$, the time- t numerical solution map R_h^t is the n -fold composition $R_h^t = (R^h)^n$.

For this special case, we now outline the arguments in the proof of Theorem 2. Analogous to ordinary differential equations, there exist normal coordinates near the periodic orbit $\Gamma = \{\bar{x}^\alpha : \alpha \in \mathbf{R}\}$. As is known from Hale [21, Ch. 10], every function $x \in \mathcal{C}$ in some neighbourhood of Γ can be written as $x = \bar{x}^\alpha + \beta$, where $\alpha \in \mathbf{R}$ is unique up to integer multiples of the period ω , and β is unique in the maximal invariant subspace of $DS^\omega(\bar{x}(\alpha))$ that does not contain the eigenfunction to the eigenvalue 1. It can be verified that the exact flow map S^t written in normal coordinates, $(\alpha, \beta) \mapsto (\hat{\alpha}, \hat{\beta})$, satisfies the conditions of the attractive invariant manifold theorem Theorem A.1 in a strip of $\mathbf{R} \times \mathcal{C}$, clearly with the periodic orbit Γ as attractive invariant curve. Consider now the closed bounded set in \mathcal{C} ,

$$B_{r,L} = \{\beta \in \mathcal{C} : \|\beta\| \leq r, \beta \text{ is Lipschitz bounded by } L\} .$$

Using the above *nonsmooth-data error bound* and a uniform Lipschitz bound of numerical solutions $x_h^t \in \mathcal{C}$, it is seen, for appropriately chosen r and L , that together with S^t also the Runge-Kutta map R_h^t written in normal coordinates satisfies the conditions of Theorem A.1 on $\mathbf{R} \times B_{r,L}$ for sufficiently

small step size h . This yields the existence of an exponentially attractive invariant curve Γ_h for R_h^t , and subsequently also for the one-step map R^h . Since the periodic orbit \bar{x} is arbitrarily differentiable, the *smooth-data error bound* yields, uniformly for $\alpha \in \mathbf{R}$,

$$\|R_h^t(\bar{x}^\alpha) - S^t(\bar{x}^\alpha)\| \leq C h^p .$$

Corollary A.2 requires just this bound of the difference of R_h^t and S^t on the periodic orbit Γ , and hence it yields the optimal-order distance estimate $\text{dist}_H(\Gamma_h, \Gamma) = O(h^p)$.

2.5 Related Results

The persistence of (not necessarily stable) hyperbolic periodic orbits under discretization has been studied also for semilinear parabolic differential equations. For implicit Euler time discretizations of such problems, Alouges and Debussche [2] show the existence of invariant closed curves approximating the hyperbolic periodic orbit with a sub-optimal order smaller than 1. In [43], it is shown for Runge-Kutta time discretizations that the approximation order of the invariant curve is actually that of high-order finite-time error bounds for the Runge-Kutta approximation of smooth solutions of the parabolic problem. As in the case of delay differential equations, the result relies on both low-order nonsmooth-data and high-order smooth-data finite-time error bounds.

3 Hopf Bifurcation of Semilinear Parabolic Differential Equations

Following [44], we study the long-time behaviour of numerical discretizations in a situation where hyperbolicity gets lost, in the neighbourhood of a bifurcation point. We consider Runge-Kutta time discretization of semilinear parabolic equations near a generic, supercritical Hopf bifurcation. The phase portrait is shown to persist under the discretization, and in particular, the bifurcation point and the Hopf orbits are approximated with the high order of finite-time approximations to smooth solutions of the parabolic equation. The analysis uses a reduction to two-dimensional center manifolds of both the continuous problem and its discretization, and a comparison of the dynamics on the center manifolds via normal forms. The existence, smoothness, and approximation properties of the center manifold of the discretization are obtained by studying the discretization, by the same numerical method, of a boundary value problem on the negative half-line.

3.1 Analytical Framework

We consider reaction-diffusion equations and incompressible Navier-Stokes equations in the abstract setting of sectorial evolution equations in a Banach

space as given in Henry's book [24]. We let the equation be parametrized by a real bifurcation parameter λ ,

$$\frac{du}{dt} + A(\lambda)u = F(u, \lambda) . \quad (12)$$

We assume that the system can be transformed, via suitable spectral projections, to a block-diagonal form

$$\begin{aligned} \frac{dy}{dt} + B(\lambda)y &= f(y, v, \lambda) \\ \frac{dv}{dt} + L(\lambda)v &= g(y, v, \lambda) \end{aligned} \quad (13)$$

with the following specifications. The real 2×2 -matrix $B(\lambda)$ has a pair of complex conjugate eigenvalues which cross the imaginary axis at the parameter value λ^* with non-vanishing speed, i.e.,

$$\sigma(-B(\lambda)) = \{\alpha(\lambda) \pm i\omega(\lambda)\}, \quad \text{with } \alpha(\lambda^*) = 0, \quad \frac{d\alpha}{d\lambda}(\lambda^*) > 0, \quad \omega(\lambda^*) > 0 .$$

