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Numerical convergence for semilinear parabolic equations

Robert Huth

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Weierstrass Institute
Mohrenstr. 39
10117 Berlin
Germany
E-Mail: Robert.huth@wias-berlin.de

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Weierstraß-Institut für Angewandte Analysis und Stochastik (WIAS)
Leibniz-Institut im Forschungsverbund Berlin e. V.
Mohrenstraße 39
10117 Berlin
Germany

Fax: +49 30 20372-303
E-Mail: preprint@wias-berlin.de
World Wide Web: <http://www.wias-berlin.de/>

We present a convergence result for finite element discretisations of semilinear parabolic equations, in which the evaluation of the nonlinearity requires some high order of regularity of the solution. For example a coefficient might depend on derivatives or pointevaluation of the solution. We do not rely on high regularity of the exact solution itself and as a payoff we can not deduce convergence rates. As an example the convergence result is applied to a nonlinear Fokker–Planck type battery model.

1 Introduction

The existing literature provides numerical convergence results for semilinear parabolic problems. One can easily find results for reaction-diffusion equations, Allen-Cahn or Cahn-Hilliard equations, see for example [JLTW87, TW75, Tho06, CH02, FP03, EL92]. The prototype of an reaction-diffusion equations without specifying further details like boundary conditions or assumptions on appearing expressions, is

$$\partial_t u = \Delta u + f(u) \quad \text{and} \quad f : \mathbb{R} \rightarrow \mathbb{R} .$$

The key difference to our setting is that in the reaction-diffusion equation f maps from L^p to L^q when interpreted as an operator acting on functions. On the other hand, the nonlinear problem in our consideration, see the example in Section 4, has the form

$$\partial_t u = \Delta u + N(u, t) , \quad \text{and} \quad N : H^\theta \times \mathbb{R} \rightarrow H^{-1} .$$

Here the nonlinearity maps from an interpolation space H^θ into H^{-1} . Hence some steps when attempting to prove numerical convergence are not possible for this setting, because the convergence of some u_h in L^p does not allow us to conclude convergence of $N(u_h, t)$. Another helpfull tool used for standard convergence results is not available for us. It is the method of deriving error estimates by exploiting high regularity of the exact solution. This could be the use of an interpolation estimates in H^1 which exploit the boundedness of the solution in H^2 . In our application we do not have such a regularity.

Our arguments are of abstract form. We are able to state that for a sequence of space discretisation fineness $h_j \rightarrow 0$ and a sequence of time step-size $k_j \rightarrow 0$ the numerical solutions converge to the exact solution. For this, h_j and k_j must vanish together in a suitable way. As our arguments are abstract and not constructive, we lack to say what this suitable way might be. Nevertheless, the achieved convergence result gives confidence that numerical solutions are related to an exact solutions of a PDE at hand. This is a nontrivial question for nonlinear problems.

We deduce the desired convergence in two steps. First, we show convergence of a semi-discretised system, which is a discretisation in space only, but not in time. To do so, we derive a priori bounds for the discrete solutions U_{h_j} , which do not depend on the discretisation parameter. Hence for $h_j \rightarrow 0$ a subsequence of U_{h_j} converges weakly. We identify the limit as the exact solution of the original problem. The uniqueness of the exact solution gives the weak convergence of the whole sequence. In the second step we employ standard arguments for the numerical integration of ODEs in \mathbb{R}^n . Thus, we carry the convergence of the semi-discretised problem over to the fully discretised one. We do not derive convergence rates or necessary relations between space and time discretisation. The difficulty is here, the convergence of the semi-discrete problem when discretised only in space. If one is able to improve the convergence results presented here and derive a priori estimates for the error of the semi-discrete solutions, then one could use techniques of Lubich and Ostermann [LO96] to further derive estimates for the error of the time discretisation.

The use of semigroup techniques to show numerical convergence, is motivated by a paper by Bakaev [Bak02]. The author exploits, for linear parabolic problems, the connection of the discrete operators to their undiscretised counterparts. Considering only linear problems, Bakaev is able to derive error estimates for the discrete semigroup and even for the fully discretised problem. Earlier works that consider only linear problems go back to Eriksson et al. [EJL98]. The usage of semigroup techniques for semilinear problems was also done by Geissert in [Gei07]. Geissert derives error estimates for the semi-discretised problem. The allowed nonlinearities in [Gei07] exclude explicitly the nonlinear dependence on the solution in high regularity, which is the aim of this work.

In the following we first introduce our notation, define a problem prototype and state the necessary assumptions in Section 2. Then we derive the numerical convergence result in Section 3. It is presented in an abstract way such that it can be applied to a wide range of problems. In Section 4 we apply the numerical convergence result to an example problem which stems from the modelling of the charging of a lithium-ion battery. This problem demonstrates the appearance of a nonlinearity which does not allow to apply known results. It also demonstrates how one can weaken the assumption of linear growth for the nonlinear term, in the case, where the exact solution stays bounded in a suitable way.

2 Assumptions and Definitions

We consider a complex Hilbert space \mathbb{X} with norm $\|\cdot\|_0$ and inner product $(\cdot, \cdot)_0$. Furthermore we denote by \mathbb{V} a dense subspace of \mathbb{X} , equipped with norm $\|\cdot\|_1$. The subspace \mathbb{V} shall also be a Hilbert space and we denote its dual by \mathbb{V}^{-1} with norm $\|\cdot\|_{-1}$. The spaces form a cascade of canonical embeddings

$$\mathbb{V} \hookrightarrow \mathbb{X} = \mathbb{X}^{-1} \hookrightarrow \mathbb{V}^{-1} .$$

In the sequel we will also use $\|\cdot\|_e$ and $(\cdot, \cdot)_e$ for the Euclidean norm and inner product. The spaces \mathbb{V} and \mathbb{V}^{-1} are closely related to the operator A .

Assumption 2.1. Let $-A : D(A) \subset \mathbb{V} \rightarrow \mathbb{V}^{-1}$ be a linear and sectorial operator with compact resolvent and densely embedded domain $D(A) = \mathbb{V} \hookrightarrow \mathbb{V}^{-1}$, such that there exist constants $m > 0$, $\omega < 0$ and $\theta \in]\pi/2, \pi[$, satisfying

$$\begin{aligned} \rho(-A) \supset S_{\theta, \omega} &:= \{\lambda \in \mathbb{C} : \lambda \neq \omega, |\arg(\lambda - \omega)| \leq \theta\}, \\ \|R(\lambda, -A)v\|_{-1} &\leq \frac{m}{|\lambda - \omega|} \|v\|_{-1} \quad \text{for all } v \in \mathbb{V}, \lambda \in S_{\theta, \omega}. \end{aligned}$$

By $\rho(-A)$ we denote the resolvent set of $-A$. Furthermore we assume, that A is selfadjoint and gives the norm and scalar product in \mathbb{V} by

$$\|v\|_1 := \sqrt{(v, v)_1}, \quad (v, w)_1 := \langle Av, \bar{w} \rangle,$$

which results into the identity $\|v\|_1 = \|Av\|_{-1}$.

The operator A shall also be weakly closed. This means, that for any sequence $v_j \in \mathbb{V}$ such that $Av_j \rightharpoonup w$ in \mathbb{V}^{-1} , there must exist $v \in \mathbb{V}$ such that $v_j \rightarrow v$ in \mathbb{V}^{-1} and $Av = w$.

Note that a simple consequence of $m > 0$ and $\omega < 0$ is the existence of a constant c_A , such that

$$\|v\|_1 = \|Av\|_{-1} \geq c_A \|v\|_{-1}. \quad (1)$$

Whenever calculations will depend on m , ω , θ or c_A , we say that they depend on the sectorial properties of A . With this notion we can also define intermediate spaces for $\theta \in [-1, 1]$ as the domains of fractional powers of A , by

$$\mathbb{V}^\theta = D(A^{\frac{\theta+1}{2}}) \quad \text{with norm: } \|v\|_\theta := \|A^{\frac{1+\theta}{2}} v\|_{-1}, \quad (2)$$

which are compactly embedded into each other, such that

$$\mathbb{V}^{\theta_2} \hookrightarrow \mathbb{V}^{\theta_1} \quad \text{for all } 0 \leq \theta_1 \leq \theta_2 \leq 1. \quad (3)$$

This compact embedding can be deduced from the assumption of compact resolvents. A usual setting when working with parabolic PDEs is $\mathbb{X} = L^2(\Omega)$, $A = \Delta$, the Laplacian, and $\mathbb{V} = H_0^1(\Omega)$.

