

Backward error analysis of a full discretization scheme for a class of parabolic partial differential equations

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Abstract

A numerical method for reaction-diffusion equations with analytic nonlinearity is presented, for which a rigorous backward error analysis is possible. We construct a modified equation, which describes the behavior of the full discretization scheme up to exponentially small errors in the step size. The construction is based on embedding into nonautonomous equations and the use of averaging techniques. The long-time behavior near hyperbolic equilibria is analyzed.

1 Introduction

For an illustration of backward error analysis of differential equations, we consider first an ordinary differential equation with analytic right hand side

$$\dot{x} = f(x), x(0) = x_0 \in \mathbf{R}^m. \quad (1.1)$$

We want to compare the flow $\Phi(t, u)$ with numerical methods e.g. some Runge-Kutta method with step-size h , which defines a local diffeomorphism

$$x_{n+1} = \Phi(h, x_n). \quad (1.2)$$

Our main intention is to compare these perturbations with the flow of (1.1) of some modified equation $\dot{x} = \tilde{f}(x)$, with \tilde{f} inside the same class as f , rather than compare it to the flow of the original equation.

For ordinary differential equations there is a strong relationship between backward analysis of numerical schemes and the averaging of nonautonomous equations. One-step methods for equation (1.1) with step-size h can be interpreted as the exact time- h -map of a rapidly forced ordinary differential equation as

$$\dot{x} = f(x) + h^p g(x, \frac{t}{h}, h), x(0) = x_0 \in \mathbf{R}^m. \quad (1.3)$$

with $g(\cdot, \tau, \cdot)$ periodic in $\tau = \frac{t}{h}$ with period 1, see [FS96].

For such rapidly forced equations like (1.3) Neishtadt [Nei84] proved, that the equation can be transformed to :

$$\dot{y} = \tilde{f}(y) + \alpha(y, \frac{t}{h}, h) \quad (1.4)$$

with $\|\alpha\| < c_2 \exp(-c_1/h)$ and $\|\tilde{f} - f\| < c_3 h^p$ on a bounded domain.

Hence there is modified autonomous vector field near f , which describes very accurately the behavior of the numerical method. Instead of going via the embedding into nonautonomous vector fields and using the Neishtadt theorem, there are more recent direct methods. For real analytic f bounded on some poly-disc around x_0 , Hairer and Lubich [HL97, theorem 1] construct directly a $\tilde{f}(h, \tilde{x})$ such that

$$\|x_1 - \tilde{x}(h)\| \leq c_1 \exp(-\frac{c_2}{h}) \quad (1.5)$$

for $h < h_0$ with explicit estimates of c_1, c_2 and h_0 . If $x(t)$ remains inside some compact set K , where f is also real analytic and bounded, then such an extremely good approximation also holds for finite times $T = O(h^{-1})$

$$x_n - \tilde{x}(nh) = O(\exp(-\frac{c}{h})) \text{ for } nh \leq T. \quad (1.6)$$

These exponential estimates can be used to explain, why several qualitative effects are well replicated by numerical schemes. Some of these properties are local behavior near steady states, stable periodic orbits, homoclinic orbits [FS96] and energy conservation for symplectic integrators [BG94, San92]. There is a vast literature on different aspects of backward error analysis for ordinary differential equations, see [HL97, Rei99] and the review article [HL99] and references therein. Some ideas for backward error analysis of partial differential equations can be found in [EDHJ95], especially in a modeling context. However no rigorous theorems on backward error analysis are given.

We will consider semilinear parabolic partial differential equations, see e.g. [Hen83]. As a model take a system of reaction-diffusion equations with $U = (u_1, \dots, u_n)$, $D = \text{diag}(d_1, \dots, d_n)$ with $d_i > 0$, and $F = (f_1, \dots, f_n)$:

$$\frac{\partial}{\partial t} U(x, t) - D \Delta U(x, t) = F(U(x, t)) \quad (1.7)$$

with periodic boundary conditions on $\Omega = [0, l]^d$, $d = 1, 2, 3$ and initial conditions $U(0) = U_0$ in the Sobolev space $H_{per}^s(\Omega, \mathbf{R}^n) \subset C^0(\Omega, \mathbf{R}^n)$, i.e. $s > \frac{d}{2}$, for a definition see e.g. [Tem88, p.48]. The nonlinearity F is assumed to be an entire function $\mathbf{R}^n \rightarrow \mathbf{R}^n$. Equation (1.7) defines a semiflow on $H_{per}^s(\Omega, \mathbf{R}^n) = D(A^{\frac{s}{2}})$ with the differential operator $A = -D\Delta$.

The solutions of this equation are extremely regular, they are in Gevrey classes $G_{\sigma}^{\frac{s}{2}}(\Omega, \mathbf{R}^n)$ as shown in [FT98]. The Fourier coefficients $V_j, j \in \mathbf{Z}^d$ of a function V in the Gevrey class $G_{\sigma}^{\frac{s}{2}}(\Omega, \mathbf{R}^n)$ decay like $\|j\|^{-s} \exp(-\sigma\|j\|)$. A norm of $G_{\sigma}^{\frac{s}{2}}(\Omega, \mathbf{R}^n)$ is given by

$$|V|_{G_{\sigma}^{\frac{s}{2}}} = \left(\sum_{k=1}^n \sum_{j \in \mathbf{Z}^d} v_k^j v_k^j (1 + d_k \|j\|^2)^s \exp(2\sigma\|j\|) \right)^{\frac{1}{2}}. \quad (1.8)$$

where v_k^j is the k^{th} component of the Fourier coefficient of the spatial Fourier expansion into $\exp(i\frac{2\pi}{l}j \cdot x)$ of the periodic functions V . Alternatively we can define Gevrey classes as

$$G_{\sigma}^{\frac{s}{2}}(\Omega, \mathbf{R}^n) = D \left(A^{\frac{s}{2}} \exp(\sigma(-\Delta)^{\frac{1}{2}}) \right) \quad (1.9)$$

with $A = -D\Delta$. The spatial Fourier modes decay exponentially fast, where the exponent depends on time. In [FT98] it is shown for the solution $S(t, U_0)$ of 1.7, that

$$\begin{aligned} S(t, U_0) &\in G_t^{\frac{s}{2}} \text{ for } 0 \leq t \leq T^* \\ S(t, U_0) &\in G_{T^*}^{\frac{s}{2}} \text{ for } t \geq T^*. \end{aligned} \quad (1.10)$$

holds for some maximal Gevrey exponent $T^* > 0$. Furthermore

$$|S(t, U_0)|_{G_{\min(t, T^*)}^{\frac{s}{2}}} \leq C_0,$$

as long as $|S(t, U_0)|_{H_{per}^s} \leq M_0$, i.e. only if a suitable Sobolev norm of the solution remains bounded, see [FT98].

We consider a special discretization scheme of (1.7). We will construct modified equations, which describe the behavior of the scheme up to exponentially small errors. We have to stress that the analyzed scheme is hardly used in practise due to very strict rules on the size of the time-steps. Anyway, this scheme will give a first example of a numerical scheme in parabolic partial differential equations for which a rigorous backward error analysis is possible. So for this discretization scheme very accurate predictions about the long-time behavior can be made. A scheme of full discretization of (1.7) in space and time is analyzed. In space we use a Galerkin spectral method, which defines a system of analytic ordinary differential equations for

$$U_N(x, t) = \sum_{\|j\| \leq N} U_N^j(t) \exp(i \frac{2\pi}{l} jx).$$

with multi-index $j \in \mathbf{Z}^d$. As we consider periodic boundary conditions, the eigenfunctions for the Galerkin space are cos and sin functions. Or when using the above complex notation they have the form $\exp(i \frac{2\pi}{l} jx)$. We define the approximation space H_N in this complex notation, but $U_N(x) \in \mathbf{R}^n$ for all $x \in \Omega$ and $U_N \in H_N$:

$$H_N = H_N^l = \left\{ \sum_{j \in \mathbf{Z}^d, \|j\| \leq N} U^j \exp(i \frac{2\pi}{l} jx) \mid U^j \in \mathbf{C}^n, U^j = \overline{U^{-j}} \right\} \quad (1.11)$$

The equation in the Galerkin space is given by

$$\begin{aligned} \dot{U}_N &= P_N \Delta U_N + P_N F(U_N) \\ U_N(0) &= P_N U_0 \end{aligned} \quad (1.12)$$

where P_N denotes the L^2 projection on the real Galerkin approximation space H_N , which is spanned by eigenfunctions of A . The ordinary differential equation (1.12) defines a local flow on H_N denoted by $S_N(t, U_N)$.