We further assume, with $\omega^* = \omega(\lambda^*)$,

$$B(\lambda^*) = \begin{pmatrix} 0 & -\omega^* \\ \omega^* & 0 \end{pmatrix} .$$

The linear operator $L(\lambda)$ in (13) is a densely defined closed operator on a Banach space X , with domain $D(L)$ independent of λ . The spectrum of $-L(\lambda)$ is in a sector lying strictly in the left half-plane, and $L(\lambda)$ satisfies the sectorial resolvent bound, with an angle $\phi < \pi/2$ and a positive abscissa $\ell > 0$,

$$\|(z + L(\lambda))^{-1}\|_{\mathcal{L}(X)} \leq \frac{K}{|z + \ell|} \quad \text{for all complex } z \text{ with } |\arg(z + \ell)| \geq \phi$$

uniformly for λ in an interval A around λ^* . The functions

$$\begin{aligned} \lambda &\mapsto B(\lambda) \in \mathbf{R}^{2 \times 2} \\ \lambda &\mapsto L(\lambda) \in \mathcal{L}(D(L), X) \end{aligned} \quad \text{are arbitrarily differentiable.}$$

The nonlinearities f and g , taking values in \mathbf{R}^2 and X , respectively, are arbitrarily differentiable on $\mathbf{R}^2 \times V \times A$, where $V = D(L(\lambda)^\alpha)$ for some $\alpha < 1$. (Note, V is independent of λ because of the uniform resolvent condition.) We assume that the left-hand side of (13) represents the linearization of the equation at the stationary point $(0, 0)$, i.e.,

$$\begin{aligned} f(0, 0, \lambda) &= 0, \quad g(0, 0, \lambda) = 0 \\ D_y f(0, 0, \lambda) &= 0, \quad D_v f(0, 0, \lambda) = 0, \quad D_y g(0, 0, \lambda) = 0, \quad D_v g(0, 0, \lambda) = 0 . \end{aligned}$$

It is known [24,59] that the system (13) has a *center manifold*

$$\mathcal{M}_\lambda = \{(y, s(y, \lambda)) : y \in \mathbf{R}^2\} ,$$

with a defining function $s : \mathbf{R}^2 \times \Lambda \rightarrow V$ which, for arbitrary integer k , is k times continuously differentiable in a k -dependent neighbourhood of $(0, \lambda^*)$. The center manifold is locally invariant and attracts solutions at an exponential rate. The dynamics of the system (13) in a neighbourhood of the stationary point $(0, 0)$ is determined by the equation reduced to the center manifold,

$$\frac{dy}{dt} + B(\lambda)y = \varphi(y, \lambda) , \quad (14)$$

where $\varphi(y, \lambda) = f(y, s(y, \lambda), \lambda)$ satisfies $\varphi(0, \lambda) = 0$, $D_y \varphi(0, \lambda) = 0$. A near-identity change of coordinates transforms (14) to *normal form* [60, Sections 2.2B and 3.1B], which in polar coordinates reads for $\lambda = \lambda^* + \rho^2$

$$\begin{aligned} \frac{dr}{dt} &= (a\rho^2 + cr^2)r + O(r(\rho^4 + r^4)) \\ \frac{d\theta}{dt} &= \omega^* + b\rho^2 + dr^2 + O(\rho^4 + r^4) , \end{aligned} \quad (15)$$

where $a = d\alpha/d\lambda(\lambda^*) > 0$, $b = d\omega/d\lambda(\lambda^*)$, and where the coefficients c and d depend on second and third derivatives of φ at the bifurcation point. The normal form yields that the dynamical behaviour passes for λ growing across λ^* from an asymptotically stable equilibrium to an asymptotically stable periodic orbit if $c < 0$, and such a change in the dynamics is possible only if $c \leq 0$. In the following we assume

$$c < 0 .$$

The periodic orbits of the reduced equation (14) are close to circles centered at 0 with radius $r = \rho\sqrt{-a/c}$, where again $\rho = \sqrt{\lambda - \lambda^*}$. It will be convenient to parametrize the periodic orbits by ρ via $\lambda(\rho) = \lambda^* + \rho^2$. We denote the periodic orbit of Eq. (12) with parameter $\lambda(\rho)$ by $\Gamma(\rho)$. This periodic orbit lies on the center manifold to the parameter $\lambda(\rho)$.

3.2 Numerical Method

A Runge-Kutta time discretization of (12) reads

$$\begin{aligned} u_{n+1} &= u_n + h \sum_{i=1}^m b_i U'_{ni} , \quad U_{ni} = u_n + h \sum_{j=1}^m a_{ij} U'_{nj} , \\ U'_{ni} + A(\lambda)U_{ni} &= F(U_{ni}, \lambda) \quad (i = 1, \dots, m) . \end{aligned}$$

The stability condition we need here is a weakened form of the strong A-stability defined in Section 1.2. For an angle $\theta \leq \frac{1}{2}\pi$, the method is called

strongly $A(\theta)$ -stable if all eigenvalues of the Runge-Kutta matrix \mathcal{Q} lie outside the closed complex sector $|\arg(-z)| \leq \theta$, and if the stability function of the method satisfies

$$|R(z)| \leq 1 \quad \text{for } |\arg(-z)| \leq \theta$$

and

$$|R(\infty)| < 1.$$

We assume that the method is strongly $A(\theta)$ -stable with $\theta > \phi$, where ϕ is the angle in the sectorial resolvent condition. As in Section 1.2, we assume that the method has classical order p and stage order q . We let

$$k = \min(p, q + 1).$$

3.3 Statement of the Result

Theorem 3. [44] *In the above situation, there exist $h_0 > 0$, $\lambda_0 < \lambda^*$, $\rho_0 > 0$, and constants C and C^* , such that for all positive time steps $h \leq h_0$, there is a parameter value λ_h^* with*

$$|\lambda_h^* - \lambda^*| \leq C^* h^p$$

such that the following holds:

(i) *For every $\lambda \in [\lambda_0, \lambda_h^*)$, the Runge-Kutta discretization has the asymptotically stable equilibrium point 0.*

(ii) *For every $\rho \in (0, \rho_0]$, the Runge-Kutta discretization with parameter $\lambda_h(\rho) = \lambda_h^* + \rho^2$ has an attractive invariant closed curve $\Gamma_h(\rho)$. Its Hausdorff distance to the periodic orbit $\Gamma(\rho)$ with parameter $\lambda(\rho) = \lambda^* + \rho^2$ satisfies*

$$\text{dist}_H(\Gamma_h(\rho), \Gamma(\rho)) \leq C \rho h^k.$$

3.4 Discussion and Comparison with the ODE Case

For ordinary differential equations

$$\frac{dx}{dt} = f(x, \lambda)$$

the question of the behaviour of Hopf bifurcation under numerical discretization was first considered by Brezzi, Ushiki and Fujii [8]. They state an analogue of Theorem 3 for the explicit Euler method and give an outline of a proof for the two-dimensional case.

Hairer and Lubich [16] study the behaviour of Runge-Kutta methods near a Hopf bifurcation of ordinary differential equations with real-analytic right-hand side via a *backward analysis* of numerical integrators. It is shown in [3, 16] that there exists a modified differential equation

$$\frac{d\tilde{x}}{dt} = f_h(\tilde{x}, \lambda)$$

such that the numerical solution map R_h^t departs from the flow S_h^t of the modified differential equation by only exponentially small terms in the step size: for a fixed $t = nh$,

$$R_h^t(x) - S_h^t(x) = O(e^{-\gamma/h})$$

uniformly for x in any complex compact subset of the domain of analyticity. The constant $\gamma > 0$ is inversely proportional to a Lipschitz constant of f . The real-analytic function f_h is $O(h^p)$ close to f , again uniformly on complex compact sets. The modified differential equation undergoes a Hopf bifurcation at a parameter $\lambda_h^* = \lambda^* + O(h^p)$. Although the hyperbolicity of the Hopf orbits deteriorates as λ approaches the bifurcation point, the exponential smallness of the error allows us to use the approximation result of hyperbolic periodic orbits (see Sect. 2.4) down to parameters that are exponentially close to the bifurcation point: $\lambda \geq \lambda_h^* + e^{-\gamma/(2h)}$. For such a λ , we thus obtain the existence of an attractive invariant closed curve of the discretization which is exponentially close to the periodic orbit of the modified equation for the same parameter value.

Backward analysis is a powerful tool for studying numerical discretizations even in non-hyperbolic situations in nonstiff ordinary differential equations. However, it is not applicable to partial differential equations due to the unboundedness of the operator. (See, however, [45] for some partial results in that direction when very strong smoothing properties such as Gevrey regularity are available.)

The proof of Theorem 3 follows a standard procedure in the analysis of bifurcations [33, 58, 59] outlined already in Section 3.1: reduction of the dynamics to a center manifold and analysis of the normal form of the reduced equation. The first step is to construct a center manifold of the discretization, and to study its relationship to the center manifold of the continuous problem. In [44], the center manifold is constructed from a boundary value problem on the negative half-line,

$$\begin{aligned} \frac{dy}{dt} + B(\lambda)y &= f(y, v, \lambda), & y(0) &= \eta \\ \frac{dv}{dt} + L(\lambda)v &= g(y, v, \lambda), & \limsup_{t \rightarrow -\infty} \|v(t)\| &< \infty, \end{aligned}$$

from which the function $s : \mathbf{R}^2 \times \Lambda \rightarrow V$ defining the center manifold \mathcal{M}_λ is obtained by setting

$$s(\eta, \lambda) = v(0).$$

Similarly, the center manifold of the Runge-Kutta discretization is obtained by formally applying the Runge-Kutta method to this boundary value problem. Existence, attractivity, smoothness and approximation properties of the

discrete center manifold then follow from studying the numerical discretization of the boundary value problem. Using the convolution quadrature interpretation of the Runge-Kutta method [42] and exploiting the temporal smoothness of the solution of the boundary value problem, which follows from the smoothness of the function s , the following result is obtained.

There exists a center manifold

$$\mathcal{M}_{\lambda,h} = \{(y, s_h(y, \lambda)) : y \in \mathbf{R}^2\}$$

which is invariant under the numerical method and uniformly in h and λ exponentially attractive. The defining function $s_h : \mathbf{R}^2 \times \Lambda \rightarrow V$ has the same regularity properties as s , with derivatives bounded uniformly in h . There is the approximation estimate

$$\|s_h(y, \lambda) - s(y, \lambda)\| \leq C |y| h^k$$

in the norm of the space V , and the same order of approximation is valid for any fixed number of derivatives of $s_h - s$ with respect to y and λ .

The next step is to compare the normal forms of the time- h flow map of the reduced differential equation on \mathbf{R}^2 and of the Runge-Kutta map reduced to the discrete center manifold, giving another map on \mathbf{R}^2 . This comparison uses the above estimates for s_h and leads to a situation to which Theorem A.1 and Corollary A.2 can be applied. This yields the existence of invariant curves and the approximation properties as stated in Theorem 3.