We also introduce a general form of a discretisation of A on a finite dimensional subspace. For $n \in \mathbb{N}$ and a set of linear independent elements $\{\varphi_j\}_j \subset \mathbb{V}$, we define

$$\mathbb{V}_h = \text{span}\{\varphi_1, \varphi_2, \dots, \varphi_n\} \subset \mathbb{V}, \quad (4)$$

which is by construction isomorph to \mathbb{C}^n . We define the matrices A_h , M_h and D_h as

$$A_{hi,j} = \langle A\varphi_i, \varphi_j \rangle, \quad M_{hi,j} = (\varphi_i, \varphi_j)_0, \quad D_h = M_h^{-1} A_h. \quad (5)$$

Note that M_h and A_h are invertible, symmetric and positive definite matrices. Thus D_h exists and is also invertible. First, we introduce some notation. We define suitable norms in the finite

dimensional subspaces and give relations to norms in spaces, in which they are embedded. Let $v_h \in \mathbb{C}^n$, then we define the canonical embedding operator

$$T_h : \mathbb{C}^n \rightarrow \mathbb{V}, \quad T_h v_h = \sum_{j=1}^N (v_h)_j \varphi_j. \quad (6)$$

Next to T_h , we introduce the projection $P_h : \mathbb{V}^{-1} \rightarrow \mathbb{C}^n$, which is for any given $w \in \mathbb{V}^{-1}$ defined as the solution of

$$\langle w, T_h v_h \rangle_{\mathbb{V}} = (P_h w, M_h v_h)_e \quad \text{for all } v_h \in \mathbb{C}^n. \quad (7)$$

By the identity $(T_h P_h w, T_h v_h)_0 = (P_h w, M_h v_h)_e$, we see that $T_h P_h$ is the \mathbb{X} -orthogonal projection into \mathbb{V}_h . Furthermore we need that the projection P_h is stable in the \mathbb{V} norm. The precise meaning of stability is formulated in the following assumption.

Assumption 2.2. *There exists a constant c_P , such that for any $v \in \mathbb{V}$ there holds*

$$\|T_h P_h v\|_1 \leq c_P \|v\|_1. \quad (8)$$

The crucial point is, that c_P does in general depend on the choice or construction of the discrete space \mathbb{V}_h . Consequently, the inequality (8) imposes extra conditions when considering a family of discrete spaces \mathbb{V}_{h_j} , namely that there is a c_P independent of j . For sufficient conditions to satisfy this stability for the L^2 projection, we refer to Bramble, Pasciak and Steinbach [BPS02]. In practice quasiuniform meshes satisfy this condition, but Bramble et al. prove that even weaker conditions suffice.

We define for $v_h \in \mathbb{C}^n$ discrete versions of norms,

$$\|v_h\|_{h,1} := \|T_h v_h\|_1, \quad \|v_h\|_{h,-1} := \sup_{w_h \in \mathbb{V}_h^1, \|w_h\|_{h,1}=1} (T_h v_h, T_h w_h)_0, \quad (9)$$

$$\|v_h\|_{h,M} := \|T_h v_h\|_0. \quad (10)$$

Imitating the notation for the original space \mathbb{V} and \mathbb{V}^{-1} , we will use the following names for \mathbb{C}^n when equipped with the above norms

$$\mathbb{V}_h^{-1} := (\mathbb{C}^n, \|\cdot\|_{h,-1}), \quad \mathbb{V}_h^M := (\mathbb{C}^n, \|\cdot\|_{h,M}), \quad \mathbb{V}_h^1 := (\mathbb{C}^n, \|\cdot\|_{h,1}).$$

The discrete norms $\|\cdot\|_{h,M}$ and $\|\cdot\|_{h,1}$ are standard for this type of methods and they simply result from the mapping T_h . The more interesting definition is the norm $\|\cdot\|_{h,-1}$. It stems from the question of how a vector $v_h \in \mathbb{C}^n$ can be interpreted as an element of the dual space of $\mathbb{V}_h^1 := (\mathbb{C}^n, \|\cdot\|_{h,1})$. Such an interpretation is defined by the action of $w_h \in \mathbb{V}_h^{-1}$ on another element $v_h \in \mathbb{V}_h^1$. The definition of the norm above belongs to the choice

$$\langle w_h, v_h \rangle_{\mathbb{V}_h^1} := (T_h v_h, T_h w_h)_0 = (M_h v_h, w_h)_e.$$

This mimics the canonical embedding $\mathbb{V} \hookrightarrow \mathbb{X} \hookrightarrow \mathbb{V}^{-1}$. Furthermore this allows us to fit the discretised setting in the context of sectorial operators and express the norm $\|\cdot\|_{h,1}$ by $\|\cdot\|_{h,-1}$

and D_h . Note that we have the identity $\|v_h\|_{h,1} = \|A_h^{\frac{1}{2}}v_h\|_e$ and so we can deduce from (9) by changing w_h to $z_h := A_h^{\frac{1}{2}}w_h$,

$$\begin{aligned} \|v_h\|_{h,-1} &= \sup_{z_h \in \mathbb{C}^N, \|z_h\|_e=1} (M_h A_h^{-\frac{1}{2}} z_h, v_h)_e = \|A_h^{-\frac{1}{2}} M_h v_h\|_e, \\ \Rightarrow \|D_h v_h\|_{h,-1} &= \|A_h^{-\frac{1}{2}} M_h M_h^{-1} A_h v_h\|_e = \|v_h\|_{h,1}. \end{aligned}$$

The norm $\|v_h\|_{h,-1}$ is only bounded from above by $\|T_h v_h\|_{-1}$ because by (9)

$$\|v_h\|_{h,-1} \leq \sup_{w \in \mathbb{V}, \|w\|_1=1} (T_h v_h, w)_0 = \|T_h v_h\|_{-1}. \quad (11)$$

By the assumed stability of the projection P_h in (8), we can also achieve a bound from below. Take any $v_h \in \mathbb{V}_h^{-1}$, then

$$\begin{aligned} \|T_h v_h\|_{-1} &= \sup_{w \in \mathbb{V}, \|w\|_1=1} (w, T_h v_h)_0 = \sup_{w \in \mathbb{V}, \|w\|_1=1} (M_h P_h w, v_h)_e \\ &= \sup_{w \in \mathbb{V}, \|w\|_1=1} \langle v_h, P_h w \rangle_{\mathbb{V}_h^{-1}} \leq \sup_{w \in \mathbb{V}, \|w\|_1=1} \|v_h\|_{h,-1} \|P_h w\|_{h,1} \leq \|v_h\|_{h,-1} c_P, \end{aligned}$$

and hence

$$\frac{1}{c_P} \|T_h v_h\|_{-1} \leq \|v_h\|_{h,-1} \leq \|T_h v_h\|_{-1}. \quad (12)$$

Now we state the general form of problems and their discretised versions, for which we want to show the desired convergence of the approximative solutions. We define the finite time interval $S =]0, T_0]$, $0 < T_0 < \infty$, and let N be a mapping from $\mathbb{V}^\gamma \times S$ into \mathbb{V}^{-1} for a $\gamma \in [-1, 1[$. Then we seek for solutions to the operator differential equation

$$\partial_t u(t) = -Au(t) + N(u(t), t), \quad u(0) = u_0, \quad (13)$$

for some $u_0 \in \mathbb{V}^{-1}$. Its discretised version is an ODE in \mathbb{C}^n ,

$$\partial_t U(t) = -D_h U(t) + P_h N(T_h U(t), t), \quad U(0) = Q_h u_0, \quad (14)$$

with a suitable mapping Q_h . Thus, the discretised version of N is $P_h N(T_h \cdot, \cdot)$, which maps $\mathbb{C}^n \times \mathbb{R}$ into \mathbb{C}^n . The possibly nonlinear mapping N must satisfy the following assumption.

Assumption 2.3. *Let $\gamma \in]0, 1[$. The mapping $N : \mathbb{V}^\gamma \times S \rightarrow \mathbb{V}^{-1}$ is locally Lipschitz continuous in the first argument and Hölder continuous with Hölder exponent $\alpha_N > \frac{1}{2}$ in the second. This means there exists an increasing function g , such that for all $v_1, v_2 \in \mathbb{V}^\gamma$ and $s_1 < s_2 \in \mathbb{R}$,*

$$\|N(v_1, s_1) - N(v_2, s_2)\|_{-1} \leq g(\|v_1\|_\gamma + \|v_2\|_\gamma) \left(\|v_1 - v_2\|_\gamma + |s_1 - s_2|^{\alpha_N} \right). \quad (15)$$

We also assume that there exist constants $c_1 \geq 0, c_2 \geq 0$, such that for all $s \in S$ and $v \in \mathbb{V}^\gamma$ there holds

$$\|N(v, s)\|_{-1} \leq c_1 + c_2 \|v\|_\gamma. \quad (16)$$

This assumption guarantees the existence of solutions for both problems, (13) and (14), since it permits to deduce a priori bounds to the solution for any finite time.

