Efficient computation of time-periodic solutions of partial differential equations

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1 Introduction

Many dynamical systems admit a solution with a periodic state $u(t) = u(t + T)$ where T is the length of one period. Such problems appear in fluid-dynamics in the regime of moderate Reynolds numbers, either by an oscillatory forcing of known periodicity [14, 10] or by the von Kármán vortex street arising in the flow around an obstacle [9]. Other examples are found in chemical process engineering, where so called cyclic steady states are the desired operation modes in moving bed processes [22] for chromatographic separation [16]. In various chemical applications, periodic solutions are more efficient than stationary outputs [28]. In some of these examples the periodicity is known and enforced by means of the problem data (like the frequency of moving bed devices), other configurations like the flow around an obstacle yield a certain periodicity by the inner dynamics of the coupling.

The necessity to compute cyclic solutions also arises in temporal multiscale methods, where the problem features temporal microscales, that are oscillating at a high frequency. A typical example is found in damage mechanics, e.g., the deterioration of a mechanical structure (bridge or house) that will suffer slow decay and accumulation of damage over a very long period (time scale t), caused by high frequent oscillatory impulses (time scale $\tau \ll t$). Another example is found in the fluid dynamical forces (the oscillating wall shear stress) of the pulsating blood flow (time scale τ) on vessel walls that can cause damages and long time growth of stenosis [26] (time scale $t \gg \tau$). Often it is not possible to resolve the temporal microscale while performing long-time simulations and stationary simplifications are considered [27]. Temporal multiscale techniques for such long-term problems with short-term influences can be based on the solution of effective long-term equations that are obtained by averaging and that depend on the input of periodic short-term problems [6, 7]. Such an approach has been undertaken in [8] for the plaque formation problem. It has however proven to be essential to determine the periodic microscale problems up to low tolerances.

The computation of periodic states by brute-force forward simulation may take an excessive number of cycles to be run. Given a periodic forcing the convergence to the cyclic state will mainly depend on an interplay of energy conservation and smoothing properties of the underlying system of equations. In [19] a scheme is developed to approximate periodic solutions by a monotone iteration scheme. In literature several approaches are discussed for accelerating this solution procedure. [21] showed that under certain conditions an undamped Newton scheme converges towards a periodic solution. In [13] the authors formulate a Newton scheme for the periodicity error $F(q) := u(t + T) - q \stackrel{!}{=} 0$ where $u(t) = q$ is the initial value. This results in a technique similar to the shooting method that requires the solution of a matrix-valued sensitivity system. The authors of [20] propose a global space-time discretization for a direct computation of the cyclic state, formulating the periodic equation as a boundary value problem in space and time. Both approaches have to face the challenge of dimensionality: the shooting approach requires to compute M steps of a matrix valued sensitivity system of size N^2 (where N is the number of spatial unknowns, M the number of time steps), the global space-time approach results in a coupled system of size $M \times N$. Both approaches are difficult to extend to 2d or 3d problems involving partial differential equations requiring high spatial resolution with $N \gg 1\,000\,000$.

In [16] the authors present a cascadic multilevel method to accelerate the forward simulation by using approximated systems in space and time. Although this approach might suffer from long transition times its extension to PDEs with high dimension of the spatial problem is straightforward.

In this contribution, we will formulate the cyclic steady state problem as a constrained minimization problem: we search for initial data $q \in Q$ such that

$$\|u_q(T) - q\|_Q^2 \to 0,$$

where $u_q(t)$ is given as the solution of the dynamical system $u_q'(t) = f(t, u_q(t))$ with $u_q(0) = q$. Similar, to our approach [1] considered the computation of time periodic solutions of the Benjamin-Ono equation, but their analysis of the optimization problem is limited to the calculation of the derivatives of the above functional. The approach corresponds to single-shooting for the boundary-value problem in time, and can easily be extended to multiple-shooting intervals, cf., [5].

The outline of the paper is as follows. In Section 2, we will provide an abstract framework for the above minimization problem, for the determination of the periodic states. In particular, we show that for equations satisfying a smoothing property the minimization of the above problem is possible without any further regularization terms in the functional, and that the unique minimizer is indeed a periodic solution. We will show in Section 3, that the requirements of the abstract setting are met by a strongly damped wave equation. In the context of time periodic problems hyperbolic equations are often found, e.g., in damage mechanics where elastic structure are excited by periodic forcing. Quick identification of periodic solutions is important as small changes in material parameters can result in completely different resonance regimes. In Section 4, we will discuss how the resulting minimization problem can be solved numerically. Besides the description of the gradient method and the Newton scheme for approximating the minimization problem introduced in Section 2, we shortly describe the discretization in space and time. Section 5 discusses two numerical test cases, the linear strongly damped wave equation and a nonlinear problem where an additional nonlinear coupling term is introduced. We finally provide some conclusions in Section 6.