We remark that this construction can of course be carried out also in the ODE situation. In that case, the approximation estimate in Theorem 3 improves to the full order $k = p$.

A related construction can be used also for finite element space discretizations of reaction-diffusion equations and subsequently for full discretizations [joint work by S. Larsson and the author, in preparation]. There are additional difficulties due to the fact that the method is then no longer invariant under the transition from (12) to (13), and that the equilibrium point of the differential equation need not lie in the finite element space. Multistep time discretization is studied by H. Selhofer [doctoral thesis in preparation].

4 Inertial Manifolds of Semilinear Parabolic Equations

Following [11], we show high-order approximation of the inertial manifold of a semilinear parabolic equation by inertial manifolds of full discretizations combined of a spectral Galerkin method in space and a Runge-Kutta method in time. The result follows by a combination of low-order nonsmooth-data error bounds and high-order error bounds for smooth data over finite time intervals, and once more with the invariant manifold theorem of the appendix. The smoothness of solutions on the inertial manifold, as implied by time analyticity and Gevrey regularity, renders the high order of approximation possible.

4.1 Analytical Framework

The following applies to the complex Ginzburg-Landau and Kuramoto-Sivashinsky equations and to classes of reaction-diffusion equations with analytic nonlinearities in one or two space dimensions; cf. [57] and references therein. The limitation of the space dimension is due to a spectral gap condition, which is needed in the proof of existence of an inertial manifold and which is not satisfied by the three- (or higher-) dimensional Laplacian.

We consider the evolution equation

$$\frac{du}{dt} + Au = F(u) \quad (16)$$

under the following assumptions: the operator A is of the form $A = (1 + ia)L$, where $a \in \mathbf{R}$ and L is a self-adjoint, densely defined linear operator on a separable Hilbert space H , with a compact inverse and eigenvalues

$$0 < \lambda_1 \leq \lambda_2 \leq \dots \nearrow +\infty .$$

For some $\alpha < 1$, the nonlinearity is defined on $V = D(L^\alpha)$. The function $F : V \rightarrow H$ is at least twice continuously Fréchet differentiable.

We denote the norm on H by $|\cdot|$, that on V by $\|\cdot\|$. Let P_m denote the orthogonal projection on the space spanned by the first m eigenfunctions of L , and let $Q_m = I - P_m$ be the projection on the orthogonal complement. $B(\rho)$ denotes the ball of radius ρ in V centered at the origin. As in previous sections, S^t denotes the time- t flow of the evolution equation.

We are interested in an *inertial manifold* \mathcal{M} for (16) as introduced by Foias, Sell and Temam [15]. This is a positively invariant set (more precisely, for a fixed $\rho > 0$, \mathcal{M} satisfies $S^t(\mathcal{M} \cap B(\rho)) \subset \mathcal{M}$ for all $t \geq 0$) defined through a Lipschitz continuous function $s : P_m V \rightarrow Q_m V$ via

$$\mathcal{M} = \{v \in V : Q_m v = s(P_m v)\} .$$

\mathcal{M} is exponentially attracting: there exist $\nu > 0$ and a constant C (depending on ρ) such that for all $u_0 \in V$ with $\|u_0\| \leq \rho$,

$$\text{dist}(S^t(u_0), \mathcal{M}) \leq C e^{-\nu t} \quad \text{for all } t \geq 0 .$$

The dynamics of the infinite-dimensional evolution equation (16) is then determined by its restriction to the inertial manifold, which is a finite-dimensional ordinary differential equation.

The existence of an inertial manifold is known under the following conditions: (16) has an *absorbing ball*, i.e., there exist $r > 0$ and, for every $\rho > 0$, a $\tau(\rho) > 0$ such that

$$\|v\| \leq \rho \quad \text{implies} \quad \|S^t(v)\| \leq r \quad \text{for all } t \geq \tau(\rho) .$$

The second condition is a *spectral gap condition*: for a sufficiently large constant K ,

$$\lambda_{m+1} - \lambda_m \geq K \lambda_{m+1}^\alpha .$$

Finally, it is needed that λ_m is sufficiently large compared to a Lipschitz constant of F . Under these conditions, the existence of an inertial manifold of dimension m actually follows directly from Theorem A.1, used with $\Phi = S^t$ for $t = c/\lambda_{m+1}$ with a sufficiently small constant c .

For our approximation results, we make use of strong regularity results in time and space, which are known to hold for the differential equations mentioned in the beginning of this subsection; cf. [52].

Analyticity in time: for every $v \in V$ of norm bounded by ρ , the function $t \mapsto S^t(v)$ is analytic on the intersection of a complex sector $|\arg t| < \phi$ with a strip $|\operatorname{Im} t| < c$, and is bounded there by $\|S^t(v)\| \leq C$ uniformly for $\|v\| \leq \rho$.