3 Numerical Convergence in a general framework

In order to derive a priori bounds of solutions to (14), which are independent of the specific choice of \mathbb{V}_h , we use the notion of sectorial operators. We transform techniques from the existence proofs for semilinear parabolic PDEs to the semi-discretised setting. For this we need knowledge about the discretised operator as stated in the following lemma. For simple Problems one could use known results for the eigenvalues of special matrices, as they appear in the stiffness matrices for the discretised Laplacian, see for example [Yue05]. In order to keep the results applicable for various problems and types of discretisations, we derive properties of the discretised elliptic operator in a rather abstract form.

Lemma 3.1. *The matrix $-D_h$, as defined in (5), considered as an operator*

$$D_h : \mathbb{V}_h^{-1} \rightarrow \mathbb{V}_h^{-1} ,$$

is sectorial. That means there exist constants $\theta \in]\pi/2, \pi[$, $m > 0$ and $\omega \in \mathbb{R}$ such that

$$\begin{aligned} \rho(-D_h) \supset S_{\theta, \omega} &:= \{ \lambda \in \mathbb{C} : \lambda \neq \omega, |\arg(\lambda - \omega)| \leq \theta \} , \\ \|R(\lambda, -D_h)v_h\|_{h,-1} &\leq \frac{m}{|\lambda - \omega|} \|v_h\|_{h,-1} \quad \text{for all } v_h \in \mathbb{V}_h^{-1}, \lambda \in S_{\theta, \omega}. \end{aligned}$$

The constants θ , m and $\omega < 0$ are independent from the exact choice of the subspace \mathbb{V}_h and depend on the sectorial properties of $-A$.

Proof. The Matrix D_h inherits properties from A . This can be seen by the following estimate, where we used $\|\cdot\|_{h,-1} \leq \|\cdot\|_{-1}$,

$$\inf_{v_h \in \mathbb{C}^n} \frac{\|D_h v_h\|_{h,-1}}{\|v_h\|_{h,-1}} = \inf_{v_h \in \mathbb{C}^n} \frac{\|T_h v_h\|_1}{\|v_h\|_{h,-1}} \geq \inf_{v_h \in \mathbb{C}^n} \frac{\|T_h v_h\|_1}{\|T_h v_h\|_{-1}} \geq \inf_{v \in \mathbb{V}^1} \frac{\|v\|_1}{\|v\|_{-1}} \geq c_A > 0 .$$

The constant c_A stems from (1) and obviously does not depend on the choice of the subspace \mathbb{V}_h , but on the sectorial properties of A .

Before we deduce estimates for the resolvent of D_h , we want to show that D_h is a selfadjoint and positive definite operator. We denote the inner product in \mathbb{V}_h^{-1} by $(\cdot, \cdot)_{h,-1}$. It satisfies the equality

$$(\cdot, \cdot)_{h,-1} = (A_h^{-\frac{1}{2}} M_h \cdot, A_h^{-\frac{1}{2}} M_h \cdot)_e = (A_h^{-1} M_h \cdot, M_h \cdot)_e ,$$

and so for any $v_h \in \mathbb{V}_h^{-1} \sim \mathbb{C}^N$ which is not zero, there holds

$$(D_h v_h, v_h)_{h,-1} = (v_h, M_h v_h)_e = \|v_h\|_{h,M}^2 = (M_h v_h, v_h)_e = (v_h, D_h v_h)_{h,-1} > 0 .$$

Now we consider for any $\lambda \in \mathbb{C}$ satisfying $\operatorname{Re} \lambda \geq -c_A/2$, the resolvent $R(\lambda, -D_h) = (\lambda + D_h)^{-1}$. For this we inspect the expression

$$\begin{aligned} \|(\lambda + D_h)v_h\|_{h,-1}^2 &= |\lambda|^2 \|v_h\|_{h,-1}^2 + (D_h v_h, \lambda v_h)_{h,-1} + (\lambda v_h, D_h v_h)_{h,-1} + \|D_h v_h\|_{h,-1}^2 , \\ &= |\lambda|^2 \|v_h\|_{h,-1}^2 + 2\operatorname{Re}(\lambda) (D_h v_h, v_h)_{h,-1} + \|D_h v_h\|_{h,-1}^2 . \end{aligned}$$

In the case of $\text{Re}\lambda \geq 0$ one easily deduces that

$$\|(\lambda + D_h)v_h\|_{h,-1}^2 \geq |\lambda|^2 \|v_h\|_{h,-1}^2 .$$

In the case of $\text{Re}\lambda < 0$ we use that $(D_h v_h, v_h)_{h,-1} \leq \|D_h v_h\|_{h,-1} \|v_h\|_{h,-1}$ and employ the estimate $\|D_h v_h\|_{h,-1}^2 \geq c_A \|D_h v_h\|_{h,-1} \|v_h\|_{h,-1}$ to get

$$\|(\lambda + D_h)v_h\|_{h,-1}^2 \geq \|v_h\|_{h,-1}^2 \lambda^2 + \|D_h v_h\|_{h,-1} \|v_h\|_{h,-1} (2\text{Re}(\lambda) + c_A) .$$

Since by assumption $2\text{Re}(\lambda) + c_A > 0$ and $\|D_h v_h\|_{h,-1} \|v_h\|_{h,-1} \geq c_A \|v_h\|_{h,-1}^2$ we arrive at

$$\begin{aligned} \|(\lambda + D_h)v_h\|_{h,-1}^2 &\geq \|v_h\|_{h,-1}^2 [(\text{Re}(\lambda) + c_A)^2 + \text{Im}(\lambda)^2] \geq \|v_h\|_{h,-1}^2 [\text{Re}(\lambda)^2 + \text{Im}(\lambda)^2] , \\ &\geq \|v_h\|_{h,-1}^2 |\lambda|^2 . \end{aligned}$$

Thus, we deduced that $(\lambda + D_h)$ is invertible for all $\lambda \in \mathbb{C}$ with $\text{Re}\lambda \geq -c_A/2$ and furthermore for $R(\lambda, -D_h) = (\lambda + D_h)^{-1}$ we get

$$\|\lambda R(\lambda, -D_h)v_h\|_{h,-1} \leq \|v_h\|_{h,-1} , \quad \text{for all } \lambda \in \mathbb{C}, \text{Re}\lambda \geq -c_A/2 .$$

According to [Lun95, Prop.2.1.11], this estimate is sufficient for D_h to be sectorial with constants $\omega = -c_A/2 < 0$, $m = 2$ and $\theta = \frac{3}{4}\pi$ independent of the exact choice of \mathbb{V}_h . \square

This insight allows us to use semigroup techniques for further estimates. In order to do this we need to connect the norm in \mathbb{V}^θ , $\theta \in [-1, 1]$, for which we want to derive bounds, with the norms $\|\cdot\|_{h,-1}$ and $\|\cdot\|_{h,1}$, which are related to the mentioned semigroup in \mathbb{C}^n . We do so by using that $\|T_h \cdot\|_1 = \|\cdot\|_{h,1}$ and the estimate for $\|T_h \cdot\|_{-1}$ in (12). Thus for $\theta \in [-1, 1]$ and $\sigma \geq 0$ there holds for all $v_h \in \mathbb{C}^n$

$$\|T_h v_h\|_\theta \leq c \|T_h v_h\|_{-1}^{\frac{1-\theta}{2}} \|T_h v_h\|_1^{\frac{1+\theta}{2}} \leq c \|v_h\|_{h,-1}^{\frac{1-\theta}{2}} \|v_h\|_{h,1}^{\frac{1+\theta}{2}} \leq c \|v_h\|_{h,1} . \quad (17)$$

One identity, which we will exploit extensively, is the variation of constants formula. This formula is satisfied for U , the solution to (14), and for all t in the existence interval of the solution. It reads

$$U(t) = e^{-D_h t} U(0) + \int_0^t e^{-D_h(t-s)} P_h N(T_h U(s), s) ds . \quad (18)$$

Even though $e^{-D_h t}$ is the well defined exponential function of a sectorial matrix, we interpret it at the same time with the semigroup generated by the sectorial operator D_h with domain \mathbb{V}_h^1 . This allows us to use various techniques to derive estimates for the solutions depending on the sectorial properties of D_h . Those properties do not depend on the exact construction of \mathbb{V}_h , i.e. the choice and number of basis functions, see Lemma 3.1. We thus derive uniform bounds which must hold for any discretisation \mathbb{V}_h . The most essential inequality is an estimate for the semigroup $e^{-D_h t}$. It is derived from the estimate $\|D_h^\sigma e^{-D_h t} v_h\|_{h,-1} \leq c t^{-\sigma} \|v_h\|_{h,-1}$, $\sigma \geq 0$, which holds for any sectorial operator D_h which generates a contractive semigroup. Then there exists a constant c such that for any $v_h \in \mathbb{C}^N$ there holds

$$\|T_h D_h^\sigma e^{-D_h t} v_h\|_\theta \leq c t^{-\sigma} t^{\frac{1-\theta}{2}} t^{-(1+\sigma)\frac{1+\theta}{2}} \|v_h\|_{h,-1} = c t^{-\sigma - \frac{1+\theta}{2}} \|v_h\|_{h,-1} , \quad (19)$$

where the constant c depends on the sectorial properties of D_h and c_p from (8), because we used (17). As a consequence we formulate the following Lemma.