2 Abstract Setting

In order to analyze the method under consideration, we first provide an abstract form for the control to state mapping. To this end, let $\Omega \subset \mathbb{R}^d$, with $d \in \mathbb{N}$, be a, sufficiently smooth, domain and let $I = (0,T)$ be a given time interval. Let Q be a Hilbert-space of admissible initial values, i.e., Q contains functions $q\colon \Omega \to \mathbb{R}^c$, $c \in \mathbb{N}$, of a certain regularity. Further, let W be another Hilbert-space of functions $u\colon I \times \Omega \to \mathbb{R}^c$ satisfying $W \subset C(\bar{I}, Q) \cap C(\bar{I}, L^2(\Omega))$.

We are concerned with periodic solutions, $u(T) = u(0)$, to the evolutionary PDE

$$\begin{aligned} \partial_t u(t,x) + \mathcal{A}u(t,x) &= f(t,x) && \text{in } I \times \Omega,\\ u(0) &= q && \text{in } \Omega, \end{aligned}$$

together with appropriate boundary values on $I \times \partial\Omega$.

For convenience, we define a corresponding variational form. Let $(\cdot,\cdot)_Q$ and $\|\cdot\|_Q$ be the scalar product and norm on Q, $(\!(\cdot,\cdot)\!)$ and $|\!|\!|\cdot|\!|\!|$ be the scalar product and norm on $L^2(I, L^2(\Omega))$ and $A\colon W \times W \to \mathbb{R}$ be a given continuous bilinear mapping. Then given an initial-value $q \in Q$, we associate a state $u = u_q \in W$ as a solution to

$$(\!(\partial_t u, \phi)\!) + A(u,\phi) = (\!(f,\phi)\!) + (q, \phi(0))_Q \qquad \forall \phi \in W \tag{1}$$

where $f \in L^2(I, L^2(\Omega))$ is a given right-hand side. In order for this mapping to be well defined, we assume the following

Assumption 1. *For any given $q \in Q$ there exists a unique solution u_q with $u_q(0) = q$ of (1). Further, this solution satisfies the stability estimate*

$$\|u(T)\|_Q \le c(\|q\|_Q + c_F)$$

with a constant c_F depending on the chosen data f, where $c_0 = 0$.

Example 2. The most simple example for the above setting is the heat equation

$$\begin{aligned} \partial_t u(t,x) - \Delta u(t,x) &= f(t,x) && \text{in } I \times \Omega,\\ u(0,x) &= q(x) && \text{in } \Omega,\\ u(t,x) &= 0 && \text{on } \partial\Omega. \end{aligned}$$

Here $Q = L^2(\Omega)$ and $W = W(0,T) = \{v \in L^2(I, H_0^1) \,|\, \partial_t v \in L^2(I, (H_0^1(\Omega))^*)\}$ and the weak form of the initial value problem is given by

$$(\!(\partial_t u, \phi)\!) + (\!(\nabla u, \nabla\phi)\!) + (u(0), \phi(0)) = (\!(f,\phi)\!) + (q, \phi(0))$$

for any $\phi \in W$, where $(\cdot,\cdot)$ denotes the $L^2(\Omega) = Q$ scalar product - here the H_0^1-$(H_0^1)^*$ duality pairing is identified with the L^2-scalar product. It is then well-known that Assumption 1 is satisfied, see, e.g., [25, Chapter 26].

Based upon the well-posed forward problem, we can now formulate an optimization problem for the time-periodic setting.

$$\begin{aligned} \min_{q\in Q, u\in W} \ & \frac{1}{2}\|q-u(T)\|_Q^2 \\ \text{s.t. } & u,\ q \text{ solve (1).} \end{aligned} \tag{2}$$

It is clear, that the minimal value of (2) is zero if and only if the corresponding minimizer q, u satisfy $q = u(0) = u(T)$.

When considering this problem, the difficulty lies in the fact, that while $\|\cdot\|_Q^2$ is uniformly convex the composed mapping $(q, u) \mapsto \|q - u(T)\|_Q^2$ is not. Consequently, a small trick is needed to assert that indeed a minimum exists.