Gevrey regularity: for a given $\rho > 0$, there exist a constant C and a time $\bar{t} > 0$ such that $S^t(v)$ is in the domain of $\exp(+ (tA)^{1/2})$ and

$$\|\exp((tA)^{1/2})S^t(v)\| \leq C \quad \text{for} \quad \|v\| \leq \rho, \quad 0 \leq t \leq \bar{t}.$$

4.2 Numerical Method

We consider a spectral Galerkin discretization in space combined with Runge-Kutta discretization in time. The spectral Galerkin method yields an approximation to the solution of (16) in the space V_N spanned by the first N eigenfunctions of A . With P_N denoting the orthogonal projection on V_N , the method solves

$$\frac{du_N}{dt} + Au_N = P_N F(u_N), \quad u_N(0) = P_N u_0.$$

This problem is discretized in time by a strongly $A(\theta)$ -stable Runge-Kutta method of order p and stage order q ; cf. Section 3.2. The angle θ should be larger than $\arg(1 + ia)$. We set again

$$k = \min(p, q + 1).$$

The time step is again denoted by h , and we let for brevity

$$\Delta = (N, h).$$

The numerical approximation at time $t = nh$ is written as $R_\Delta^t(u_0)$.

4.3 Statement of the Result

Theorem 4. [11] *In the above situation, for given $\rho > 0$, there exist positive constants $C_0, C_1, C_2, c, \ell, \kappa$ (independent of the dimension m of the inertial manifold \mathcal{M}) such that the following holds for N and h with $\lambda_m/\lambda_{N+1} \leq \kappa$ and $h\lambda_m \leq \kappa$. There exists a manifold \mathcal{M}_Δ that is positively invariant under the numerical method (more precisely, $R_\Delta^t(\mathcal{M}_\Delta \cap B(\rho)) \subset \mathcal{M}_\Delta$ for $t = nh \geq$*

0). It is defined by a function $s_\Delta : P_m V \rightarrow Q_m V$, which is Lipschitz bounded by ℓ , via

$$\mathcal{M}_\Delta = \{v \in V : Q_m v = s_\Delta(P_m v)\} .$$

\mathcal{M}_Δ attracts all numerical solutions starting with $\|u_0\| \leq \rho$ exponentially,

$$\text{dist}(R_\Delta^t(u_0), \mathcal{M}_\Delta) \leq C_0 e^{-t\nu/2} \quad \text{for all } t = nh \geq 0 .$$

The Hausdorff distance to the inertial manifold of (16) is bounded by

$$\text{dist}_H(\mathcal{M}_\Delta, \mathcal{M}) \leq C_1 e^{-c\sqrt{\lambda_{N+1}/\lambda_m}} + C_2 (\lambda_m h)^k .$$

4.4 Discussion

Theorem 4 gives exponential convergence in space and high order in time. We have included the dependence on the dimension m because the spectral gap condition is usually satisfied for infinitely many m , leading to a nested sequence of inertial manifolds with growing attractivity exponents ν . Moreover, even the smallest possible m may be quite large in applications. The way the distance estimate depends on m shows that only the time and length scales of the differential equation reduced to the inertial manifold need to be resolved properly by the discretization for an accurate approximation of the inertial manifold.

We outline a proof of Theorem 4 that uses Theorem A.1 and Corollary A.2, whereas [11] employs a Hadamard graph transform adopted from [30].

The existence of an inertial manifold of the discretization can be proved using Theorem A.1 and a *nonsmooth-data* error bound. Combining the results of [43] and [55, Sect. 3.3] on time and space discretizations, respectively, the following finite-time error bound is obtained: uniformly for $\|u_0\| \leq \rho$ and $0 < t \leq T$,

$$\|R_\Delta^t(u_0) - S^t(u_0)\| \leq C (t^{-\alpha} h |\log h| + (h/t)^k + (t\lambda_{N+1})^{\alpha-1}) .$$

The same bound holds also for the derivative, $\|DR_\Delta^t(u_0) - DS^t(u_0)\|_{\mathcal{L}(V)}$. The error bound implies the existence of an absorbing ball of the discretization for sufficiently small h and large N . Consequently, the dynamics is not changed if the scheme is modified outside a sufficiently large ball in V , say of radius \hat{r} . We can then achieve that the above error bounds hold globally on V . In the light of Theorem A.1, R_Δ^t is thus a small Lipschitz perturbation of S^t . Hence, for $t = c/\lambda_{m+1}$ with sufficiently small c , together with S^t also R_Δ^t satisfies the conditions of that theorem. This yields the existence of the inertial manifold of the discretization.

The distance estimate between the inertial manifolds \mathcal{M} and \mathcal{M}_Δ can be based on Corollary A.2. This requires to estimate $R_\Delta^t(u_0) - S^t(u_0)$ only for $u_0 \in \mathcal{M}$, which is achieved via a study of the regularity of solutions

on \mathcal{M} and using *smooth-data* finite-time error bounds. Theorem 4.1 of [42] gives the following error bound. If the solution $u(t) = S^t(u_0)$ satisfies, with $d(t) = Q_N F(u(t)) = Q_N(du/dt + Au(t))$,

$$\begin{aligned} \|u^{(k)}(0)\| + \int_0^T \|u^{(k+1)}(t)\| dt &\leq \mu, \\ \|A^{-1}d(0)\| + \int_0^T \|A^{-1}d'(t)\| dt &\leq \delta_N, \end{aligned}$$

(where $u^{(k)}$ denotes the k th time derivative of u , and d' the time derivative of d), then

$$\|R_\Delta^t(u_0) - S^t(u_0)\| \leq C(\mu h^k + \delta_N)$$

for $0 \leq t \leq T$. Solutions on the inertial manifold $\mathcal{M} \cap B(r)$ can be continued backward in time, and they stay in $\mathcal{M} \cap B(\hat{r})$ at least for a time that is inverse proportional to λ_m (recall that the equation and the scheme were modified outside \hat{r}). With a time $t \sim \lambda_m^{-1}$, we can thus employ the time analyticity and Gevrey regularity estimates to obtain

$$\mu = O(\lambda_m^k), \quad \delta_N = O(e^{-c\sqrt{\lambda_{N+1}/\lambda_m}})$$

uniformly for $u_0 \in \mathcal{M} \cap B(r)$. Corollary A.2 then yields the desired high-order distance bound.