Let λ_N be the largest eigenvalue of $-Id\Delta$ restricted to H_N . Equation (1.12) is then discretized in time by some analytic one-step method (e.g. Runge-Kutta) with step size h and order k . The full discretization defines a local discrete semigroup on H_N which is analytic in U_0 and its j^{th} iterate is denoted by

$$\Phi_{h,N}^j(U_0), j = 0, 1, 2, \dots$$

We will couple the step size h and the number of Galerkin modes via

$$h \cdot \lambda_N^{1+\beta} \approx 1 \quad (1.13)$$

for $\beta > 0$. This means, we choose N for given h , such that $|h \cdot \lambda_N^{1+\beta} - 1|$ is minimal. Our main theorem for this kind of discretization is the infinite-dimensional counterpart of (1.6).

Theorem 1 Consider equation (1.7) where $F : \mathbf{R}^n \rightarrow \mathbf{R}^n$ is an entire function. Suppose, that the local semiflow $S(t, U_0)$ with $|U_0|_{H_{per}^s} \leq M_1$, defined by (1.7), remains inside the ball $B_{H_{per}^s}(M_0, 0)$ for times t with $0 < t < \tilde{T} \leq \infty$.

Let the full discretization $\Phi_{h,N}$ be real analytic in U . Let the discretization be of order p for a complex extended domain, i.e. there is $C : \mathbf{R}^+ \rightarrow \mathbf{R}^+$ with $C(r)$ bounded for $r \rightarrow 0$ independent of σ with $N(h)$ defined by (1.13)

$$|\Phi_{h,N}(U_0) - S_N(h, U_0)|_{G_\sigma^{s/2}} \leq C(|P_N U_0|_{G_\sigma^{s/2}}) h^{p+1} \quad (1.14)$$

for U_N in a complex extension of $H_N \cap B_{G_\sigma^{s/2}}(R, 0)$.

Then there exist h^* , t^* , T and a modified equation on $B_{H_{per}^s}(R, 0)$

$$\dot{\bar{U}} + A\bar{U} = F(\bar{U}) + \bar{F}(\bar{U}, h, N(h)) \quad (1.15)$$

$$\bar{U}(0) = U_0 \quad (1.16)$$

which defines a local semiflow $\bar{S}_{h,N}(t, U_0)$, such that for $0 < h \leq h^*$ and $N(h)$ defined by (1.13):

$$|\Phi_{h,N}^j(U_0) - \bar{S}_{h,N}(j \cdot h, U_0)| \leq C \left(\exp\left(-c_1 \min(t, t^*) \sqrt{\lambda_N}\right) + \exp\left(-c_2 h^{-\frac{\beta}{1+\beta}}\right) \right) \quad (1.17)$$

for $0 < t = j \cdot h < T$ with

$$T = \begin{cases} \tilde{T} & , \text{ if } \tilde{T} < \infty \\ O(h^{-\frac{\beta}{1+\beta}}, \sqrt{\lambda_N}) & , \text{ if } \tilde{T} = \infty \end{cases}$$

The constants C, c_1, c_2, t^* are independent of h and N , when choosing $N = N(h)$ as above. The possible non-local perturbation

$$\bar{F} : H_{per}^s \times [0, h^*] \times \mathbf{N} \rightarrow H_{per}^s$$

is uniformly bounded in $h \rightarrow 0, N = N(h) \rightarrow \infty$ for $U \in B_{H^s}(M_0, 0)$:

$$|\bar{F}(U)|_{H^s} \leq C_1 h^p. \quad (1.18)$$

- Remark 1**
1. The exponential estimates are fully developed after a transient time t^* . But we have to stress, that exponential estimates hold for any fixed positive time
 2. The correction \bar{F} is nonlocal, i.e. to evaluate $\bar{F}(U, h)(x)$ at a $x \in \Omega$ one has to evaluate $\bar{F}(U, h)$ in the Sobolev space first. While to evaluate the local nonlinearity $F(U)(x)$ it suffices to compute $F(U(x))$.
 3. The assumptions on $\Phi_{h,N}$ are fulfilled, when we are discretizing the equation in time by some implicit discretization schemes (e.g. higher order Runge-Kutta methods). But the order k , that these methods have as integrators of ordinary differential equations cannot be achieved, see section 2.
 4. The constant t^* is given by $t^* = \min(T^*, \frac{1}{2L})$, where T^* is the maximal Gevrey exponent as in (1.10). L is the Lipschitz constant of $F + \bar{F}$ on the ball of radius M_1 in H_{per}^s . This is up to an error $O(h^p)$ close to the Lipschitz constant of F .
 5. The essential difficulty to consider other equations is to prove Gevrey regularity. Such results hold e.g. for Navier Stokes equations with periodic boundary conditions [FT89] and for reaction diffusion equations on the sphere S^2 [CRT00].

We will prove this theorem in section 4. The main ingredient will be the embedding of the numerical scheme into a nonautonomous equation. Then we can apply the averaging techniques of [Mat99].

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2 Time integrators

Although the assumption (1.14) is standard for ordinary differential equations, it does not hold in general for parabolic partial differential equations. We give examples of discretization schemes, which fulfill the approximation assumption (1.14) of the theorem for some $p > 0$. It assumes the convergence of the method independent of N and independent of the Banach space $G_\sigma^{s/2}$. In the proof of theorem 2 we furthermore need estimates when extending $H_N \cap B_{G_\sigma^{s/2}}$ to a complex neighborhood, i.e. we have to complexify $G_\sigma^{s/2}$ for $\sigma \geq 0$. Error estimates for strongly $A(\theta)$ stable Runge-Kutta methods were given by Lubich and Ostermann in [LO93] and [LO96] in a general setting of semilinear parabolic equations on some Banach space X

$$\frac{d}{dt}U + AU = F(U), U(0) = U_0 \in X^\alpha. \quad (2.1)$$

Here A is a sectorial operator, $X^\alpha = D(A^\alpha)$ a fractional power space and $f : X^\alpha \rightarrow X$ a Lipschitz nonlinearity, see [Hen83].

The equation (1.7) fits in this setting even when posing it on Gevrey classes, since A is sectorial on $G_\sigma^{s/2}$ by the following lemma and the nonlinearity is a Lipschitz map from $G_\sigma^{s/2}$ to itself by lemma 2 in [Mat99], so we can choose $\alpha = 0$ and can take initial values in $X = G_\sigma^{s/2}$.

Lemma 2 *The operator*

$$A = -\text{diag}(d_1, \dots, d_n)\Delta$$

is sectorial on $G_\sigma^{s/2}(\Omega, \mathbf{C}^n)$ with $D(A) = G_\sigma^{s/2+1}(\Omega, \mathbf{C}^n)$.

Proof: We use definition 1.3.1 of Henry [Hen83]. A is densely defined on $G_\sigma^{s/2}$, as it is defined on finite Fourier series. To check closeness, let $u_k \xrightarrow{G_\sigma^{s/2}} u$ and $Au_k \xrightarrow{G_\sigma^{s/2}} v$. We have to show $u \in D(A)$ and $Au = v$. The convergence of Au_k in $G_\sigma^{s/2}$ gives, that u_k converges in $G_\sigma^{s/2+1}$, hence $u \in D(A)$. As A is closed on L^2 , we have by $|v - Au|_{L^2} = 0$, that the Fourier series of v and Au coincide and thus $Au = v$ in $G_\sigma^{s/2}$.

A is sectorial on $L^2(\Omega)$, the resolvent can be estimated

$$|(\lambda - A)^{-1}|_{L(L^2, L^2)} \leq M(\lambda) = \frac{M}{|\lambda + 1|},$$

for $\lambda \in \{\lambda | \phi \leq |\arg(\lambda + 1)| \leq \pi\}$ for some $\phi \in (0, \frac{\pi}{2})$ with M depending on ϕ ; see e.g. [Hen83].