Lemma 3.2. Let $\gamma \in [0, 1[$. If Assumption 2.3 holds and there is a bound K , such that

$$\|T_h U_0\|_{h,1} \leq K, \quad (20)$$

then we know that the solution $U : S \rightarrow \mathbb{C}^n$ to (14) is bounded in the sense that there is a constant c , such that

$$\|T_h U(t)\|_\gamma \leq c, \quad \text{for all } t \in S \quad (21)$$

and c does not depend on the choice or dimension of \mathbb{V}_h .

Proof. We use (18), (17) and (19) to get for any $t \in S$

$$\begin{aligned} \|T_h U(t)\|_\gamma &\leq \|T_h e^{-tD_h} U(0)\|_\gamma + \|T_h \int_0^t e^{-(t-s)D_h} P_h N(U(s), s) \, ds\|_\gamma \\ &\leq c \|U(0)\|_{h,1} + c \int_0^t (t-s)^{-\frac{1+\gamma}{2}} \|P_h N(T_h U(s), s)\|_{h,-1} \, ds. \end{aligned}$$

Then we employ Assumption 2.3 to get the inequality

$$\|T_h U(t)\|_\gamma \leq c(\|U(0)\|_{h,1} + t^{\frac{1-\gamma}{2}}) + c \int_0^t (t-s)^{-\frac{1+\gamma}{2}} \|T_h U(s)\|_\gamma \, ds,$$

which allows us to use Gronwall's lemma. This then results by the boundedness of the time interval S , into the existence of a uniform bound to $\|T_h U(t)\|_\gamma$ for all times $t \in S$. The constants which appeared in the estimates along the way depended on the sectorial properties of D_h . These are independent of the choice and dimension of \mathbb{V}_h , see Lemma 3.1. Hence, as asserted in this lemma, the quality of the final bound in (21) does not depend on them as well. \square

The bound for the numerical solution, which we derived in the last lemma, helps us to treat the locally Lipschitz continuity of N as Lipschitz, i.e. drop the *locally* in *locally Lipschitz continuous*. This gives rise to better regularity of the discrete solution.

Lemma 3.3. Define the bounded time interval $S := [0, T_0]$. Let $U : S \rightarrow \mathbb{C}^n$ be the solution to ODE (14), and let Assumptions 2.1 to 2.3 hold. If there exists a bound K such that

$$\|U(0)\|_{h,1} \leq K \quad (22)$$

then $T_h U$ is Hölder continuous in \mathbb{V}^θ for any $\theta \in [-1, 1[$ in the sense that for all $t_1, t_2 \in S$

$$\|T_h U(t_1) - T_h U(t_2)\|_\theta \leq C |t_1 - t_2|^{\frac{1-\theta}{2}}. \quad (23)$$

We even have for $\sigma := \min(\alpha_N, \frac{1-\gamma}{2})$ the time regularity of

$$U \in C^1(S, \mathbb{V}_h^{-1}) \cap C(S, \mathbb{V}_h^1), \quad (24)$$

$$T_h \partial_t U \in C(S, \mathbb{V}^{-1}), \quad (25)$$

$$\{t \mapsto P_h N(T_h U(t), t)\} \in C^\sigma(S, \mathbb{V}_h^{-1}). \quad (26)$$

The bounds in these spaces, as well as C , depend on N and the sectorial properties of A , but not on the exact choice or dimension of \mathbb{V}_h .

Proof. In the proof we follow the reasoning in the book of Lunardi, [Lun95]. The main adjustment is that we consider two kinds of spaces. On the one hand there are the spaces \mathbb{V} , \mathbb{V}^{-1} and the interpolation spaces \mathbb{V}^θ whereas on the other hand we have the discretised spaces \mathbb{V}_h^1 , \mathbb{V}_h^{-1} and the interpolation spaces \mathbb{V}_h^θ defined by D_h . We use identities and estimates between the norms of those two types to switch between them when needed. For convenience we will carry out the proof of (23), following the proof of Proposition 4.2.1 in [Lun95]. Note that indeed all constants do not depend on the exact choice of \mathbb{V}_h .

We use the fact that the solution U must satisfy the variation of constants formula. For $0 < t_1 < t_2 < T_0$ this gives rise to

$$\begin{aligned} \|T_h U(t_2) - T_h U(t_1)\|_\theta &\leq \|T_h \left(e^{-D_h t_2} - e^{-D_h t_1} \right) U(0)\|_\theta \\ &\quad + \|T_h \int_0^{t_1} \left(e^{-D_h(t_2-s)} - e^{-D_h(t_1-s)} \right) P_h N(T_h U(s), s) \, ds\|_\theta \\ &\quad + \|T_h \int_{t_1}^{t_2} e^{-D_h(t_2-s)} P_h N(T_h U(s), s) \, ds\|_\theta \\ &\leq I + II + III. \end{aligned}$$

We estimate the three terms separately. Note that the following estimates use integrals which only exist if $\theta < 1$ and so this is a necessary bound for θ .

The first term is not very critical and we can easily deduce an estimate by (19),

$$\begin{aligned} I &= \|T_h \int_0^{t_2-t_1} -D_h e^{-D_h s} e^{-D_h t_1} U(0) \, ds\|_\theta, \\ &\leq c \int_0^{t_2-t_1} s^{-\frac{1+\theta}{2}} \|D_h e^{-D_h s} e^{-D_h t_1} U(0)\|_{h,-1} \, ds, \leq c(t_2 - t_1)^{\frac{1-\theta}{2}} \|U(0)\|_{h,1}. \end{aligned}$$

Note that even though the generic constant c might change from step to step, it only depends on the sectorial properties of D_h , which themselves depend on the sectorial properties of A , see Lemma 3.1.

The second and third term can be estimated by additionally exploiting the boundedness of $P_h N(T_h U(t), t)$ in the \mathbb{V}_h^{-1} -norm. This is true according to Assumption 2.3, Lemma 3.2 and the simple inequality $\|P_h v\|_{h,-1} \leq \|v\|_{-1}$. This uniform inequality for P_h is true for any $v \in \mathbb{V}^{-1}$ and can easily be deduced by the definition of P_h in (7). Using these ingredients we get

$$\begin{aligned} II &\leq \int_0^{t_1} \int_{t_1-s}^{t_2-s} \|T_h D_h e^{-D_h r} P_h N(T_h U(s), s)\|_\theta \, dr \, ds, \\ &\leq c \int_0^{t_1} \int_{t_1-s}^{t_2-s} r^{-\frac{3+\theta}{2}} \, dr \, ds \leq c(t_2 - t_1)^{\frac{1-\theta}{2}}, \\ III &\leq c \int_{t_1}^{t_2} (t_2 - s)^{-\frac{1+\theta}{2}} \, ds \leq c(t_2 - t_1)^{\frac{1-\theta}{2}}. \end{aligned}$$

These three estimates combined, result in a constant c independent of the choice of the subspace \mathbb{V}_h , such that

$$\|T_h U(t_2) - T_h U(t_1)\|_\theta \leq c |t_1 - t_2|^{\frac{1-\theta}{2}}. \quad (27)$$

This proves the first assertion in this lemma.

We use the boundedness of $T_h U$ in \mathbb{V}^γ and deduce from the Hölder continuity of $T_h U$ in (27) and the locally Lipschitz continuity of N in Assumption 2.3, that $f(t) := P_h N(U(t), t) \in C^\sigma(S, \mathbb{V}_h^{-1})$ with $\sigma = \min(\alpha_N, \frac{1-\theta}{2})$. The norm of f in $C^\sigma(S, \mathbb{V}_h^{-1})$ is bounded from above independent of the choice of \mathbb{V}_h . This is the proof of (26).