4.5 Related Results

The existence of inertial manifolds for spectral discretizations in space was studied by Foias, Sell and Temam [15] and Jones and Stuart [30]. The distance estimate of Theorem 4.1 of [15], in a framework which corresponds to the case $\alpha = 1/2$, is $O(\lambda_{N+1}^{-1/4})$. The bound of [30] is $O(\lambda_{N+1}^{\alpha-1})$, which corresponds to the nonsmooth-data finite-time error bound. (The dependence on m is considered explicitly in these papers, but is not reproduced here.)

The first results on the existence of inertial manifolds of time discretizations were given by Demengel and Ghidaglia [10]. Full discretizations were subsequently studied by Jones and Stuart [30]. Those authors consider linearly implicit Euler and fractional step time discretizations and obtain distance estimates of the low order of nonsmooth-data error bounds. Shardlow [54] studies multistep time discretizations and also obtains low-order distance estimates of an order not exceeding 1.

Lord [39] establishes discrete Gevrey regularity for finite difference methods for the complex Ginzburg-Landau equation and uses it to study approximation of the inertial manifold.

C^1 -approximation of inertial manifolds has been studied by Jones, Stuart and Titi [31].

5 Attractors of Damped Wave Equations

For a specially constructed time discretization combined with a spectral Galerkin space discretization of a dissipative wave equation, we show the existence of an attractor of the discretization which lies close to that of the partial differential equation. The result relies on a nonsmooth-data finite-time error bound, which is not available for usual time discretizations.

5.1 Analytical Framework

We consider the abstract damped wave equation

$$\frac{d^2 u}{dt^2} + \alpha \frac{du}{dt} + Au = g(u) \quad (17)$$

with a positive damping parameter $\alpha > 0$. The linear operator A is assumed to be a self-adjoint, densely defined operator on a Hilbert space H , with a compact inverse and eigenvalues $0 < \lambda_1 \leq \lambda_2 \leq \dots$. We let $V = D(A^{1/2})$ and set $X = V \times H$. The norm on X is denoted by $\|\cdot\|$, viz. $\|(u, v)\|^2 = |A^{1/2}u|^2 + |v|^2$, where $|\cdot|$ is the norm on H .

For the nonlinearity we assume that for some $\gamma > 0$,

$$\begin{aligned} g : V &\rightarrow D(A^{\gamma/2}) \\ g : D(A^{(1-\gamma)/2}) &\rightarrow H \end{aligned} \quad \text{are continuously Fréchet differentiable,}$$

and that it permits unique solutions $S^t(u_0, v_0) = (u(t), du/dt(t))$ of (17) in X for all times t and initial values $(u_0, v_0) \in X$.

We further assume that (17) has a (global) *attractor*, that is, a compact set $\mathcal{A} \subset X$ which is invariant under the flow, viz. $S^t(\mathcal{A}) = \mathcal{A}$ for all t , and which attracts bounded sets in X . The latter means that for every bounded set B in X and for every $\varepsilon > 0$, there is a t_0 (which depends on ε and B), such that $S^t(B)$ is in an ε -neighbourhood of \mathcal{A} for $t \geq t_0$.

We refer to Temam [57, Ch. IV] for conditions which ensure the existence of an attractor, and for concrete examples of damped wave equations having an attractor.

5.2 Numerical Method

The choice of time discretization requires more care than in the preceding sections. In contrast to the parabolic case, standard numerical integration schemes for (17) do not admit convergent nonsmooth-data error bounds, which are needed here. Instead we consider a time-stepping method in the spirit of [17, 28]. To motivate the method, we start from the variation-of-constants formula

$$\begin{pmatrix} A^{1/2}u(t+h) \\ v(t+h) \end{pmatrix} = E(hA^{1/2}) \begin{pmatrix} A^{1/2}u(t) \\ v(t) \end{pmatrix}$$

$$+ h \int_0^1 E((1-\theta)hA^{1/2}) \begin{pmatrix} 0 \\ -\alpha v(t+\theta h) + g(u(t+\theta h)) \end{pmatrix} d\theta ,$$

where $v = du/dt$ and

$$E(\xi) = \begin{pmatrix} \cos \xi & \sin \xi \\ -\sin \xi & \cos \xi \end{pmatrix} .$$

Expressing the term $v(t+\theta h)$ under the integral once more by the same formula and dropping terms of formal order $O(h^2)$ leads to the following method:

$$\begin{pmatrix} A^{1/2}u_{n+1} \\ v_{n+1} \end{pmatrix} = \left(E(hA^{1/2}) - h\alpha\Phi(hA^{1/2}) \right) \begin{pmatrix} A^{1/2}u_n \\ v_n \end{pmatrix} \\ + h\Psi(hA^{1/2}) \begin{pmatrix} 0 \\ g(u_n) \end{pmatrix}$$

with

$$\Phi(\xi) = \int_0^1 E((1-\theta)\xi) \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} E(\theta\xi) d\theta \\ \Psi(\xi) = \int_0^1 E((1-\theta)\xi) d\theta .$$

The integrals can be evaluated analytically. They are such that the entries of the transformed matrices $D(\xi)^{-1}(\Phi(\xi), \Psi(\xi))D(\xi)$ with $D(\xi) = \text{diag}(\xi, 1)$ are entire functions of ξ^2 .