Theorem 3. *Let Assumption 1 be satisfied with $c < 1$. Then Problem (2) has exactly one minimizer.*

Proof. Clearly, the functional is convex, and thus any local minimizer is global. We will now see, that the functional is strictly convex. This asserts that there is at most one minimizer of (2).

To this end, let $q, \tilde{q} \in Q$ be arbitrary with corresponding states $u, \tilde{u}$. Then for any $\lambda \in (0, 1)$ it is

$$\begin{aligned} \|\lambda(q-u(T)) + (1-\lambda)(\tilde{q}-\tilde{u}(T))\|_Q^2 &= \lambda\|q-u(T)\|_Q^2 + (1-\lambda)\|\tilde{q}-\tilde{u}(T)\|_Q^2 \\ &\quad - \lambda(1-\lambda)\|q-u(T)-\tilde{q}+\tilde{u}(T)\|_Q^2. \end{aligned}$$

Clearly, if $q - u(T) - \tilde{q} + \tilde{u}(T) \neq 0$ a strict inequality, and thus strict convexity, holds. Assume, to the contrary that the above would be zero, then

$$q - \tilde{q} = u(T) - \tilde{u}(T)$$

and moreover it holds

$$\begin{aligned} \partial_t(u-\tilde{u}) + \mathcal{A}(u-\tilde{u}) &= 0 && \text{in } I \times \Omega, \\ (u-\tilde{u})(0) &= q - \tilde{q} && \text{in } \Omega. \end{aligned}$$

By the stability estimate of Assumption 1, we have

$$\|(u-\tilde{u})(T)\|_Q \le c\|q-\tilde{q}\|_Q < \|q-\tilde{q}\|_Q$$

since $c < 1$ contradicting the equality $(u - \tilde{u})(T) = q - \tilde{q}$. Thus the functional is strictly convex, and at most one minimizer exists.

To show existence of a minimizer, we abbreviate $j(q, u) = \frac{1}{2}\|q - u(T)\|_Q^2$, and see immediately that $0 \le j(q, u)$ and hence there exists $\bar{j} = \inf_{q,u} j(q, u)$. Consequently, there exists a minimizing sequence (q_k, u_k) with $u_k = u_{q_k}$. With the same calculation as above (and $\lambda = \frac{1}{2}$), we get the following for the minimizing sequence:

$$\begin{aligned}
\frac{1}{4}\|q_l - q_m + u_m(T) - u_l(T)\|_Q^2 &= \frac{1}{2}\|q_l - u_l(T)\|_Q^2 + \frac{1}{2}\|q_m - u_m(T)\|_Q^2 \\
&\quad - \|\frac{1}{2}(q_l - u_l(T)) + \frac{1}{2}(q_m - u_m(T))\|_Q^2 \\
&= j(q_l, u_l) + j(q_m, u_m) \\
&\quad - 2\frac{1}{2}\|\frac{1}{2}(q_l + q_m) - \frac{1}{2}(u_l + u_m)\|_Q^2 \\
&= j(q_l, u_l) + j(q_m, u_m) \\
&\quad - 2j(\frac{1}{2}(q_l + q_m), \frac{1}{2}(u_l + u_m)) \\
&\leq j(q_l, u_l) + j(q_m, u_m) - 2\bar{j} \\
&\to 0 \qquad (l, m \to \infty).
\end{aligned}$$

Now, by the reverse triangle inequality

$$\big|\|q_l - q_m\|_Q - \|u_l(T) - u_m(T)\|_Q\big| \leq \|q_l - q_m + u_m(T) - u_l(T)\|_Q \to 0.$$

By the stability estimate $\|u_m(T) - u_l(T)\|_Q \leq c\|q_l - q_m\|_Q$, we see that

$$\begin{aligned}
0 &\leq (1-c)\|q_l - q_m\|_Q \\
&\leq (1-c)\|q_l - q_m\|_Q + c\|q_l - q_m\|_Q - \|u_m(T) - u_l(T)\|_Q \\
&= \|q_l - q_m\|_Q - \|u_m(T) - u_l(T)\|_Q \\
&= \big|\|q_l - q_m\|_Q - \|u_m(T) - u_l(T)\|_Q\big|.
\end{aligned}$$

Hence the minimizing sequence q_k is a Cauchy-sequence and the assertion follows. □

Remark 4. The assumption $c < 1$ made in the statement of the theorem is only needed for the case $f \equiv 0$. Here it is a reasonable assumption. For example, if considering the heat equation

$$((\partial_t u, \phi)) + ((\nabla u, \nabla \phi)) + (u(0), \phi(0)) = (q, \phi(0)),$$

one can test with $\phi = tu$ to get the estimate

$$T \int_\Omega |u(T,x)|^2 \,\mathrm{d}x \leq \int_I \int_\Omega |u(t,x)|^2 dx.$$

Together with a stability estimate for $\int_I \int_\Omega |u(t,x)|^2 dx$ one obtains the result

$$\int_\Omega |u(T,x)|^2 \,\mathrm{d}x \leq \frac{c}{T}\|q\|^2$$

showing that $c < 1$ is reasonable once T is sufficiently large.