We can then apply known regularity results for non-homogeneous equations of the form $\partial_t u = -D_h u + f(t)$, see [Lun95, thm.4.3.1]. Exploiting the regularity of the initial value, see (22), we then know that

$$U \in C^1(S, \mathbb{V}_h^{-1}) \cap C(S, \mathbb{V}_h^{-1}), \quad (28)$$

with norm bounded from above depending on the sectorial properties of D_h . This gives the desired quality (24). Consequently, $\partial_t U$ is bounded and continuous in \mathbb{V}_h^{-1} , which gives by (12) the continuity and boundedness of $T_h \partial_t U$ in \mathbb{V}^{-1} . \square

With the previous lemmata we can derive the convergence of approximations U_j , where each U_j is the solution to a discretisation of the PDE (13) on a space \mathbb{V}_{h_j} in the form of (14). The sequence of spaces \mathbb{V}_{h_j} fills up the whole space in the limit for $j \rightarrow \infty$. The subscript h_j shall suggest that this is usually accomplished by a space discretisation with a grid size $h_j \rightarrow 0$.

Theorem 3.4. *Assume that the mapping $N : \mathbb{V}^\gamma \times \mathbb{C} \rightarrow \mathbb{V}^{-1}$ is locally Lipschitz in the first argument and locally Hölder continuous in the second, as described in Assumption 2.3. We consider a sequence of finite dimensional subspaces $\mathbb{V}_{h_j} \subset \mathbb{V}$ of the form (4), which in the limit are dense in \mathbb{V} . By this we mean*

$$\begin{aligned} & \text{for all } v \in \mathbb{V} \text{ there exists a sequence } v_{h_j} \in \mathbb{V}_{h_j}^1, j = 1, 2, \dots, \text{ such that,} \\ & T_{h_j} v_{h_j} \rightarrow v \text{ in } \mathbb{V}. \end{aligned} \quad (29)$$

Furthermore, we need for the sequence \mathbb{V}_{h_j} that the respective projections P_{h_j} are stable, as described in Assumption 2.2. Additionally let Assumption 2.1 and 2.3 hold.

For each j we discretise the operator differential equation (13) to get an ODE of the form (14) on a finite time interval $S := [0, T_0]$. Let $U_j(0) = Q_{h_j} u_0 \in \mathbb{V}_{h_j}$ be the sequence of initial data for the discretised problems. We assume that $u_0 \in \mathbb{V}^1$ and that there is a constant K such that

$$T_{h_j} Q_{h_j} u_0 \rightarrow u_0, \quad \text{in } \mathbb{V}^{-1}, \quad (30)$$

$$\|Q_{h_j} u_0\|_{h_j,1} \leq K. \quad (31)$$

The functions $U_j : S \rightarrow \mathbb{C}^{N_j}$, which are the solutions to the set of ODE's of the form (14), then converge to the solution u of the PDE (13), in the sense that for all $\theta \in [-1, 1]$,

$$T_{h_j} U_j \xrightarrow{j \rightarrow \infty} u \quad \text{in } C(S, \mathbb{V}^\theta). \quad (32)$$

Proof. Since the proof is quite long, we give a sketch of the proof in a table of contents manner first.

- (i) gather results of previous lemmata

- (ii) show convergence of $T_{h_j}U_j$ to some u_∞ in $C(S, \mathbb{V}^\theta)$ for any $\theta \in [-1, 1[$
- (iii) deduce weak $L^2(S, \mathbb{V}^{-1})$ convergence of each term in the discretised formulation
 - (iii.a) deduce the convergence $\partial_t T_{h_j}U_j \rightarrow \partial_t u_\infty$
 - (iii.b) deduce the convergence $\{t \mapsto T_{h_j}P_{h_j}N(U_j(t), t)\} \rightarrow \{t \mapsto N(u_\infty(t), t)\}$
 - (iii.c) deduce the convergence $T_{h_j}D_{h_j}U_j \rightarrow Au_\infty$
- (iv) final consequence, u_∞ is a solution to (13)

(i) gather results of previous lemmata. Our assumptions allow us to apply Lemma 3.3. Then for $f(t) := T_{h_j}P_{h_j}N(U_j(t), t)$ and any $\theta \in [-1, 1]$ there is a $\delta > 0$ and an upper bound K , independent of j , such that

$$\|T_{h_j}U_j\|_{C^{\frac{1-\theta}{2}}(S, \mathbb{V}^\theta)} \leq K, \quad (33)$$

$$\|f(t)\|_{C^\delta(S, \mathbb{V}^{-1})} \leq K, \quad (34)$$

$$\|T_h\partial_t U_j(t)\|_{C(S, \mathbb{V}^{-1})} \leq K. \quad (35)$$

(ii) show convergence of $T_{h_j}U_j$ to some u_∞ in $C(S, \mathbb{V}^\theta)$. Take any $\theta \in [-1, 1[$. By the uniform bound of $T_{h_j}U_j$ in \mathbb{V}^1 , see (33), and the assumed compact embedding, see (3), we deduce that for any $t \in S$ the sequence $\{T_{h_j}U_j(t)\}_j$ is precompact in \mathbb{V}^θ . Additionally, the family of functions $T_{h_j}U_j : S \rightarrow \mathbb{V}^\theta$ is equicontinuous as a consequence of the equi Hölder continuity in (33). This allows us to employ a variant of the Arzela Ascoli theorem for families of functions with values in general Banach spaces, see [Kel75, p. 233]. Hence, $T_{h_j}U_j$ must converge in $C(S, \mathbb{V}^\theta)$ (along a not relabelled subsequence)

$$T_{h_j}U_j \rightarrow u_\infty \quad \text{in } C(S, \mathbb{V}^\theta). \quad (36)$$

(iii) deduce suitable convergence of each term in their discretised formulation.

We are left to prove, that u_∞ is a solution to the original problem (13). For this we show that the terms in the discretised version (14) converge piecewise to their corresponding counterparts in (13). To be precise, we have to show that their images under the mapping T_h converge in \mathbb{V}^{-1} . In order to connect this to the convergence in (36), we consider the subsequence of $T_{h_j}U_j$, such that (36) holds. We do so without relabelling.

(iii.a) deduce the convergence $\partial_t T_{h_j}U_j \rightarrow \partial_t u_\infty$ in $L^2(S, \mathbb{V}^{-1})$

By (35) we have the uniform boundedness of $\partial_t T_{h_j}U_j(t) = T_{h_j}\partial_t U_j(t)$ in \mathbb{V}^{-1} for all t and j . Together with (33) this gives that the function $T_{h_j}U_j$ is bounded in $H^1(S, \mathbb{V}^{-1})$ uniformly in j . Thus, a subsequence must converge weakly to some $\tilde{u} \in H^1(S, \mathbb{V}^{-1})$. This \tilde{u} must then coincide with the limit u_∞ in (36), which means that the weak limit \tilde{u} is unique. Therefore, the whole sequence $\partial_t T_{h_j}U_j(t)$ converges weakly to $\partial_t u_\infty \in L^2(S, \mathbb{V}^{-1})$.

(iii.b) deduce the convergence $\{t \mapsto T_{h_j}P_{h_j}N(U_j(t), t)\} \rightarrow \{t \mapsto N(u_\infty(t), t)\}$.

By the convergence in (36) and the continuity of N , see Assumption 2.3, we have

$$N(T_{h_j}U_j(t), t) \rightarrow N(u_\infty(t), t) \quad \text{in } C(S, \mathbb{V}^{-1}). \quad (37)$$

From this we will deduce the weak convergence of $T_{h_j} P_{h_j} N(T_{h_j} U_j(t), t)$ to $N(u(t), t)$ in \mathbb{V}^{-1} for all fixed $t \in S$. First we show a boundedness in \mathbb{V}^{-1} as follows,

$$\begin{aligned} \|T_{h_j} P_{h_j} N(U_j(t), t)\|_{-1} &= \sup_{v \in \mathbb{V}} \frac{\left(T_{h_j} P_{h_j} N(U_j(t), t), v \right)_X}{\|v\|_1} = \sup_{v \in \mathbb{V}} \frac{\left(N(U_j(t), t), v \right)_X}{\|v\|_1}, \\ &\leq \sup_{v \in \mathbb{V}} \|N(U_j(t), t)\|_{-1} \frac{\|P_{h_j} v\|_1}{\|v\|_1}. \end{aligned}$$

The assumption (8) gives the boundedness of the quotient $\|P_{h_j} v\|_1 / \|v\|_1$. Employing (37), we deduce the uniform boundedness of $\|T_{h_j} P_{h_j} N(U_j(t), t)\|_{-1}$ for all j . The space \mathbb{V}^{-1} is a Hilbert space and so this boundedness results in the weak convergence of a subsequence.