As space discretization we take a standard spectral Galerkin method. With P_N denoting the orthogonal projection on the space H_N (or V_N) spanned by the first N eigenfunctions, and with A_N the restriction of A to H_N , this space discretization is obtained by replacing A by A_N and g by $P_N g$ in the above formula.

The numerical solution starting from $(u_0, v_0) \in X_N = V_N \times H_N$ is denoted by $R_\Delta^t(u_0, v_0) = (u_n, v_n)$ at $t = nh$, where again Δ symbolizes the pair (N, h) of discretization parameters.

Remark. The above method is just a particular example of a class of methods that are exact solvers for $d^2u/dt^2 + Au = 0$. It is a first-order method when applied to initial value problems (17) that admit a smooth solution. A second-order method could be constructed along similar lines.

Remark. Even in cases where an eigendecomposition of the matrix arising from the space discretization is computationally not feasible, as in finite element methods, the method can be efficiently implemented using superlinearly convergent Krylov subspace approximations of matrix function times vector products; cf. [28].

5.3 Statement of the Result

Theorem 5. *If the discretization is sufficiently fine, it has a (local) attractor \mathcal{A}_Δ . The semi-distance to the attractor \mathcal{A} converges to 0 as $h \rightarrow 0$, $N \rightarrow \infty$. More precisely, for every $\varepsilon > 0$ and every bounded set B in X , there exist positive h_0 , N_0 , t_0 such that*

$$\text{dist}(R_\Delta^t(u_0, v_0), \mathcal{A}) < \varepsilon \quad \text{for } t > t_0$$

whenever $(u_0, v_0) \in B \cap X_N$ and $N > N_0$, $h < h_0$.

5.4 Discussion and Related Results

Theorem 5 is apparently the first result on the dynamics of a fully discretized dissipative wave equation. An analogue of Theorem 5 for spectral Galerkin semi-discretization in space was obtained already by Hale, Lin and Raugel [22]. However, the derivation of a corresponding result for time discretizations was hampered by the fact that standard time discretization methods admit no convergent error bounds where the error is measured in the same norm in which bounds for the initial data are specified. Such a *nonsmooth-data error bound* does exist for the numerical method of Section 5.2:

For every $\rho > 0$ and $T > 0$, there exists C such that

$$\|R_\Delta^t(u_0, v_0) - S^t(u_0, v_0)\| \leq C(h^\gamma + \lambda_{N+1}^{-\gamma})$$

for all $(u_0, v_0) \in X_N$ with $\|(u_0, v_0)\| \leq \rho$ and for $0 \leq t = nh \leq T$.

This is proved below. With this error bound, the distance estimate of Theorem 5 then follows by an argument given by Larsson [35]: Let $\varepsilon > 0$ and let B be a bounded set in X , of which we may assume that it contains the ε -neighbourhood of \mathcal{A} . We choose T such that

$$\text{dist}(S^t(B), \mathcal{A}) := \sup_{x \in B} \text{dist}(S^t(x), \mathcal{A}) < \frac{1}{2}\varepsilon \quad \text{for } t \geq \frac{1}{2}T.$$

If the discretization is sufficiently fine, the above error bound yields for $B_N = B \cap X_N$

$$\text{dist}(R_\Delta^t(B_N), \mathcal{A}) < \varepsilon \quad \text{for } \frac{1}{2}T \leq t \leq T,$$

and in particular, $R_\Delta^t(B_N) \subset B_N$ for such t . Hence, the bound must hold for all $t \geq \frac{1}{2}T$. This proves the distance estimate of Theorem 5. The existence of an attractor \mathcal{A}_Δ of the discretization then follows from the discrete-time version of Theorem I.1.1 in [57].

Like other results in the spirit of [22], such as [13, 26, 35, 39] on parabolic problems, Theorem 5 gives no estimate for the distance between \mathcal{A}_Δ and \mathcal{A} , nor for the dimension of \mathcal{A}_Δ , and no information about the discrete flow on \mathcal{A}_Δ . It also does not ensure that \mathcal{A}_Δ lies close to every point on the attractor \mathcal{A} . The latter has been shown for gradient flows by Hale and Raugel

[23], but is not true in general. Hill and Süli [27] study set convergence $\mathcal{A}_\Delta \rightarrow \mathcal{A}_0$, where \mathcal{A}_0 is a compact invariant subset of \mathcal{A} . The shadowing results cited in Section 1.5 relate the dynamics on the discrete attractor to those of the partial differential equation in situations where the attractor is a hyperbolic invariant set or where the system has Morse-Smale structure.