Finally, we remark, that if the analog of Assumption 1 holds for the adjoint problem

$$\begin{aligned} -\partial_t z(t,x) + \mathcal{A}^* z(t,x) &= 0 && \text{in } I \times \Omega, \\ z(T) &= u(T) - q && \text{in } \Omega, \end{aligned}$$

i.e., the estimate

$$\|z(0)\|_Q \le c\|u(T) - q\|_Q$$

holds for some $c < 1$, then the unique minimize of (2) is indeed a periodic solution. To see this, we note, that Lagrange calculus asserts that for the minimizer $\bar{q}, \bar{u}$ of (2) there is a corresponding adjoint $\bar{z}$ solving the above adjoint problem with data $\bar{u}(T) - \bar{q}$. With this, standard calculus, see, e.g., [23], gives the first order necessary optimality condition

$$\bar{u}(T) - \bar{q} + \bar{z}(0) = 0.$$

Assuming that the minimizer is not periodic, i.e., $\bar{u}(T) - \bar{q} \neq 0$, the stability estimate with $c < 1$ asserts,

$$\|\bar{z}\|_Q \le c\|\bar{u}(T) - \bar{q}\|_Q < \|\bar{u}(T) - \bar{q}\|_Q$$

contradicting the optimality condition.

3 The damped wave equation

As a typical example of an equation with oscillatory behavior, we discuss the strongly damped wave equation.

$$\begin{aligned} \partial_t v - \mu\Delta u - \lambda\Delta v &= f && \text{in } I \times \Omega, \\ \partial_t u - v &= 0 && \text{in } I \times \Omega, \\ u(0) &= q_u && \text{in } \Omega, \\ v(0) &= q_v && \text{in } \Omega, \\ u(t,x) &= 0 && \text{on } I \times \partial\Omega \end{aligned} \tag{3}$$

where $I = (0,T)$ and $\Omega \subset \mathbb{R}^d$ is a domain with sufficiently smooth boundary, $f \in L^2(I, H^{-1}(\Omega))$, and $\mu, \lambda > 0$. It is well known, that for any initial data $q_v \in L^2(\Omega)$ and $q_u \in H_0^1$ this equation admits a solution $v \in C(\overline{I}, L^2(\Omega)) \cap L^2(I, H_0^1(\Omega))$ and $u \in C(\overline{I}, H_0^1(\Omega))$, see, e.g., [24, 2] also allowing for a potential nonlinearity in the equation.

We will now see, that indeed Assumption 1 is satisfied on the space

$$Q = \{(q_v, q_u) \in L^2(\Omega) \times H_0^1(\Omega)\}$$

with corresponding norm

$$\|q\|_Q^2 = \|q_v\|^2 + \|\nabla q_u\|^2. \tag{4}$$

Theorem 5. *There exists a constant $c > 0$ such that the unique solution (u,v) of (3) with $f \equiv 0$ satisfies the estimate*

$$\|(v(T), u(T))\|_Q^2 \le \frac{c}{T}\|(v(0), u(0))\|_Q^2,$$

where $c > 0$ depends on the domain Ω and on the parameters μ, λ, e.g., $c = \mathcal{O}(\lambda + \lambda^{-1})$.

Proof. To see the assertion, we multiply the first equation in (3) with a function $\phi \in L^2(I, H_0^1(\Omega))$ and integrate over $I \times \Omega$ to get

$$((\partial_t v, \phi)) + \mu((\nabla u, \nabla \phi)) + \lambda((\nabla v, \nabla \phi)) = 0. \tag{5}$$

Now, selecting $\phi = v = \partial_t u$, we obtain

$$\begin{aligned} 0 &= ((\partial_t v, v)) + \mu((\nabla u, \nabla v)) + \lambda((\nabla v, \nabla v)) \\ &= \frac{1}{2}\|v(T)\|^2 - \frac{1}{2}\|v(0)\|^2 + \frac{\mu}{2}\|\nabla u(T)\|^2 - \frac{\mu}{2}\|\nabla u(0)\|^2 + \lambda|||\nabla v|||^2. \end{aligned}$$