We analyse for fixed $t \in S$ the weak limit of $N_j(t) := T_{h_j} P_{h_j} N(U_j(t), t)$ (in a not relabelled subsequence) by the following estimate. Take an arbitrary element $v \in \mathbb{V}$ and choose a recovery sequence v_{h_j} as in (29). We use the identity

$$\langle T_{h_j} P_{h_j} N(T_{h_j} U_j(t), t), T_{h_j} v_{h_j} \rangle = \langle N(T_{h_j} U_j(t), t), T_{h_j} v_{h_j} \rangle$$

to get

$$\begin{aligned} |\langle N_j(t), v \rangle - \langle N, v \rangle| &= |\langle N_j(t), v \rangle \pm \langle N_j(t), T_{h_j} v_{h_j} \rangle \pm \langle N, T_{h_j} v_{h_j} \rangle - \langle N, v \rangle|, \\ &\leq |\langle N_j(t), v - T_{h_j} v_{h_j} \rangle| + |\langle N(T_{h_j} U_j(t), t) - N(u_\infty(t), t), T_{h_j} v_{h_j} \rangle| \\ &\quad + |\langle N(u_\infty(t), t), v - T_{h_j} v_{h_j} \rangle|, \\ &\leq (\|N_j(t)\|_{-1} + \|N(u_\infty(t), t)\|_{-1}) \|v - T_{h_j} v_{h_j}\|_1 \\ &\quad + \|N(U_j(t), t) - N(u_\infty(t), t)\|_{-1} \|T_{h_j} v_{h_j}\|_1. \end{aligned}$$

The first addend vanishes for $j \rightarrow \infty$ by the boundedness of $N(u(t), t)$ and $N_j(t)$ and the convergence of $T_{h_j} v_{h_j}$. The second addend vanishes by the convergence in (36). Thus, we have the weak convergence $T_{h_j} P_{h_j} N(U_j(t), t) \rightharpoonup N(u(t), t)$. By the uniqueness of the limit we deduce that the whole subsequence must converge weakly to this limit for any fixed t . In combination with the boundedness of $T_{h_j} P_{h_j} N(U_j(t), t)$ on \mathbb{V}^{-1} , which is uniform for all t , this results in the weak convergence

$$\{t \rightarrow T_{h_j} P_{h_j} N(U_j(t), t)\} \rightharpoonup \{t \rightarrow N(u(t), t)\} \quad \text{in } L^2(S, \mathbb{V}^{-1}). \quad (38)$$

(iii.c) *deduce convergence $T_{h_j} D_{h_j} U_j \rightarrow Au_\infty$.* We have already shown the weak convergence of the discrete time derivative and of the nonlinear term. This immediately gives, by equality (14), that there is a $w \in \mathbb{V}^{-1}$ such that

$$\partial_t T_{h_j} U_j - T_{h_j} P_{h_j} N(T_{h_j} U_j(t), t) = T_{h_j} D_{h_j} U_j \rightharpoonup w, \quad \text{in } L(S, \mathbb{V}^{-1}). \quad (39)$$

We are left to show that $w = Au_\infty$.

By the uniform (in j and t) boundedness of $\|T_{h_j} U_j(t)\|_1$ we know that along a subsequence $T_{h_j} U_j$ must converge weakly in $L^2(S, \mathbb{V}^1)$. Consequently, $AT_{h_j} U_j$ must converge weakly in

$L^2(S, \mathbb{V}^{-1})$. We show that this weak limit must coincide with w . For this purpose we investigate the following. Take any $v \in \mathbb{V}^1$, $t_1 < t_2 \in S$, consider $v_{h_j} \in \mathbb{V}_{h_j}^1$ to be a recovery sequence for v as in (29). We derive the estimate

$$\begin{aligned} \left| \int_{t_1}^{t_2} \langle T_{h_j} D_{h_j} U_j(t) - AT_{h_j} U_j(t), v \rangle dt \right| &\leq \int_{t_1}^{t_2} |\langle T_{h_j} D_{h_j} U_j(t) - AT_{h_j} U_j(t), T_{h_j} v_{h_j} \rangle| \\ &\quad + |\langle T_{h_j} D_{h_j} U_j(t) - AT_{h_j} U_j(t), v - T_{h_j} v_{h_j} \rangle| dt. \end{aligned}$$

Due to the construction of D_{h_j} we know, when acting on functions in the image of T_h , that $T_{h_j} D_{h_j} U_j(t)$ and $AT_{h_j} U_j(t)$ coincide. Therefore, the first term vanishes and we get

$$\begin{aligned} \left| \int_{t_1}^{t_2} \langle T_{h_j} D_{h_j} U_j(t) - AT_{h_j} U_j(t), v \rangle dt \right| \\ \leq \int_{t_1}^{t_2} \|T_{h_j} D_{h_j} U_j(t) - AT_{h_j} U_j(t)\|_{-1} \|v - T_{h_j} v_{h_j}\|_1 dt. \end{aligned} \quad (40)$$

Having shown the boundedness of the left hand side of (39) uniformly in j and t , we know that $\|T_{h_j} D_{h_j} U_j(t)\|_{-1}$ is also uniformly bounded. Furthermore, by (33), the term $\|AT_{h_j} U_j(t)\|_{-1} = \|U_j(t)\|_{h,1}$ stays bounded as well. Thus, we deduce from (40) with the help of (29),

$$\left| \int_{t_1}^{t_2} \langle T_{h_j} D_{h_j} U_j(t) - AT_{h_j} U_j(t), v \rangle dt \right| \leq c \int_{t_1}^{t_2} \|v - T_{h_j} v_{h_j}\|_1 dt \rightarrow 0. \quad (41)$$

Consequently, for any function $v : S \rightarrow \mathbb{V}^1$, which is piecewise constant in time, we get the equality

$$\int_S \langle w(t), v(t) \rangle dt = \lim_{j \rightarrow \infty} \int_S \langle T_{h_j} D_{h_j} U_j(t), v(t) \rangle dt = \lim_{j \rightarrow \infty} \int_S \langle AT_{h_j} U_j(t), v(t) \rangle dt. \quad (42)$$

Since those piecewise constant functions are dense in $L^2(S, \mathbb{V}^{-1})$, we have by [HN01, Thm 8.40] that $AT_{h_j} U_j$ converges weakly in $L(S, \mathbb{V}^{-1})$ to w as well.

By Assumption 2.1, A is a weakly closed operator, and thus there holds

$$Au_\infty = (\text{weak}) \lim_{j \rightarrow \infty} AT_{h_j} U_j = (\text{weak}) \lim_{j \rightarrow \infty} T_{h_j} D_{h_j} U_j = w \quad \text{in } L^2(S, \mathbb{V}^{-1}). \quad (43)$$

Note that this limit is again unique and hence, the whole sequence must converge weakly.

(iv) final consequence, u_∞ is a solution to (13). We have shown that all discrete terms in (14) converge (in $L^2(S, \mathbb{V}^{-1})$) to their continuous counterpart in (13) along a subsequence as chosen in part (ii) of the proof. Thus we get the equality in $L^2(S, \mathbb{V}^{-1})$,

$$\partial_t u_\infty(t) = -Au_\infty(t) + N(u_\infty(t), t). \quad (44)$$

By the convergence (30) we also know that $u_\infty(0) = u_0$. The limit function $u_\infty : S \rightarrow \mathbb{V}^1$ is thus a solution to (13). At first glance, u_∞ seems to be a weaker type of solution than the classical solution which we actually seek, because (44) holds in the $L^2(S, \mathbb{V}^{-1})$ sense. But according to L_p -regularity results, see for example Prüss [Prü03], such a weaker solution is also

unique and therefore must coincide with the original solution $u \in C^1(S, H^{-1}) \cap C(S, H_m^1)$. By this uniqueness we also deduce that the whole sequence converges in the sense of (32). This proves the assertion of this theorem. Note that by (30) and (31) and the compact embedding of the interpolation spaces, see (3), $T_h U_j(0)$ converges in all spaces \mathbb{V}^θ , $\theta \in [-1, 1[$ to u_0 . In \mathbb{V}^1 it still converges weakly. But it suffices to demand only (30) and (31), as this implies convergence in all \mathbb{V}^θ . \square

4 Application of Numerical convergence result to an example

We will use the achieved convergence result to prove the convergence of numerical solutions to the exact solutions of a selected nonlinear PDE. The PDE stems from [DGH11, DHM⁺11] and models the loading of a rechargeable lithium ion battery. We define the spatial domain $\Omega :=]0, 1[$, the time interval $S :=]0, T]$ and furthermore $\mathbb{L} : C(\bar{\Omega}) \rightarrow \mathbb{R}$ as

$$\mathbb{L}(v) := \int_{\Omega} \psi'(x)v(x) \, dx + (v(1) - v(0)), \quad \forall v \in C(\bar{\Omega}). \quad (45)$$