As each Fourier monomial $\exp(i\frac{2\pi}{l}jx)$ is an eigenfunction of $(\lambda - A)^{-1}$, we have

$$|(\lambda - A)^{-1} \exp(i\frac{2\pi}{l}jx)|_{G_\sigma^{s/2}} \leq M(\lambda) |\exp(i\frac{2\pi}{l}jx)|_{G_\sigma^{s/2}}.$$

Thus for all $v \in G_\sigma^{s/2}(\Omega, \mathbf{C}^n)$ we get the same resolvent estimate as in L^2 :

$$|(\lambda - A)^{-1}v|_{G_\sigma^{s/2}} \leq \frac{M}{|\lambda + 1|} |v|_{G_\sigma^{s/2}}$$

for λ in a sector $\{\lambda | \phi \leq |\arg(\lambda + 1)| \leq \pi\}$ for some $\phi \in (0, \frac{\pi}{2})$. \square

In the setting of abstract semilinear parabolic equations (2.1) there are two different kind of error estimates. First there are nonsmooth error estimates for general initial values as in [LO96]. Uniform estimates for finite times can only be given after some transient: The constant in front of the expected order h^k will depend on a transient time and tend to infinity for small times. Whereas in ordinary differential equations we get as in (1.14) an estimate of order h^{k+1} for the first time step. Furthermore the order of convergence is even then too small. So they are not applicable to assure (1.14).

Secondly there are smooth error estimates. For higher order estimates we need smoothness in time starting at $t = 0$, which in general cannot be assumed for arbitrary initial conditions. Even then the full order of convergence known from the theory of ordinary differential equations is not realized in general. We will use these smooth error estimates, but instead of assuming smoothness we use the coupling of λ_N and h . We use results of Lubich and Ostermann [LO93, theorem4.1]. They consider a large class of semidiscretization in time (strongly $A(\theta)$ stable Runge-Kutta methods with internal stage order q and order k for $k \geq q + 1$). Hence the estimates will also hold uniformly in N when using the full discretization.

$$|\Phi_{h,N}(U_0) - S_N(h, U_0)|_{G_\sigma^{s/2}} \leq C \cdot (|U_N^{(q+1)}(0)|_{G_\sigma^{s/2}} + \int_0^h |U_N^{(q+1)}(t)|_{G_\sigma^{s/2}} dt) h^{q+1},$$

where $U_N^{(q+1)}(t)$ denotes the $(q + 1)$ th time derivative, which can be bounded by $C\lambda_N^{q+1}$. Using $\lambda_N^{1+\beta} h \leq 1$ gives

$$|\Phi_{h,N}(U_0) - S_N(h, U_0)|_{G_\sigma^{s/2}} \leq C(\lambda_N h)^{q+1} = Ch^{\frac{\beta(q+1)}{1+\beta}}.$$

Hence assumption (1.14) holds for full discretization with Galerkin discretization in space and some higher order strongly $A(\theta)$ stable Runge-Kutta methods like higher order Radau methods in time, when they are coupled by $\lambda_N^{1+\beta} h \leq C$ with appropriate $\beta > 0$. If we use a 3-stage RadauIIa method, then $q = 3$. To apply theorem 1, we choose $\beta = \frac{1}{2}$ and get the exponential estimates $Ch^{\frac{3}{2}} \exp(-ch^{-\frac{1}{3}})$ and $|\bar{F}| \leq Ch^{\frac{1}{3}}$ with $p = \frac{3}{2}$ in the theorem.

For linear parabolic equations with periodic boundary conditions with semigroup $S(t, U)$ and semidiscretization Φ of step size h , Lubich and Ostermann showed in [LO95] that the full order of convergence p can be achieved for finite times $t = nh \leq T$:

$$|S(n \cdot h, U_0) - \Phi^n(U_0)| \leq Ch^p$$

So perhaps the above error estimates are not optimal, because we do not use the periodic conditions.

Convergence results for discretization in space by spectral Galerkin methods can be found e.g. in [Stu95] and [DT93]. In [DT93] the Gevrey regularity is used to show exponential convergence of the Galerkin approximation, if one already starts with Gevrey regular initial values. In this paper we consider general initial values and take also the effect of time discretization into account.

3 Embedding into nonautonomous equations

An essential tool in the proof of the theorem is the embedding into a nonautonomous equation. For that we rewrite equation (1.7) as

$$\begin{aligned}\frac{\partial}{\partial t}U &= -AU + F(U) \\ U(0) &= U_0 \in H_{per}^s(\Omega, \mathbf{R}^n)\end{aligned}\tag{3.1}$$

with $A = -\text{diag}(d_1\Delta, \dots, d_n\Delta)$ on $\Omega = [0, l]^d$ with $d = 1, 2, 3$, periodic boundary conditions and $s \geq \frac{d}{2}$.

To compare the numerical scheme $\Phi_{h,N}$ with equations of type (3.1) we are going to embed $\Phi_{h,N}$ into a rapidly forced ordinary differential equation

$$\begin{aligned}\frac{\partial}{\partial t}U_N &= -AU_N + P_N F(U_N) + h^p G(U_N, \frac{t}{h}, h, N) \\ U_N(0) &= P_N U_0.\end{aligned}\tag{3.2}$$

The discretization scheme coincides exactly with the time-h map $\Psi(h, 0, \cdot)$ of a nonautonomous equation like in (3.2):

$$\Phi_{h,N}^n(U_0) = \Psi(n \cdot h, 0, P_N U_0; h, N).$$

In proposition 3 we will construct a time-periodic perturbation G of (3.2), such that its evolution $\Psi(t, 0, U_N; h, N)$ has the desired property.

The nonautonomous ordinary differential equation (3.2) can easily be extended to a partial differential equation with nonlinearities, which are non-local

$$\begin{aligned}\frac{\partial}{\partial t}U &= -AU + P_N F(P_N U) + h^p G(P_N U, \frac{t}{h}, h, N) \\ U(0) &= P_N U_0.\end{aligned}$$

Applying a theorem like the Neishtadt theorem for ordinary differential equations for our class of equations as in [Mat99], we will complete the proof of theorem 2 in section 4.

We consider the ordinary differential equation (1.12) with associated flow $S_N(t, U)$. As an adaption of [FS96, proposition 2.1] and its refinement in [ZB98] we construct a nonautonomous perturbation G as in (3.2) for our special discretization scheme with estimates uniform on its Gevrey norm in $h \rightarrow 0, N(h) \rightarrow \infty$.

Proposition 3 *Let the assumptions of theorem 1 on the nonlinearity F and the full discretization scheme $\Phi_{h,N}$ hold: $F : \mathbf{R}^n \rightarrow \mathbf{R}^n$ is real analytic in U and $\Phi_{h,N}$ is real analytic in U and h for fixed N and fulfills (1.14). Furthermore N and h are coupled as in (1.13) by setting $\lambda_N^{1+\beta} h \approx 1$ with $\beta > 0$.*

Then there exist $h^ > 0$, a nonautonomous vector field $G = G(U_N, \theta, h, N)$, a non-increasing continuous function $\rho : [0, h^*] \rightarrow (0, \infty]$ with $\rho(0) = \infty$ and a continuous non-decreasing function $r : \mathbf{R}^+ \rightarrow \mathbf{R}^+$ such that:*

- (i) $G(U_N, \theta, h, N) \in H_N$ is defined for all real θ and $0 \leq h \leq h^*$ and $U_N \in H_N$ with $|U_N|_{H_{per}^s} \leq \rho(h)$.
- (ii) For fixed N the perturbation G is C^∞ -smooth in θ and analytic in h, U_N .
- (iii) The vector field G is periodic in θ with period 1.

(iv) $\Phi_{h,N}(h, U_0) = \Psi(h, 0, P_N U_0; h, N)$, where Ψ is the evolution of (3.2).

(v) $|G(U_N, \theta, h, N)|_{G_\sigma^{s/2}} \leq r(|U_N|_{G_\sigma^{s/2}})$ independent of σ, θ, h and N .