Utilizing Poincaré's inequality this shows

$$\begin{aligned} \|(v(T), u(T))\|_Q^2 + \lambda|||\nabla v|||^2 &\le c\|(v(0), u(0))\|_Q^2, \\ \lambda|||v|||^2 &\le c\|(v(0), u(0))\|_Q^2 \end{aligned}$$

with a constant c depending on μ. Now, testing (5) with $\phi = u$, we assert

$$\begin{aligned} 0 &= ((\partial_t v, u)) + \mu((\nabla u, \nabla u)) + \lambda((\nabla v, \nabla u)) \\ &= -((v, \partial_t u)) + (v(T), u(T)) - (v(0), u(0)) + \mu|||\nabla u|||^2 \\ &\quad + \frac{\lambda}{2}\|\nabla u(T)\|^2 - \frac{\lambda}{2}\|\nabla u(0)\|^2. \end{aligned}$$

Together with the estimate for $((v, \partial_t u)) = |||v|||^2$ and $\|(v(T), u(T))\|_Q^2$, we assert

$$\mu|||\nabla u|||^2 + \frac{\lambda}{2}\|\nabla u(T)\|^2 \le c(1 + \lambda + \lambda^{-1})\|(v(0), u(0))\|_Q^2.$$

Finally, we test with $\phi = tv$ and obtain

$$\begin{aligned} 0 &= ((\partial_t v, tv)) + \mu((\nabla u, t\nabla v)) + \lambda((\nabla v, t\nabla v)) \\ &= \frac{T}{2}\|v(T)\|^2 - \frac{1}{2}|||v|||^2 + \frac{T\mu}{2}\|\nabla u(T)\|^2 - \frac{\mu}{2}|||\nabla u|||^2 + \lambda|||t^{1/2}\nabla v|||^2. \end{aligned}$$

Together with the estimates for $|||v|||$ and $|||\nabla u|||$ this shows the assertion. □

For the following numerical treatment, we can define a weak form for the solution of (3). To this end, let $U = (v, u)$, $q = (q_v, q_u)$, $\Phi := (\phi, \psi)$ and define

$$\begin{aligned} B(U, \Phi) &= ((\partial_t U, \Phi)) + ((\mathcal{A}U, \Phi)) \\ &= ((\partial_t v, \phi)) + \mu((\nabla u, \nabla \phi)) + \lambda((\nabla v, \nabla \phi)) \\ &\quad + ((\partial_t u - v, \psi)) + (v(0), \phi(0)) + (u(0), \psi(0)), \\ F(q; \Phi) &= ((f, \phi)) + (q_v, \phi(0)) + (q_u, \psi(0)) \end{aligned} \tag{6}$$

where, again, $((\cdot, \cdot))$ is the space-time integral. Then the solution U of (3) solves the problem

$$B(U, \Phi) = F(q; \Phi) \quad \forall \Phi \in W := C(\bar{I}, H_0^1(\Omega)) \times C(\bar{I}, L^2(\Omega)).$$

4 Solving the Optimization Problem

We refer to the setting introduced in Section 2. Let $u \in W$ be the solution on $I = [0, T]$ given by the variational formulation

$$B(U, \Phi) = F(q; \Phi) \qquad \forall \Phi \in W, \tag{7}$$

that has been introduced in (6). We aim to find $U(0) = q \in Q$ that minimizes

$$J(q; U(T)) := \min_{q \in Q, U \in W} \frac{1}{2} \|q - U(T)\|_Q^2,$$

such that $U = U_q$ solves (7). It is now straightforward to derive first order necessary optimality conditions, cf., [15, 23, 12]. In order to briefly write the resulting system, we introduce the Lagrangian $L : W \times W \times Q \to \mathbb{R}$ by

$$L(U, Z, q) = J(q; U(T)) + F(q, Z) - B(U, Z).$$

Differentiating the Lagrangian with respect to Z, U, and q gives the optimality system

$$\begin{aligned} B(U, \Phi) &= F(q; \Phi), \\ B(\Phi, Z) &= J'_U(q; U(T))(\Phi) = (q - U(T), \Phi(T))_Q, \\ 0 &= J'_q(q; U(T))(\delta q) + F'_q(q; Z)(\delta q) = (q - U(T), \delta q)_Q + (\delta q, Z(0)) \end{aligned}$$