Let $\psi' \in L^2(\Omega)$ and $p \in C^{\frac{1}{2}+\varepsilon}(S)$ be given, then the PDE reads

$$\begin{cases} \partial_t u(t, x) = \partial_x \left(\partial_x u(t, x) + u(t, x) \left[\psi'(x) - \mathbb{L}(u(t)) - p(t) \right] \right) & \text{for } x \in \Omega, t \in S, \\ \partial_x u(t, x) + u(t, x) \left[\psi'(x) - \mathbb{L}(u(t)) - p(t) \right] = 0 & \text{for } x \in \partial\Omega, t \in S, \end{cases} \quad (46)$$

accompanied with an initial value $u_0 \in H^1(\Omega)$ for the unknown solution $u : \Omega \times S \rightarrow \mathbb{R}$, which satisfies $u_0 \geq 0$ and $\int_{\Omega} u_0 \, dx = 1$. The solution $u(t) := u(t, \cdot) : \Omega \rightarrow \mathbb{R}$ describes at each fixed time $t \in S$ the distribution of the loading state of nanosized storage particles, which form the cathode of the battery. The average loading state gives then the overall loading state of the whole battery at time t . The Hölder continuous function p describes the rate at which the battery is charged or discharged. We assume that for all times $t \in S$ it is true that $\int_{\Omega} x u_0(x) \, dx + \int_0^t p(t) \in]0, 1[$ as this implies the global existence and boundedness of solutions to (46) in $C(S, H^1(\Omega))$, as shown in [DHM⁺11]. We also know that u stays non-negative keeps its mean value of one. This is consistent with the interpretation of $u(t)$ being a probability distribution for any fixed $t \in S$.

In order to apply the above convergence results, we modify our problem, such that it satisfies Assumption 2.3. We define for a positive number $K > 0$ the cut-off function

$$\zeta_K(s) := \begin{cases} s, & \text{if } |s| \leq k. \\ \text{sgn}(s)K, & \text{if } |s| > K. \end{cases} \quad (47)$$

We then substitute in (46), $\zeta_K(\mathbb{L})$ for \mathbb{L} . When choosing K large enough, this does not alter the problem, since we can guarantee that $u(t) \in C(\bar{\Omega})$ and $\mathbb{L}(u(t)) \in \mathbb{R}$ stays bounded. We can do so because of the global boundedness in $H^1(\Omega)$ of the original solution u . The modified (weak) problem formulation reads for all $t \in S$ and for all $v \in H^1(\Omega)$

$$\left(\partial_t u(t), v \right)_{L^2} = - \left(\partial_x u(t), \partial_x v(t) \right)_{L^2} - \left([\psi' - p(t) - \zeta_K(\mathbb{L}(u(t)))] u(t), \partial_x v(t) \right)_{L^2}. \quad (48)$$

Note that the solution is also unique, since the original existence theory in [DHM⁺11] still applies for it.

We consider a spatial finite element discretisation with piecewise affine functions. So we get a semi discretised version of (46), which is

$$M_h \dot{U}(t) = -A_h U(t) - [\widehat{B}_h - p(t)B_h - \zeta_K \left((L, U(t))_e \right) B_h] U(t) + . \quad (49)$$

The appearing matrices are defined as with the help of the finite element basis functions φ_j as $(M_h)_{i,j} = (\varphi_i, \varphi_j)_{L^2}$, $(A_h)_{i,j} = (\partial_x \varphi_i, \partial_x \varphi_j)_{L^2}$, $(B_h)_{i,j} = (\partial_x \varphi_i, \varphi_j)_{L^2}$ and $(B_h)_{i,j} = (\partial_x \varphi_i, \psi' \varphi_j)_{L^2}$. The vector L is defined by $L_i := \mathbb{L}(\varphi_i)$.

We still need to define the choice of the mapping which gives for a $u_0 \in H^1(\Omega)$ a corresponding discrete initial value $U_h(0)$. Our choice is

$$U_h(0) = P_h u_0 , \quad (50)$$

where P_h is the L^2 -projection on the space of all piecewise affine functions having a mean value of one. We can now formulate the convergence result for this specific problem.

Lemma 4.1. *Consider $\mathcal{P}_{h_j}^1$ to be the space of continuous and piecewise linear functions on an equidistant partition of $\Omega = [0, 1]$ into intervals of length h_j which vanish for $j \rightarrow \infty$.*

Let the assumptions of the existence theorem in [DHM⁺11] hold, such that there exists a unique solution to the PDE (46) on the finite time interval $S = [0, T_0]$. Furthermore, let U_j be the solution of the ODE (49), which is the (semi)discretised version of the PDE on the space $\mathcal{P}_{h_j}^1$. The discrete initial value $U_{h_j}(0)$ be defined as in (50) for $u_0 \in H_m^1(\Omega)$.

Then the solution U_{h_j} exists on the whole time interval S and it converges to u in the sense that for any $\theta \in [-1, 1[$

$$T_{h_j} U_{h_j} \xrightarrow{j \rightarrow \infty} u \quad \text{in } C(S, H_m^\theta(\Omega)) . \quad (51)$$

Proof. We aim at showing that the PDE (46) and its discretisation (49) fit into the framework of Theorem 3.4. For this reason we have to modify the PDE (46) into an equivalent one. According to the assumptions, we have $\psi \in H^1(\Omega)$ and also $p \in C^{\alpha_N}(S, \mathbb{R})$ for an $\alpha_N > \frac{1}{2}$ as the given data of the PDE (46).

We define the complex Hilbert spaces \mathbb{V}^1 and \mathbb{X} and the operator A as

$$\begin{aligned} \mathbb{V}^1 &:= H_m^1(\Omega) , & (v_1, v_2)_1 &:= \int_{\Omega} \partial_x v_1(x) \partial_x \overline{v_2}(x) \, dx , & \mathbb{X} &:= L^2(\Omega) \\ A : \mathbb{V}^1 \subset \mathbb{V}^{-1} &\rightarrow \mathbb{V}^{-1} , & \langle Au, v \rangle &= \int_{\Omega} \partial_x u \partial_x v \, dx . \end{aligned}$$

The space \mathbb{V}^{-1} is the usual dual of \mathbb{V}^1 . The nonlinearity in the PDE is considered by defining the mappings $N, N_0 : C(\Omega) \rightarrow H^{-1}(\Omega)$, such that for all $v \in C(\Omega)$:

$$\begin{aligned} \langle N_0(v, t), w \rangle &:= \left([\psi' - p(t) - \zeta_K \left(\mathbb{L}(v) \right)] v, \partial_x w(t) \right)_{L^2} \quad \forall w \in H^1(\Omega) , & (52) \\ N(v, t) &:= N_0(v + 1, t) . \end{aligned}$$

The function ζ_K is the cut-off function as described in (47). According to [DHM⁺11], the solution u is in the space $C(S, H_m^1(\Omega))$. We define the cut-off barrier to be $K := 1 + \max_{t \in S} \{|\mathbb{L}u(t)|\}$ and deduce that u , the solution to (46), coincides with the unique solution to the modified version $\partial_t u = -Au + N_0(u, t)$, $u(0) = u_0$. In order to work in the spaces of mean-value free functions we switch to the equivalent problem of seeking w , such that

$$\partial_t w = -Aw + N(w, t), \quad w(0) = u_0 - 1, \quad (53)$$

and clearly $u \equiv w + 1$. We also switch in the discretised version from (49) to

$$\partial_t W_{h_j} = -D_{h_j} W_{h_j} + P_{h_j} N(T_{h_j} W_{h_j}, t), \quad W_{h_j}(0) = Q_{h_j}(u_0 - 1), \quad (54)$$

where D_{h_j} is defined as in (5). Similar to the case of (53), we have the identity $U_{h_j} = W_{h_j} + (1, 1, \dots, 1) \in \mathbb{C}^{n_j}$. As a remark we note that for real valued vectors $U_{h_j}(0)$ the solution is also real valued for all times.