(vi) For $D_N = H_N \cap B_{G_\sigma^{s/2}}(R, 0) \subset \mathbf{R}^k$ the perturbation G can be extended to a complex δ -neighborhood taking distances in the $G_\sigma^{s/2}$ norm:

$$\sup_{U_N \in D_N + \delta, \theta \in \mathbf{R}} |G(U_N, \theta, h, N)|_{G_\sigma^{s/2}} \leq B_2.$$

Proof:

The basic idea of the construction is to interpolate for fixed N between the identity and the numerical scheme Φ by a family $t \mapsto \Psi(t, 0, U; h, N)$ of diffeomorphisms with

$$\begin{aligned} \Psi(0, 0, U; h, N) &= 0 \\ \Psi(h, 0, U; h, N) &= \Phi_{h,N}(h, U). \end{aligned}$$

An evolution is then defined, omitting the other arguments, by

$$\Psi(t, s) = \Psi(t, 0) \circ \Psi(s, 0)^{-1}.$$

This can be extended to $t \notin [0, h]$ by iteration. We repeat the construction of [FS96]. This interpolation is done in step 1. In step 2 we will construct G , such that $-A + P_N F + G$ is the time derivative of Ψ . The properties (i)-(iv) will be checked in step 3. The estimates in (v) and (vi) will be derived in step 4.

Step 1: Interpolation

Choose $\chi : \mathbf{R} \rightarrow [0, 1]$ a C^∞ cut-off function analytic in $\tau \neq 0, 1$ with

$$\chi(\tau) = \begin{cases} 1 & \text{for } \tau \leq 0 \\ 0 & \text{for } \tau \geq 1. \end{cases}$$

Then we define Ψ by interpolation for $t \in [0, h]$

$$\Psi(t, 0, U_N; h, N) := \chi\left(\frac{t}{h}\right) S_N(t, U_N) + (1 - \chi\left(\frac{t}{h}\right)) S_N(t - h, \Phi_{h,N}(h, U_N)). \quad (3.3)$$

As S_N is only a local flow in time, we need the restriction $|U_N|_{H^s} \leq \rho(h)$, then

$$\Psi(0, 0, U_N; h, N) = S_N(0, U_N) = U_N \quad (3.4)$$

$$\Psi(h, 0, U_N; h, N) = S_N(0, \Phi_{h,N}(U_N)) = \Phi_{h,N}(U_N). \quad (3.5)$$

We can then extend the definition to all $t \geq 0$ by

$$\Psi(t, 0, U_N; h, N) := \Psi\left(t - \left\lfloor \frac{t}{h} \right\rfloor h, 0, \Phi_{h,N}^{\left\lfloor \frac{t}{h} \right\rfloor}(U_N); h, N\right). \quad (3.6)$$

Thus Ψ is an interpolation of $\Phi(n \cdot h, U_N)$, $n \in \mathbf{Z}$. Then

$$\Psi(t, 0, \Psi(n \cdot h, 0, U_N; h, N); h, N) = \Psi(t + n \cdot h, 0, U_N; h, N)$$

and the curve $t \mapsto \Psi(t, 0, U_N; h, N)$ is clearly analytic for $\frac{t}{h} \notin \mathbf{N}$. By the recursion formula above, it is enough to check C^∞ -smoothness at $t = h$ to prove that $t \mapsto \Psi(t, 0, U_N; h, N)$ is

C^∞ . We denote by D_\pm^m the m^{th} t -derivative from above (+) and from below (-). Then we get for arbitrary m dropping dependence on h, N :

$$\begin{aligned}
& D_+^m|_{t=h}\Psi(t, 0, U_N) \\
&= D_+^m|_{t=0}\Psi(t, 0, \Phi_{h,N}(U_N)) \\
&= D_+^m|_{t=0}\left(\chi\left(\frac{t}{h}\right)S_N(t, \Phi_{h,N}(U_N)) + (1 - \chi\left(\frac{t}{h}\right))S_N(t - h, \Phi_{h,N}^2(U_N))\right) \\
&= D_+^m|_{t=0}S_N(t, \Phi(h, U_N)) = D_-^m|_{t=0}S_N(t, \Phi(h, U_N)) \\
&= D_-^m|_{t=h}\left(\chi\left(\frac{t}{h}\right)S_N(t, U_N) + (1 - \chi\left(\frac{t}{h}\right))S_N(t - h, \Phi_{h,N}(U_N))\right) \\
&= D_-^m|_{t=h}\Psi(t, 0, U_N).
\end{aligned}$$

This proves C^∞ -regularity of Ψ in t .

Step 2: Construction of G

To construct the perturbation we rescale time by $\theta = \frac{t}{h}$, then we denote

$$\tilde{\Psi}(\theta, 0, U_N; h, N) = \Psi(\theta h, 0, U_N; h, N). \quad (3.7)$$

Thus we have for $\theta \in [0, 1]$:

$$\tilde{\Psi}(\theta, 0, U_N; h, N) = \chi(\theta)S_N(h\theta, U_N) + (1 - \chi(\theta))S_N(h\theta - h, \Phi_{h,N}(h, U_N)).$$

We define

$$G(U_N, \theta; h, N) := h^{-p}\left(h^{-1}D_\theta\tilde{\Psi}(\theta, 0, V_N; h, N) - (-AU_N + P_N F(U_N))\right) \quad (3.8)$$

where $V_N = V_N(U_N, \theta; h, N)$ is defined implicitly by

$$U_N = \tilde{\Psi}(\theta, 0, V_N; h, N). \quad (3.9)$$

This can be solved for V_N by the implicit function theorem. $\tilde{\Psi}$ is analytic in h, V_N and smooth in Θ . For $h = 0$ the trivial solution is $V_N = V_N(U_N, \theta; 0, N) = U_N$ by (3.4) and the linearisation $D_{V_N}\tilde{\Psi}(\theta, 0, V_N; 0, N) = Id$ is invertible. Hence we can solve (3.9) for $V_N = V_N(U_N, \theta; h, N)$ uniformly for $0 \leq h \leq h^*$ in a ball $|U_N| \leq \rho(h)$ and $\tilde{\Psi}$ is defined. Thus V_N will be defined on a reduced domain $0 \leq \theta \leq 2, 0 \leq h \leq h^*, |U_N| \leq \rho(h)$.

Step 3: Basic properties of G

First we extend the domain of G to all real θ by 1-periodic extension to show (iii). Thus we have to check periodicity for $0 \leq \theta \leq 2$. Let $0 \leq \theta \leq 1, h > 0$ then we get from (3.6)

$$\tilde{\Psi}(\theta, 0, \Phi_{h,N}(V_N(U_N, \theta + 1; h, N))); h, N) = \tilde{\Psi}(\theta + 1, 0, V_N(U_N, \theta + 1; h, N)); h, N) = U_N$$

which implies by applying $\tilde{\Psi}(\theta, 0)^{-1}$ on both sides

$$\Phi_{h,N}(V_N(U_N, \theta + 1; h, N)) = V_N(U_N, \theta; h, N).$$

Hence we get when dropping arguments h and N :

$$\begin{aligned}
& h^{p+1}(G(U_N, \theta + 1) - G(U_N, \theta)) \\
&= D_\theta\tilde{\Psi}(\theta + 1, 0, V_N(\theta + 1)) - D_\theta\tilde{\Psi}(\theta, 0, V_N(\theta)) \\
&= D_\theta\tilde{\Psi}(\theta, 0, \Phi_{h,N}V_N(\theta + 1)) - D_\theta\tilde{\Psi}(\theta, 0, V_N(\theta)) \\
&= D_\theta\tilde{\Psi}(\theta, 0, V_N(\theta)) - D_\theta\tilde{\Psi}(\theta, 0, V_N(\theta)) = 0,
\end{aligned}$$

proving periodicity for $h > 0$. Next we will extend G down to $h = 0$. Let d_j denote various remainder terms real analytic in $0 \leq h \leq h^*$, $|U_N| \leq \rho(h)$ and C^∞ in θ . By the p^{th} order approximation property we have

$$\Phi_{h,N}(U_N) = S_N(h, U_N) + h^{p+1}d_0$$

This implies

$$\begin{aligned} \tilde{\Psi}(\theta, U_N) &= \chi(\theta)S_N(h\theta, U_N) + (1 - \chi(\theta))S_N(h\theta - h, \Phi_{h,N}(h, U_N)) \\ &= \chi(\theta)S_N(h\theta, U_N) + (1 - \chi(\theta))S_N(h\theta - h, S_N(h, U_N)) \\ &\quad + (1 - \chi(\theta)) [S_N(h\theta - h, \Phi_{h,N}(U_N)) - S_N(h\theta - h, S_N(h, U_N))] \\ &= S_N(h\theta, U_N) + h^{p+1}d_1. \end{aligned} \quad (3.10)$$