for any $\Phi \in W$ and $\delta q \in Q$. In particular, the last formula gives a representation for the gradient of the minimization problem

$$\min_{q \in Q} j(q) := J(q, U_q(T))$$

where $U_q \in W$ denotes the unique solution of (7) for the given value $q \in Q$. More precisely, for given $q \in Q$ one can calculate the Q-gradient $\nabla j(q) \in Q$ as solution of

$$(\nabla j(q), \delta q)_Q = (q - U(T), \delta q)_Q + (\delta q, Z(0)) \tag{8}$$

for all $\delta q \in Q$, where Z and U are given as solutions to the first two equations of the optimality system. Notice, that for $\|(v, u)\|_Q := \int_\Omega v^2 + u^2 \mathrm{d}x$ this means

$$\nabla j(q) = q - U(T) + Z(0),$$

while for $\|(v, u)\|_Q := \int_\Omega v^2 + |\nabla u|^2 \mathrm{d}x$ the calculation of the gradient requires the solution of a PDE for the q_u component.

The above observation allows to formulate a standard gradient-descent method

Algorithm 6 (Gradient method)**.** *Let $q^0 \in Q$ be an initial guess, and pick parameters $\gamma \in (0, 1/2)$ and $\alpha \in (0, 1)$. For $n = 1, 2, \ldots$ until $\|\nabla j(q^n)\|_Q < TOL$ iterate*

1. *Solve the primal problem*

$$B(U^n, \Phi) = F(q^{n-1}; \Phi).$$

2. *Solve the adjoint problem*

$$B(\Phi, Z^n) = J'_U(q^{n-1}; U^n(T))(\phi).$$

3. *Compute the gradient* $\nabla j(q^{n-1})$ *using* (8).

4. *Find the largest* $k \in \{0, 1, \dots\}$ *such that (Armijo-rule)*

$$j(q^{n-1} - \alpha^k \nabla j(q^{n-1})) \leq j(q^{n-1}) - \gamma \alpha^k \|\nabla j(q^{n-1})\|^2$$

holds and set $\alpha_n = \alpha^k$.

5. *Update*

$$q^n = q^{n-1} - \alpha_n \nabla j(q^{n-1}).$$

Similarly, we can construct an inexact Newton-type method, where the Newton equation

$$H(q)\delta q = -\nabla j(q)$$

is solved inexactly using a matrix-free CG-method. Here H denotes the Hessian operator $H(q)\colon Q \to Q$ of the reduced functional $j(q)$. For each subiteration of the CG-method requires the solution of two linear PDEs (the tangent and 'dual-for-hessian' equation), see, e.g., [3].

4.1 Discrete Setting

To simplify the notation, we discretize the time interval $I = (0, T)$ into discrete time steps of uniform size

$$0 = t_0 < t_1 < \cdots < t_M = T, \quad k := t_n - t_{n-1}. \tag{9}$$

We discretize in time with the backward Euler scheme. This can be interpreted as an approximation of the temporal Galerkin discretization with piecewise constant and discontinuous trial- and test-spaces on the subdivision (9), see [3, 4] for extensions to other time stepping schemes like variants of the Crank-Nicolson scheme and the necessary modifications required for dynamic time step sizes.

In the following, we give details on the discrete formulation for the strongly damped wave equation, written as first order system in $U = (v, u) \in W$ where $v = \partial_t u$. By $U_l = (v_l, u_l)$, we denote the approximation at time t_l. The control is given as $q = (q_v, q_u) \in Q$. The test function is denoted by Φ_k with $\Phi_l = (\phi_l, \psi_l)$ at time t_l. We introduce the discrete bilinear form $B_k(\cdot,\cdot)$ and the right hand sides of primal and dual problem

$$
\begin{aligned}
B_k(U_k,\Phi_k) &= \sum_{l=1}^{M}\Big\{(v_l - v_{l-1},\phi_l) + k\mu(\nabla u_l,\nabla\phi_l) + k\lambda(\nabla v_l,\nabla\phi_l) \\
&\qquad\qquad + (u_l - u_{l-1} - kv_l,\psi_l)\Big\} + (v_0,\phi_0) + (u_0,\psi_0), \\
F_k(q;\Phi_k) &= \sum_{l=1}^{M} k(f(t_l),\phi_l) + (q_v,\phi_0) + (q_u,\psi_0), \\
J_k(q,U_k;\Phi_k) &= \frac{1}{2}\Big((v_M - q_v,\phi_k) + (\nabla(u_M - q_u),\nabla\psi_l)\Big)
\end{aligned}
\tag{10}
$$

where $F_l = F(t_l)$. Apart from the approximation of this right hand side (by the box rule), the backward Euler scheme corresponds to the dG(0) Galerkin discretization, compare to (6).