5.5 Proof of the Nonsmooth-Data Error Bound

By the variation-of-constants formula, the solution $(u(t), v(t)) = S^t(u_0, v_0)$ satisfies

$$\begin{aligned} \begin{pmatrix} A^{1/2}u(t+h) \\ v(t+h) \end{pmatrix} &= \left(E(hA^{1/2}) - h\alpha\Phi(hA^{1/2}) \right) \begin{pmatrix} A^{1/2}u(t) \\ v(t) \end{pmatrix} \\ &\quad + h\Psi(hA^{1/2}) \begin{pmatrix} 0 \\ g(u(t)) \end{pmatrix} + d(t) \end{aligned}$$

with the defect

$$d(t) = h \int_0^1 E((1-\theta)hA^{1/2}) \begin{pmatrix} 0 \\ g(u(t+\theta h)) - g(u(t)) \end{pmatrix} d\theta + O(h^2) .$$

By our assumption on g we have

$$|g(u(t+\theta h)) - g(u(t))| \leq L|A^{(1-\gamma)/2}(u(t+\theta h) - u(t))| = O(h^\gamma) ,$$

where the last estimate follows again from the variation-of-constants formula of Section 5.2. Hence, $|d(t)| = O(h^{1+\gamma})$. By a standard stability estimate, this yields the error bound for the semi-discretization in time,

$$\|R_h^t(u_0, v_0) - S^t(u_0, v_0)\| \leq C h^\gamma ,$$

uniformly for $\|(u_0, v_0)\| \leq \rho$ and $0 \leq t \leq T$. The difference between the semi-discrete and the fully discrete numerical solution is estimated similarly, using

$$|(I - P_N)g(u)| = O(\lambda_{N+1}^{-\gamma}) .$$

This yields

$$\|R_\Delta^t(u_0, v_0) - R_h^t(u_0, v_0)\| \leq C \lambda_{N+1}^{-\gamma}$$

uniformly for $\|(u_0, v_0)\| \leq \rho$ and $0 \leq t \leq T$, and the desired error bound follows.

A Attractive Invariant Manifolds

Attractive invariant manifold theorems can be traced back to Hadamard a hundred years ago, and their usefulness has been rediscovered and re-established ever since. Here we give a version due to Kirchgraber, Lasagni,

Nipp, and Stoffer [32], which is particularly useful in applications because of its explicit handling of constants. A proof is contained in the report [47].

Consider a map $\Phi : A \times B \rightarrow A \times B$ defined on the Cartesian product of a Banach space A and a closed bounded subset B of another Banach space. We write $\Phi(\alpha, \beta) = (\hat{\alpha}, \hat{\beta})$ with

$$\begin{aligned}\hat{\alpha} &= \alpha + F(\alpha, \beta) \\ \hat{\beta} &= G(\alpha, \beta) .\end{aligned}$$

We assume that F and G are Lipschitz bounded, with Lipschitz constants $L_{\alpha\alpha}$, $L_{\alpha\beta}$ and $L_{\beta\alpha}$, $L_{\beta\beta}$ with respect to α , β . If these Lipschitz constants are sufficiently small, then the map Φ has an attractive invariant manifold. More precisely, the following holds.

Theorem A.1. [32,47] *If $L_{\alpha\alpha} + L_{\beta\beta} + 2\sqrt{L_{\alpha\beta}L_{\beta\alpha}} < 1$, then there is a function $s : A \rightarrow B$, Lipschitz bounded by $\ell < 2L_{\beta\alpha}/(1 - L_{\alpha\alpha} - L_{\beta\beta})$, such that*

$$\mathcal{M} = \{(\alpha, s(\alpha)) : \alpha \in A\}$$

is invariant under Φ . \mathcal{M} attracts orbits of Φ with rate $r = \ell L_{\alpha\beta} + L_{\beta\beta} < 1$, i.e., the inequality $\|\hat{\beta} - s(\hat{\alpha})\| \leq r \|\beta - s(\alpha)\|$ holds for all $(\alpha, \beta) \in A \times B$.

Remark. If $A = \mathbf{R}$, and if F , G are periodic in α with period ω , then s is again ω -periodic.

Corollary A.2. *Consider maps $\Phi, \tilde{\Phi} : A \times B \rightarrow A \times B$. Assume $\Phi, \tilde{\Phi}$ satisfy the conditions of Theorem A.1 with the same Lipschitz constants $L_{\alpha\alpha}, L_{\alpha\beta}, L_{\beta\alpha}, L_{\beta\beta}$. Let s and \tilde{s} be the functions defining the attractive invariant manifolds \mathcal{M} and $\tilde{\mathcal{M}}$, respectively. If the bound*

$$\|\tilde{\Phi}(\alpha, \beta) - \Phi(\alpha, \beta)\| \leq \delta \quad \text{for all } (\alpha, \beta) \in \mathcal{M}$$

holds in the norm $\|(\alpha, \beta)\| = \ell \|\alpha\| + \|\beta\|$ on $A \times B$, then

$$\|\tilde{s}(\alpha) - s(\alpha)\| \leq \frac{\delta}{1-r} \quad \text{for all } \alpha \in A .$$

For our applications of this result it is essential that a bound of $\tilde{\Phi} - \Phi$ is needed only on the invariant manifold \mathcal{M} , not on all of $A \times B$ (as is required in the formulation of [47]). The result as stated follows by tracing the proof in [47], or with the alternative proof in [29].

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