When replacing U_N by V_N and using $\tilde{\Psi}(\theta, 0, V_N(\theta, U_N)) = U_N$, this yields to

$$V_N(\theta, U_N) = S_N(-h\theta, U_N) + h^{p+1}d_2. \quad (3.11)$$

From (3.10,3.11) we obtain

$$\begin{aligned} h^{-1}D_\theta\tilde{\Psi}(\theta, V_N(\theta, U_N)) &= -AS_N(h\theta, V_N) + P_NF(S_N(h\theta, V_N)) + h^{-1}D_\theta h^{p+1}d_1 \\ &= -AU_N + P_NF(U_N) + h^{p+1}d_3 + h^pD_\theta d_1 \end{aligned}$$

where

$$h^{p+1}d_3 = (-A + P_NF)(S_N(h\theta, S_N(-h\theta, U_N) + h^{p+1}d_2)) - (-AU_N + P_NF(U_N)). \quad (3.12)$$

Setting $G = hd_3 + D_\theta d_1$ gives the differentiability requirements in (ii) and by continuous extension to $h = 0$ also (iii) can be proved. Then G is defined on $[0, h^*]$ for $\theta \in \mathbf{R}$ and $|U_N| \leq \rho(h)$, thus proving (i). The interpolation property (iv) is fulfilled by construction of Ψ .

Step 4: Estimates uniform in $h, N(h)$

Properties (v) and (vi) are the essential new ingredients to [FS96, proposition2.1]. We show first the estimates for $G = hd_3 + D_\theta d_1$ in (v). Starting with $D_\theta d_1$, we obtain by (3.10):

$$\begin{aligned} h^{p+1}D_\theta d_1 &= D_\theta [(1 - \chi(\theta)) (S_N(h\theta - h, \Phi_{h,N}(U_N)) - S_N(h\theta - h, S_N(h, U_N)))] \\ &= -\chi'(\theta) (S_N(h\theta - h, \Phi_{h,N}(U_N)) - S_N(h\theta - h, S_N(h, U_N))) \\ &\quad + (1 - \chi(\theta))h (-AS_N(h\theta - h, \Phi_{h,N}(U_N)) \\ &\quad + P_NF(S_N(h\theta - h, \Phi_{h,N}(U_N))) + AS_N(h\theta - h, S_N(h, U_N)) \\ &\quad - P_NF(S_N(h\theta - h, S_N(h, U_N)))). \end{aligned}$$

Using the mean value theorem we get, where

$$K = \{V \in \eta \Phi_{h,N}(U_N) + (1 - \eta)S_N(h, U_N), \eta \in [0, 1]\},$$

$$\begin{aligned} &h^{p+1}|D_\theta d_1|_{G_\sigma^{s/2}} \\ &\leq |\Phi_{h,N}(U_N) - S_N(h, U_N)|_{G_\sigma^{s/2}} \left[|\chi'(\theta)| \sup_K |DS_N(h\theta - h, V)|_{L(G_\sigma^{s/2}, G_\sigma^{s/2})} \right. \\ &\quad \left. + h|1 - \chi(\theta)| \sup_K |D(AS_N(h\theta - h, V) + P_NF(S_N(h\theta - h, V)))|_{L(G_\sigma^{s/2}, G_\sigma^{s/2})} \right]. \end{aligned}$$

So we need to estimate $|D_V S_N(h\theta - h, V)|_{L(G_\sigma^{s/2}, G_\sigma^{s/2})}$. To do this we use the variational equation, which is fulfilled by $W(t) = D_V S_N(t, V(t))$:

$$W_t + AP_N W = D_V P_N F(P_N V(t))W.$$

Thus we get

$$\begin{aligned} |D_V S_N(h\theta - h, V)|_{G_\sigma^{s/2}} &\leq |\exp(-A(h\theta - h))P_N|_{G_\sigma^{s/2}} \\ &+ \left| \int_0^{h\theta - h} \exp(-A(h\theta - h - \vartheta)) D_V P_N F(P_N V(\vartheta)) d\vartheta \right|_{G_\sigma^{s/2}}. \end{aligned} \quad (3.13)$$

To bound this expression, we first have to analyze

$$V(t) = \exp(-At)P_N V_0 + \int_0^t \exp(-A(t - \vartheta)) P_N F(V(\vartheta)) d\vartheta.$$

The linear part can be bounded using $h\lambda_N^{1+\beta} \approx 1$. $P_N F$ is locally Lipschitz on H_N with constants $L(V_N)$ uniformly bounded for $N \rightarrow \infty$ in the Gevrey norm of $G_\sigma^{s/2}$, thus we can bound $V(t)$ by a constant C for $|t| \leq h$ and $N \leq N(h)$ by the Gronwall inequality:

$$\begin{aligned} |V(t)|_{G_\sigma^{s/2}} &\leq C + \int_0^t C |P_N F(V(\vartheta))| d\vartheta \\ &\leq C + \int_0^t CL |V(\vartheta)|_{G_\sigma^{s/2}} d\vartheta \leq C. \end{aligned}$$

Then (3.13) is uniformly bounded when using $h\lambda_N^{1+\beta} \approx 1$. Using the bound (1.14) for $|\Phi_{h,N}(U_N) - S_N(h, U_N)|_{G_\sigma^{s/2}}$ we have the estimate

$$h^{p+1} |D_\theta d_1|_{G_\sigma^{s/2}} \leq (c + hC\lambda_N) C (|U_N|_{H_\sigma^{s/2}}) h^{p+1} \leq CC (|U_N|_{G_\sigma^{s/2}}) h^{p+1}, \quad (3.14)$$

as $\lambda_N h < \lambda_N^{1+\beta} h \approx 1$ is bounded.

Next we deal with

$$h^{p+1} d_3 = (-A + P_N F)(S_N(h\theta, S_N(-h\theta, U_N) + h^{p+1} d_2)) - (-AU_N + P_N F(U_N)),$$

hence we get an estimate depending on d_2 , where

$$K = \{V \in S_N(-h\theta, U_N) + \eta h^{p+1} d_2, \eta \in [0, 1]\}$$

$$\begin{aligned} h^{p+1} |d_3|_{G_\sigma^{s/2}} &\leq \sup_K |D(AS_N(h\theta, V) + P_N F(S_N(h\theta, V)))|_{L(G_\sigma^{s/2}, G_\sigma^{s/2})} h^{p+1} |d_2|_{G_\sigma^{s/2}} \\ &\leq |\lambda_N + L| C h^{p+1} |d_2|_{G_\sigma^{s/2}} \leq C h^p |d_2|_{G_\sigma^{s/2}}. \end{aligned} \quad (3.15)$$

It remains to estimate d_2 given by (3.11)

$$h^{p+1} d_2(U_N, \theta) = V_N(\theta, U_N) - S_N(-h\theta, U_N).$$

From (3.10) we get

$$S_N(-h\theta, \tilde{\Psi}(\theta, U_N) - h^{p+1} d_1(U_N)) = U_N.$$

Then replacing U_N by $V_N(U_N)$ yields to

$$S_N(-h\theta, U_N - h^{p+1}d_1(V_N)) = V_N.$$

Hence

$$h^{p+1}d_2(U_N, \theta) = S_N(-h\theta, U_N - d_1(V_N)) - S_N(-h\theta, U_N)$$

with

$$h^{p+1}|d_2(U_N, \theta)|_{G_\sigma^{s/2}} \leq Ch^{p+1}|d_1(V_N, \theta)|_{G_\sigma^{s/2}}.$$

$V_N(U_N, \theta)$ is defined by $\tilde{\Psi}(\theta, V_N(U_N, \theta), h) = U_N$, where $\tilde{\Psi}$ is a near-identity diffeomorphism. So V_N remains uniformly bounded per construction. Hence we can estimate d_1 in the way as $D_\theta d_1$ above and we get $h^{p+1}|d_1(V_N, \theta)|_{G_\sigma^{s/2}} \leq Ch^{p+1}$ and thus $h^{p+1}|d_3(U_N, \theta)|_{G_\sigma^{s/2}} \leq Ch^p$ for $U_N \in G_\sigma^{s/2}$ bounded. Hence for $G = hd_3 + D_\theta d_1$ we obtain

$$|G(U_N, \theta, h, N)|_{G_\sigma^{s/2}} \leq r(|U_N|_{G_\sigma^{s/2}})$$

and (v) is shown.