For spatial discretization, we employ a conforming finite element Galerkin scheme with $V_h \subset V$. For simplicity, we assume that V_h does not change over time. Extensions to dynamic meshes are described in the literature [4]. To keep the notation simple, we use $U_l \in V_h \times V_h$ to also denote the fully discrete approximation and skip the index 'h' referring to the spatial discretization. The control space is discretized by $V_h \times V_h \subset Q$. Given $U_0 := q = (q_v, q_u) \in V_h \times V_h$, we iterate for $l = 1, 2, \ldots, M$ to define the primal solution

$$
\begin{aligned}
(v_l,\phi_l) + k\mu(\nabla u_l,\nabla\phi_l) + k\lambda(\nabla v_l,\nabla\phi_l) &= (v_{l-1},\phi_l) + k(f_l,\phi_l) \\
(u_l,\psi_l) - k(v_l,\psi_l) &= (u_{l-1},\psi_l)
\end{aligned}
\tag{11}
$$

The discrete adjoint problem is defined by swapping the role of trial- and test-function in (10) and $Z_k = (z_k, w_k) \in V_h \times V_h$ is defined as backward in time iteration of

$$
\begin{aligned}
(z_M,\phi_M) + k\lambda(\nabla z_M,\nabla\phi_M) - k(w_M,\phi_M) &= (v_M - q_v,\phi_M) \\
(w_M,\psi_M) + k\mu(\nabla z_M,\nabla\psi_M) &= (\nabla(u_M - q_u),\nabla\psi_M) \\[1em]
(z_l,\phi_l) + k\lambda(\nabla z_l,\nabla\phi_l) - k(w_l,\phi_l) &= (z_{l+1},\phi_l) \\
(w_l,\psi_l) + k\mu(\nabla z_l,\nabla\psi_l) &= (w_{l+1},\psi_l) \\[1em]
(z_0,\phi_0) &= (z_1,\phi_0) \\
(w_0,\psi_0) &= (w_1,\psi_0),
\end{aligned}
\tag{12}
$$

where first and last steps differ from the intermediate ones.

This setting can be extended to higher order time-discretizations like the Crank-Nicolson scheme as variant of a temporal Galerkin scheme with piecewise linear continuous trial functions and piecewise constant discontinuous test-functions or to variants with better stability like the shifted θ-time stepping scheme or the fractional step theta scheme [11, 18]. Furthermore it is possible to incorporate dynamic meshes [17] and non-uniform time steps. An extension to nonlinear problems (like the Navier-Stokes equations) is described in [4].

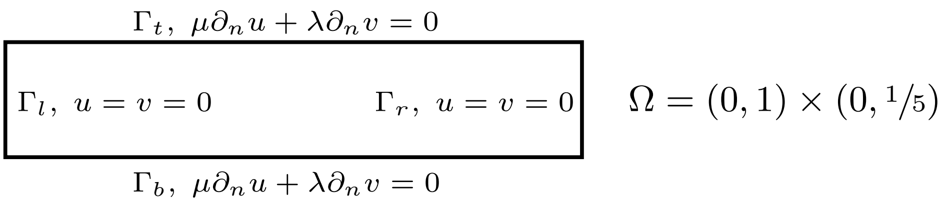

Figure 1: Configuration of the numerical test-cases. Domain of size width 1 and height 0.2. Free boundaries on the bottom and the top, homogeneous Dirichlet values on the left and the right.

5 Numerical tests

In this part, we discuss two numerical test cases following the abstract setting and the discretization introduced in the previous sections. First, we consider the damped wave equation with an oscillatory right hand side. Second, we introduce an additional nonlinearity. Both problems are given on a rectangular domain of size 1×0.2, see figure 1. On the left and the right, we prescribe homogeneous Dirichlet values for u and v, on the upper and lower boundary the solution is free, i.e.,

$$u = v = 0 \text{ on } \Gamma_{\mathrm{l/r}}, \quad \mu\partial_n u + \lambda\partial_n v = 0 \text{ on } \Gamma_{t/b}.$$

The problem is driven by the oscillatory right hand side (spatially constant)

$$f(t) = \sin(2\pi t) + \frac{1}{10}\cos(14\pi t). \tag{13}$$

It holds $f(t) = f(t+T)$ for $T = 1$. In all numerical test cases, we use piecewise bilinear elements on a quadrilateral mesh with 1 024 elements and the uniform time step size $k = 0.01$.