Now that we have clarified the setting, we need to show that the assumptions of Theorem 3.4 hold. The operator A is the well known Laplacian for mean-value free functions, and thus Assumption 2.1 is satisfied. We exploit the modification of the nonlinearity N , which we made by inserting the cut-off function ζ_K , to show Assumption 2.3. In order to do this, we inspect for $v_1, v_2 \in H_m^1(\Omega)$ and $s_1, s_2 \in S$ the difference

$$\|N(v_1, s_1) - N(v_2, s_2)\|_{-1} \leq \|N(v_1, s_1) - N(v_1, s_2)\|_{-1} + \|N(v_1, s_2) - N(v_2, s_2)\|_{-1}. \quad (55)$$

For the first difference we use the assumed Hölder continuity of p to get

$$\|N(v_1, s_1) - N(v_1, s_2)\|_{-1} \leq c \|p\|_{C^{\alpha_N}} |s_1 - s_2|^{\alpha_N} (\|v_1\|_{L^2} + 1). \quad (56)$$

For the second term in (55) we use that for any $a_1, a_2, b_1, b_2 \in \mathbb{R}$,

$$\left| \zeta_K(a_1)b_1 - \zeta_K(a_2)b_2 \right| = \left| \zeta_K(a_1)b_1 \pm \zeta_K(a_1)b_2 - \zeta_K(a_2)b_2 \right| \leq K|b_1 - b_2| + |b_2||a_1 - a_2|$$

and so we get for $c_{\mathbb{L}} := \sup\{|\mathbb{L}(v)| : v \in C(\bar{\Omega}), \|v\|_C \leq 1\}$,

$$\|N(v_1, s_2) - N(v_2, s_2)\|_{-1} \leq c \left(\|\psi'\|_{L^2} + \|p\|_{L^\infty} + K + c_{\mathbb{L}} \|v_2\|_C \right) \|v_1 - v_2\|_C. \quad (57)$$

We know that for $\gamma > \frac{1}{2}$ we have the compact embedding $H_m^\gamma \hookrightarrow C(\Omega)$. Thus, combining (55)-(57) we get the first estimate (15) in Assumption 2.3. The second inequality in this assumption follows easier. By the boundedness of ζ_K and p we get,

$$\|N(v, s)\|_{-1} \leq \left(\|\psi'\|_{L^2} + \|p\|_{L^\infty} + K \right) (\|v\|_C + 1),$$

such that by the same embedding (16) must be satisfied.

The discrete subspaces $\mathbb{V}_{h_j} = \mathcal{P}_{h_j}^1 \cap H_m^1(\Omega)$ consist of piecewise affine and mean-value free functions on an equidistant decomposition of $\Omega = [0, 1]$. It is known that for $j \rightarrow \infty$ they are dense in $H_m^1(\Omega)$ as desired in (29). The needed stability of the L^2 projection in (8) is satisfied

according to Bramble et al., see [BPS02], by choosing an equidistant grid. Hence we also satisfy the boundedness of the discrete initial values as desired in (30) and (31).

We have gathered all necessary assumptions to apply Theorem 3.4. This gives a convergence of $T_{h_j} W_{h_j} \rightarrow w$ in $C(S, \mathbb{V}^\theta)$, which is equivalent to $T_{h_j} U_{h_j} \rightarrow u$ in $C(S, \mathbb{V}^\theta)$. This convergence allows us to drop the use of the cut-off function ζ_K . By the continuity of \mathbb{L} on \mathbb{V}^γ we get that there is an j_* , such that for all $j > j_*$ there holds

$$\sup_{t \in S} |\mathbb{L}(T_h U_{h_j}(t))| \leq 1 + \sup_{t \in S} |\mathbb{L}(u(t))| = K .$$

Thus, the artificially introduced cut-off function in the nonlinear term N does not alter our problem. \square

In a final step we can deduce from the latter Lemma that also the fully discretised problem, when using the Crank-Nicolson time discretisation, converges to the exact solution. For this the space and the time discretisation must get finer in a suitable way.

Corollary 4.2. *Let the assumptions of the Lemma 4.1 hold. Then there exists a sequence $\{k(h_j)\} \subset \mathbb{R}$, such that for all pairs of space and time step sizes (h_j, k_j) , such that $0 < k_j \leq k(h_j)$ the discretisation error vanishes.*

We use the Crank-Nicolson scheme for the time discretisation and employ the notation

u for exact solution of PDE (46),

U_{h_j, k_j}^m for the FEM approximation of u at time $t_{m,j} := mk_j$ of the fully discrete problem, with spatial grid size h_j and time step size k_j ,

we state that for any $\theta \in [-1, 1[$,

$$\sup_{m \in \mathbb{N}, 0 \leq t_{m,j} \in S} \|T_{h_j} U_{h_j, k_j}^m - u(t_{m,j})\|_\theta \xrightarrow{j \rightarrow \infty} 0 . \quad (58)$$

As a consequence of the embedding $H^{\frac{1}{2} + \varepsilon}(\Omega) \hookrightarrow C(\bar{\Omega})$ this also results in convergence in the $C(\bar{\Omega})$ norm.

Proof. From Lemma 4.1 we know that there exists a sequence of solutions U_{h_j} , to the semi-discretised problem (49). Each one is an ODE of the form (14). These solutions converge in all spaces $C(S, H^\theta(\Omega))$, $\theta \in [-1, 1[$ to u .

Another consequence of Lemma 4.1 is, that there exists $K \in \mathbb{R}$ and an $j_* \in \mathbb{N}$, such that

$$\text{for all } j > j_* : \quad \sup_{t \in S} (|\mathbb{L}(T_{h_j} U_{h_j}(t))|) \leq K . \quad (59)$$

We will use this knowledge in order to transform our original ODE into an equivalent one with Lipschitz continuous right-hand side.

In the spirit of the proof of the Lemma 4.1 we modify the nonlinear part of the ODE with the cut-off function ζ_{K+1} , as defined in (47). Hence, we can use standard arguments for the numerical integration of ODE's with Lipschitz right-hand side.

We denote by $\{U_{h_j,k}^m\}_m$ the set of solution vectors of the fully discretised problem with time step size k . The time discretisation we chose, i.e. the Crank Nicholson scheme, can be interpreted as a Runge-Kutta scheme of second order or a multistep method. In both cases it is an A-stable method of order two, and so we can use known theory to state convergence of the fully discretised problem to solutions of the semi-discretised problems. We refer to a convergence result by Hairer and Wanner, [HW93, Thm.6.11], which states, assuming the Lipschitz continuity of the right hand side, that for fixed j

$$e(h_j, k) := \sup_{m \in \mathbb{N}, 0 \leq mk \leq T_0} \|T_{h_j} U_{h_j,k}^m - T_{h_j} U_{h_j}(mk)\|_{\theta} \xrightarrow{k \rightarrow 0} 0 .$$

Note that in finite dimensional spaces all norms are equivalent. Thus, for every fixed j there exists a time step size $k(h_j)$, such that for all $k \leq k(h_j)$ we can guarantee

$$e(h_j, k) \leq \frac{1}{j} . \quad (60)$$

The achieved convergence in (60) holds for the modified problem (48) and its discretisation (49), where we inserted a cut-off function ζ_K . We already showed in the proof of Theorem 3.4 that the semi-discrete problem is not altered by this modification. Now we address the modification of the fully discretised problem.

Remember that there is a constant K , such that the solution of the ODE (49), namely U_{h_j} , respects the barrier K in the sense that $|\mathbb{L}(T_{h_j} U_{h_j})| \leq k$. Therefore choosing the new cut-off barrier as $(K + 1)$, it must also be possible to satisfy for $k(h_j)$ small enough that

$$\sup_{m \in \mathbb{N}, 0 \leq mk \leq T_0} (|\mathbb{L}(T_{h_j} U_{h_j,k}^m)|) \leq K + 1 .$$

This then justifies to undo our modification in (52) and to still obtain for all $k < k(h_j)$ the bound in (60) for the unmodified version. Together with the already achieved convergence in (32) and the simple inequality

$$\|T_{h_j} U_{h_j,k}^m - u(mk)\|_{\theta} \leq \|T_{h_j} U_{h_j,k}^m - T_{h_j} U_{h_j}(mk)\|_{\theta} + \|T_{h_j} U_{h_j}(mk) - u(mk)\|_{\theta} , \quad (61)$$

this proves this corollary. □

We used a cutoff function in the discretised version of PDE (46). By the strong convergence which we get, one sees that for space and time step sizes which are small enough, we can guarantee, that we do not reach the region, where the introduced cutoff actually alters anything. Hence in practice one does not need to use the cutoff-modification if one chooses a discretisation which is fine enough. Even though the question what *fine enough* actually means might be a highly nontrivial question to answer a priori.

In the example problem of we explicitly want to include cases, where the spatially regularity of the exact solution is not better than H_m^1 . Hence we can not apply classical methods from Thomee and Wahlbin, [TW75]. Another naive way of proving numerical convergence would be to prove a priori estimates in L^2 and from there work our way up to some convergence. However this is not possible since L^2 boundedness is not enough to state anything for the nonlinearity, because this depends on the solution as a continuous function. Therefore we need to apply our result in order to verify numerical experiments.

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