It remains to check (vi). We need uniform bounds when extending G to a complex domain $D_N + \delta$. First we check that $S_N(h\theta, U_N)$ does not leave $D_N + \delta_0$ for $\theta \in [0, 1]$ and $U_N \in D_N + \delta$: For the imaginary part of U_N we get the following equation:

$$\frac{d}{dt}\text{Im}(U_N) = -A\text{Im}(U_N) + \text{Im}(F(U_N)).$$

As $\text{Im}(F(U_N)) = 0$ for $\text{Im}(U_N) = 0$, there is a linear factor of $\text{Im}(U_N)$ in $\text{Im}(F(U_N))$. Thus we can estimate using the Gronwall inequality

$$\begin{aligned} |\text{Im}(S_N(h\theta, U_N))|_{G_\sigma^{s/2}} &\leq |e^{-h\theta A}\text{Im}(U_N(0)) + \int_0^{h\theta} e^{-(h\theta-\tau)A}\text{Im}(F(U_N(\tau)))d\tau|_{G_\sigma^{s/2}} \\ &\leq \delta + \int_0^{h\theta} C\text{Im}(U_N(\tau))d\tau \leq \delta e^{h\theta C} \leq \delta e^{h^*C} = \delta_0, \end{aligned}$$

and $S_N(h\theta, U_N)$ does not leave a slightly enlarged complex extended domain. Now all estimates for (v) still hold in the extended domain, essentially because the error estimate $|\Phi_{h,N}(U_0) - S_N(h, U_0)|_{G_\sigma^{s/2}} \leq C(|U_N(0)|_{G_\sigma^{s/2}})h^{p+1}$ given in (1.14) does extend to the complex extended domain by assumption. This completes the proof of the proposition. \square

4 Proof of Theorem 1

We are now in the position to prove theorem 1. By proposition 3 the numerical scheme $\Phi_{h,N}$ coincides exactly with the time- h map of the ordinary differential equation

$$\dot{U}_N + AU_N = P_N F(U_N) + h^p G(U_N, \frac{t}{h}, h, N).$$

We extend this equation to a partial differential equation

$$\dot{\tilde{U}} + A\tilde{U} = P_N F(P_N \tilde{U}) + h^p G(P_N \tilde{U}, \frac{t}{h}, h, N(h)) \quad (4.1)$$

with a local time evolution $\tilde{S}(t, 0, \cdot)$, such that the numerical scheme and $\tilde{S}(t, 0, P_N U_0)$ coincide. We want to apply [Mat99] to (4.1). There are two groups of hypotheses, which

imply regularity in time-averaging of our class of parabolic partial differential equations. We consider equations

$$\frac{\partial}{\partial t}U - D\Delta U = F(U) + h^p G(U, \frac{t}{h}, h).$$

The first hypothesis (H.1) is to assure, that the solutions are Gevrey regular

$$\begin{aligned} U_0 &\in H_{per}^s \text{ with } s > \frac{d}{2} \\ F(\cdot), G(\cdot, t) &: B_{G_\sigma^{s/2}}(R, 0) \rightarrow G_\sigma^{s/2} \text{ differentiable in } U \\ F'(U), G'(U) &\in \dot{L}(L^2(\Omega, \mathbf{R}^n), L^2(\Omega, \mathbf{R}^n)) \text{ for } U \text{ bounded in } H_{per}^s \\ G &\text{ continuous in } t, h \\ F(\cdot), G(\cdot) &\text{ bounded with constants not depending on } \sigma, t : \\ |F(U)|_{G_\sigma^{s/2}} &\leq C_s a(C_s |U|_{G_\sigma^{s/2}}) \\ |G(U, t)|_{G_\sigma^{s/2}} &\leq C_s b(C_s |U|_{G_\sigma^{s/2}}) \\ &\text{with } a, b \text{ monotone increasing on } [0, \frac{R}{C_s}] \end{aligned} \tag{H.1}$$

The second hypothesis (H.2) describes the needed analytic properties of F and G restricted to Galerkin approximation spaces.

$$\begin{aligned} P_N F, P_N G : D_N &\rightarrow H_N \text{ is real analytic for all } N \in \mathbf{N} \\ \sup_{U_N \in D_N + \delta} |P_N F(U_N)|_{G_\sigma^{s/2}} &\leq B_1 \\ \sup_{U_N \in D_N + \delta, t \in \mathbf{R}} |P_N G(U_N, t, h)|_{G_\sigma^{s/2}} &\leq B_2 \end{aligned} \tag{H.2}$$

Then the following version of [Mat99, theorem 2 with (3.17),(3.22),(3.23), remark 9] holds:

Theorem 2 *Assume that the hypotheses (H.1) and (H.2) hold. Let G be periodic in $\tau = \frac{t}{h}$ with period 1 and fix the perturbation order $p > 0$. Suppose for initial values U_0 with $|U_0|_{H^s} \leq M_1$, that the forward orbit remains bounded, i.e. $|S(U_0, t)|_{H^s} \leq M_0 < R$ for $t \in [0, T]$. Then there exists a real analytic and time-periodic change of coordinates for $0 < h < h_1$*

$$U = V + hW(V, \frac{t}{h}, h) \tag{4.2}$$

with the following properties: W is bounded on H_{per}^s . Its image $W(H_{per}^s, \frac{t}{h}, h)$ is finite dimensional for fixed h and $W(\cdot, 0, \cdot) = 0$. The transformed nonautonomous terms are exponentially small after a transient, but the equation may contain additional non-local terms $\bar{F} = (\bar{f}_1, \dots, \bar{f}_n)$:

$$\frac{\partial}{\partial t}V - D\Delta V = F(V) + \bar{F}(V, h) + \alpha(V, \frac{t}{h}, h) + b_1(V, \frac{t}{h}, N, h) + b_2(V, \frac{t}{h}, N, h), \tag{4.3}$$

The dimension of approximation space $N(h)$ is given by $\lambda_N^{1+\beta} h \approx 1$. Then the correction terms are given by

$$b_1 = (I - P_N) \left\{ F(V + hW(P_N V)) - F(V) + h^p G(V + hP_N W(V), \frac{t}{h}, h) \right\} \tag{4.4}$$

$$\begin{aligned} b_2 &= \left[I + h \frac{\partial}{\partial P_N V} W(P_N V) \right]^{-1} P_N \{ F(V + hW(P_N V)) - F(P_N V + hW(P_N V)) \\ &\quad + h^p G(V + hW(P_N V), \frac{t}{h}, h) - h^p G(P_N V + hW(P_N V), \frac{t}{h}, h) \}. \end{aligned} \tag{4.5}$$

or can be estimated by

$$\begin{aligned} \sup_{|V|_{H_{per}^s} < M_0} |\bar{F}(V)|_{H_{per}^s} &\leq c_3 h^p \\ \sup_{|V|_{H_{per}^s} < M_1} |\alpha(V)|_{H_{per}^s} &\leq c_2 h^p \exp(-c_1 h^{-\frac{\beta}{1+\beta}}) \end{aligned}$$

Here the constants c_1, c_2, c_3, h_1 only depend on B_1 and B_2 . Furthermore \bar{F} and α are smooth in h .

We apply this theorem to (4.1). So we only have to replace $F(\cdot)$ by $P_N F(P_N \cdot)$, where N is given by the discretization scheme. First we check the assumptions of the theorem. By [Mat99, remark 6] F and therefore $P_N F$ fulfill (H.1) and (H.2). The perturbation term G satisfies (H.1) and (H.2) by proposition 3.

As the nonlinearities in (4.1) have their range in H_N only, the form (4.3) in theorem 2 can be improved. We obtain $b_1 \equiv b_2 \equiv 0$ when using the same N for the discretization and theorem 2, see (4.4,4.5). b_1 is zero, because $P_N F(P_N \cdot)$ and G have their range in $H_N = \ker(I - P_N)$. b_2 is zero, because components outside H_N do not change the values of $P_N F(P_N \cdot)$ and G . So we get by the above theorem an averaged equation

$$\begin{aligned} \dot{V} + AV &= P_N F(P_N V) + \bar{F}(V, h) + \alpha(V, \frac{t}{h}, h, N(h)) \\ V(0) &= P_N U_0 \end{aligned}$$

with local evolution $\tilde{S}_V(t, 0, P_N U_0)$ and strong estimates on the nonautonomous part:

$$\sup_{V(0) \in B_{H_{per}^s}(M_1, 0) \times \mathbf{R}^+ \times [0, h_1]} |\alpha|_{H_{per}^s} \leq c_2 h^p \exp(-c_1 h^{-\frac{\beta}{1+\beta}}).$$

We also have

$$\tilde{S}_V(n \cdot h, 0, P_N U_0) = \Phi_{h, N}^n(U_0), \quad (4.6)$$

since the coordinate change W is zero on multiples of the period h .

The modified equation (1.15) given in theorem 1 is then

$$\dot{\bar{U}} + A\bar{U} = F(\bar{U}) + \bar{F}(\bar{U}, h, N(h)) \quad (4.7)$$

$$\bar{U}(0) = U_0 \quad (4.8)$$

which defines a local semiflow $\bar{S}_{h, N}(t, U_0)$ depending on N and h . The estimates on \bar{F} in (1.18) then also follow from theorem 2.

Estimating the difference between $\bar{U}(t) = \bar{S}_{h, N}(t, U_0)$ and $V(t) = \tilde{S}_V(t, 0, P_N U_0)$ will prove the desired exponential estimate (1.17) because of (4.6). We use $P_N V(\tau) = V(\tau)$ and that $\exp(-A(t - \tau))U(\tau) \in G_t^{s/2}$, if $U(\tau) \in G_\tau^{s/2}$. The time T^* denotes the maximal Gevrey exponent as in (1.10).

$$\begin{aligned} &|\bar{U}(t) - V(t)|_{H^s} \\ &= |\bar{S}_{h, N}(t, U_0) - \tilde{S}_V(t, 0, P_N U_0)|_{H^s} \\ &= |\exp(-At)(Id - P_N)U_0|_{H^s} + \left| \int_0^t \exp(-A(t - \tau)) \{F(\bar{U}(\tau)) + \bar{F}(\bar{U}(\tau)) \right. \\ &\quad \left. - P_N F(P_N V(\tau)) - \bar{F}(V(\tau)) - \alpha(V(\tau), \frac{\tau}{h}, h, N(h))\} d\tau \right|_{H^s} \end{aligned}$$

$$\begin{aligned}
& \text{adding inside the integral } 0 = -P_N F(\bar{U}(\tau)) + P_N F(\bar{U}(\tau)) \\
\leq & |U_0|_{H_{per}^s} \exp(-\lambda_{N+1}t) + \left| \int_0^t \exp(-A(t-\tau)) \{F(\bar{U}(\tau)) - P_N F(\bar{U}(\tau)) \right. \\
& \left. + P_N F(\bar{U}(\tau)) - P_N F(V(\tau))\} d\tau \right|_{H^s} \\
& + L \int_0^t |V(\tau) - \bar{U}(\tau)|_{H^s} d\tau + tc_2 h^p \exp(-c_1 h^{-\frac{\beta}{1+\beta}}) \\
\leq & |U_0|_{H_{per}^s} \exp(-\lambda_{N+1}t) + t2B_1 \exp\left(-\sqrt{\lambda_{N+1}} \min(t, T^*)\right) + tc_2 h^p \exp\left(-c_1 h^{-\frac{\beta}{1+\beta}}\right) \\
& + L \int_0^t |V(\tau) - \bar{U}(\tau)|_{H^s} d\tau.
\end{aligned}$$

We consider first small times $t \leq \min(\frac{1}{2L}, T^*)$, where L is the Lipschitz constant of $\bar{F}(\cdot) + P_N F(P_N \cdot)$. This Lipschitz constant is close to the Lipschitz constant of F as an operator on a suitable ball in H_{per}^s . \bar{F} is analytic on a complex extension of a bounded domain in H_N . Using the Cauchy estimate, we get $D\bar{F} \leq Ch^p$ as in [Mat99].

The last inequality implies for $t \leq t^* = \min(\frac{1}{2L}, T^*)$

$$\begin{aligned}
y(t) &= \max_{0 \leq \tau \leq t} |\bar{U}(\tau) - V(\tau)|_{H^s} \leq C(t) \\
&:= 2 \left(|U_0|_{H_{per}^s} \exp(-\lambda_{N+1}t) + t2B_1 \exp\left(-\sqrt{\lambda_{N+1}} \min(t, T^*)\right) \right. \\
&\quad \left. + tc_2 h^p \exp\left(-c_1 h^{-\frac{\beta}{1+\beta}}\right) \right) \\
&\leq C \left(\exp\left(-\sqrt{\lambda_{N+1}}t\right) + \exp\left(-c_1 h^{-\frac{\beta}{1+\beta}}\right) \right).
\end{aligned}$$

For large times $t \geq t^* = \min(\frac{1}{2L}, T^*)$ we use a simple Gronwall inequality and get exponential estimates:

$$\begin{aligned}
|\bar{U}(t) - V(t)|_{H^s} &\leq C(t^*) (\exp(L(t-t^*))) \\
&\leq C \left(\exp\left(-\sqrt{\lambda_{N+1}}t^*\right) + \exp\left(-c_1 h^{-\frac{\beta}{1+\beta}}\right) \right) \exp(L(t-t^*)).
\end{aligned}$$

This implies the desired exponential estimate (1.17) on a time-scale $O\left(h^{-\frac{\beta}{1+\beta}}, \sqrt{\lambda_{N(h)}}\right)$, where the constants C, c_1, c_2, t^* do not depend on h and $N = N(h)$. The theorem is proved. \square

5 Global Errors

In this section we use the modified equation to describe some aspects of the long-time behavior of the analyzed numerical scheme. Several dynamical features of semilinear parabolic equations are replicated by numerical methods usually with an error of the order h , for a review see [Stu95].

Consider for example an equilibrium U_0 of the semi-group defined by (1.7), i.e. $S(t, U_0) = U_0, \forall t \geq 0$. It is supposed to be a hyperbolic, thus for any fixed time $t > 0$ the spectrum σ of the linearisation $DS(t, U_0)$ at U_0 splits into two parts by the unit circle: there exists $\alpha \in (0, 1)$ such that $\sigma = \sigma_s \cup \sigma_u$

$$\sigma_s = \{\lambda \in \sigma \mid |\lambda| < \alpha\} \text{ and } \sigma_u = \{\lambda \in \sigma \mid |\lambda| > \alpha^{-1}\}.$$

Then in [Stu95, chapter4] it is shown, that several numerical schemes with step size h have a hyperbolic equilibrium U_h with $|U_h - U_0| \leq Ch$. The respective phase portraits are close of order h , too. We compare the numerical scheme with the modified equation. We can show, that our discretization scheme $\Phi_{h,N}$ replicates the dynamics of a slightly modified partial differential equation near an equilibrium, with an exponentially small error.

The stable and unstable eigenspaces of the linearisation at a hyperbolic equilibrium U_0 are denoted by E^s and E^u and orthogonal projections on them by P^s and P^u . The local stable and unstable manifolds are then given by the graphs of

$$\begin{aligned} p_s &: E^s \cap B_{H^s}(\rho, 0) \rightarrow E^u \text{ for the stable and} \\ p_u &: E^u \cap B_{H^s}(\rho, 0) \rightarrow E^s \text{ for the unstable manifold.} \end{aligned}$$

Proposition 4 *Suppose the original equation (1.7) possesses a hyperbolic equilibrium at U_0 . Then the numerical scheme $\Phi_{h,N}$ with a coupling like in (1.13) with $\beta = \frac{1}{2}$ has a hyperbolic periodic orbit of period h : $\Phi_{h,N}(U_h) = U_h$, which is exponentially close to a hyperbolic equilibrium \bar{U}_h of the modified equation (1.15) with:*

$$|U_h - \bar{U}_h|_{H^s} \leq C \exp(-ch^{-\frac{1}{3}}) \quad (5.1)$$

$$|\bar{U}_h - U_0|_{H^s} \leq Ch. \quad (5.2)$$

All further results compare the discrete semigroup $\Phi_{h,N}^j(\cdot), j \geq 0$ with $\bar{S}(t, \cdot)$. There exists $\rho > 0$ such that the local stable and unstable manifolds of U_h, \bar{U}_h are given by graphs of functions

$$\begin{aligned} p_s^h(\cdot), \bar{p}_s^h(\cdot) &: E^s \cap B_{H^s}(\rho, 0) \rightarrow E^u \\ p_u^h(\cdot), \bar{p}_u^h(\cdot) &: E^u \cap B_{H^s}(\rho, 0) \rightarrow E^s \end{aligned}$$

in the following way with $u_s \in E^s \cap B_{H^s}(\rho, 0)$:

$$W^{s,loc}(U_h) = U_h + u_s + p_s^h(u_s)$$

and in the same way for the other manifolds too. Moreover the local unstable manifolds are exponentially close on $B_{H^s}(\rho, U_0)$:

$$\sup_{U \in P^u(B_{H^s}(\rho, 0))} |(p_u^h(U) + U_h) - (\bar{p}_u^h(U) + \bar{U}_h)|_{H^s} \leq C \exp(-ch^{-\frac{1}{3}}) \quad (5.3)$$

and the local stable manifolds are exponentially close on $B_{H^s}(\rho, 0)$ intersected with the image of $W^{s,loc}(U_h)$ under the regularizing map $\Phi_{h,N}^{[T^*/h]}(\cdot)$:

$$\sup_{U \in P^s(B_{H^s}(\rho, 0) \cap \Phi_{h,N}^{[T^*/h]}(W^{s,loc}(U_h)))} |p_s^h(U) + U_h - (\bar{p}_s^h(U) + \bar{U}_h)|_{H^s} \leq C \exp(-ch^{-\frac{1}{3}}). \quad (5.4)$$

On $B_{H^s}(\rho, U_0) \cap \Phi_{h,N}^{[T^*/h]}(B_{H^s}(\rho, 0))$ the orbits of $\Phi_{h,N}(\cdot)$ are exponentially followed by orbits of $\bar{S}^h(t, \cdot)$ in the following sense: For all $U \in B_{H^s}(\rho, 0) \cap \Phi_{h,N}^{[T^*/h]}(B_{H^s}(\rho, 0))$ there exists $V \in B_{H^s}(\rho, 0) \cap \bar{S}^h(T^*, B_{H^s}(\rho, 0))$, such that as long $\bar{S}^h(t, U) \in B_{H^s}(\rho, 0)$ we have that $t = j \cdot h, j \in \mathbf{N}$

$$|\Phi_{h,N}^j(U) - \bar{S}(j \cdot h, V)|_{H_{per}^s} \leq C \exp(-ch^{-\frac{1}{3}}). \quad (5.5)$$

Proof: This proposition is given for the comparison of rapidly forced equations and averaged equations in [Mat99, proposition11]. The rapidly forced equation coincides exactly with the numerical scheme at multiples of the step size h and the averaged equation is replaced by the modified equation (1.15). \square

Hence the special full discretization scheme, discussed in this paper replicates the dynamical behavior near hyperbolic equilibria with an exponentially small error – when we are comparing it with a modified equation. Using the modified equation more geometric theory of the considered discretization scheme can be developed, e.g. the analysis of the influence of rapid forcing on homoclinic orbits [Mat99, proposition14] holds in the same way for the discretization scheme. Using the modified equation one should be also able to analyze the influence of discretization on other invariant objects like periodic orbits, attractors, etc. more accurately.

References

- [BG94] G. Benettin, A. Giogilli, On the Hamiltonian interpolation of near to the identity symplectic mappings with application to symplectic integration algorithms, *J. Stat. Phys.* **74**, (1994), 1117-1143.
- [CRT00] C. Cao, M. Rammaha, E. Titi, Gevrey regularity for nonlinear analytic parabolic equations on the sphere, *Journ. Dynamics Diff. Eq.*, to appear.
- [DT93] A. Doelman, E. Titi, Regularity of solutions and the convergence of the Galerkin method in the Ginzburg-Landau equation, *Numer. Funct. Anal. Optimiz.* **143**,4 (1993), 299-321.
- [EDHJ95] K. Eriksson, D. Estep, P. Hansbo, C. Johnson, Introduction to adaptive methods for differential equations, in Iserles, A. (ed.), *Acta Numerica 1995*, Cambridge University Press, Cambridge (1995), 105-158.
- [FT98] A. Ferrari, E. Titi, Gevrey regularity for nonlinear analytic parabolic equations, *Comm. Part. Diff. Eq.* **23** (1998), 1-16.
- [FS96] B. Fiedler, J. Scheurle, *Discretization of homoclinic orbits, Rapid Forcing and "Invisible" Chaos*, Memoirs AMS, Vol. **570** (1996).
- [FT89] C. Foias, R. Temam, Gevrey Class Regularity for the solution of the Navier Stokes Equations, *J. Funct. Anal.* **87** (1989), 359-369.
- [HL97] E. Hairer, C. Lubich, The life-span of backward error analysis for numerical integrators, *Numer. Math.* **76** (1997), 441-462.
- [HL99] E. Hairer, C. Lubich, Asymptotic expansions and backward error analysis for numerical integrators, In " *Dynamics of Algorithms* (R. de la Llave, L.R. Petzold, J. Lorenz, eds.), Springer IMA Vol. **118** (2000), 91-106.
- [Hen83] D. Henry, *Geometric Theory of Semilinear Parabolic Equations*, Lecture Notes in Mathematics **840**, Springer-Verlag, New-York (1983).
- [LO93] C. Lubich, A. Ostermann, Runge-Kutta methods for parabolic equations and convolution quadrature, *Mathematics of Computation* **60** (1993), 105-131.

- [LO95] C. Lubich, A. Ostermann, Interior estimates for time discretization of parabolic equations, *Appl. Numer. Math.* **18** (1995), 241-251.
- [LO96] C. Lubich, A. Ostermann, Runge-Kutta time discretization of reaction-diffusion and Navier-Stokes equations: nonsmooth-data error estimates and long time behaviour, *Appl. Numer. Math.* **22** (1996), 279-292.
- [Mat99] K. Matthies, Time-averaging under fast periodic forcing of parabolic partial differential equations: Exponential estimates, Preprint FU Berlin 1999.
- [Nei84] A. Neishtadt, On the separation of motions in systems with rapidly rotating phase, *J. Appl. Math. Mech.* **48** (1984), 134-139.
- [Rei99] S. Reich, Backward error analysis for numerical integrators, *SIAM Num. Anal.* **36** (1999), 1549-1570.
- [San92] J.M.Sanz-Serna, Syplectic integrators for Hamiltonian problems: an overview, *Acta Numerica* **1** (1992), 243-286.
- [Stu95] A. Stuart, *Perturbation theory for infinite dimensional dynamical systems*, in M.Ainsworth, J.Levesley, W.A.Light, M.Merletta(eds), Theory and Numerics of ordinary and partial differential equations, Advances in Numerical Analysis **IV**, Clarendon Press, Oxford (1995), 181-290.
- [Tem88] R. Temam, *Infinte-dimensional dynamical systems in Mechanics and Physics*, Applied Mathematical Sciences **68**, Springer-Verlag, New-York (1988).
- [ZB98] Y. Zou, W.Beyn, Invariant Manifolds for Nonautonomous Systems with Applications to One-Step methods, *Journ. Dyn. Diff. Eq.* **10** (1998), 379-407.