In Section 3, we equipped Q with the norm $L^2(\Omega) \times H^1(\Omega)$, see (4). The numerical test-cases are mostly performed using the norm

$$\|q\|_Q^2 = \|q_v\|^2 + \|q_u\|^2,$$

for which we cannot show the smoothing property required to satisfy Assumption 1. This norm however allows for a more efficient numerics, since (8) can be solved trivially. We will add one numerical test case that highlights the use of the correct norm $L^2 \times H^1$.

5.1 Linear damped wave equation problem

We consider the wave equation written as first order system in time

$$\begin{aligned} \partial_t v - \mu\Delta u - \lambda\Delta v &= f(t) \\ \partial_t u - v &= 0, \end{aligned}$$

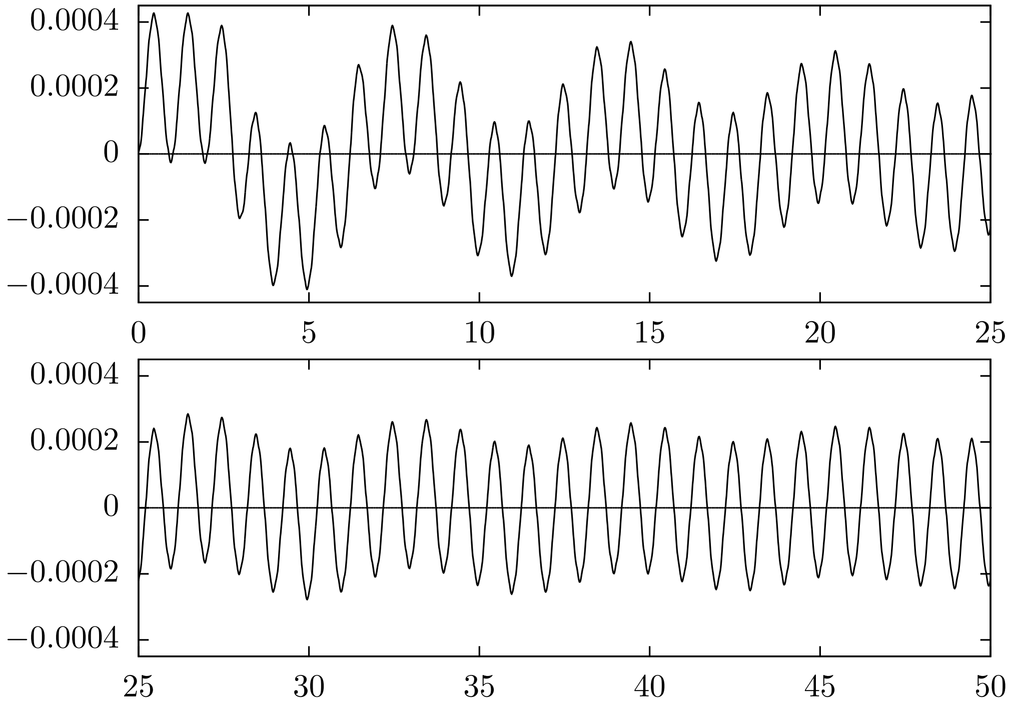

Figure 2: The functional $N(U(t))$ measuring the stress on the left and right boundaries plotted over the first 50 cycles.

with a periodic right hand side specified in (13) and the parameters

$$\mu = 0.1, \quad \lambda = 0.01$$

In Figure 2, we plot the functional

$$N\left(U(t)\right) = \int_{\Gamma_l \cup \Gamma_r} \left(\mu \partial_n u(t) + \lambda \partial_n v(t)\right) \, \mathrm{d}s$$

as function over time in for the first 50 periods, the interval $[0, 50]$. As initial solution at time $t = 0$, we used $q_v = q_u = 0$. The derivation from the periodic state is still easily visible after all 50 cycles.

Next, we directly identify the optimal initial data $q = (q_v, q_u)$ by means of the gradient method and the Newton scheme. We start the optimization routines with the initial guess $q_v = q_u = 0$. In Figure 3, we indicate the reduction of the functional

$$J(q; U_N) = \frac{1}{2}\|v_N - q_v\|^2 + \frac{1}{2}\|u_N - q_u\|^2$$

compared to the initial error in periodicity. To compare the efficiency of the gradient scheme with a direct forward solution running into the periodic solution, we plot the

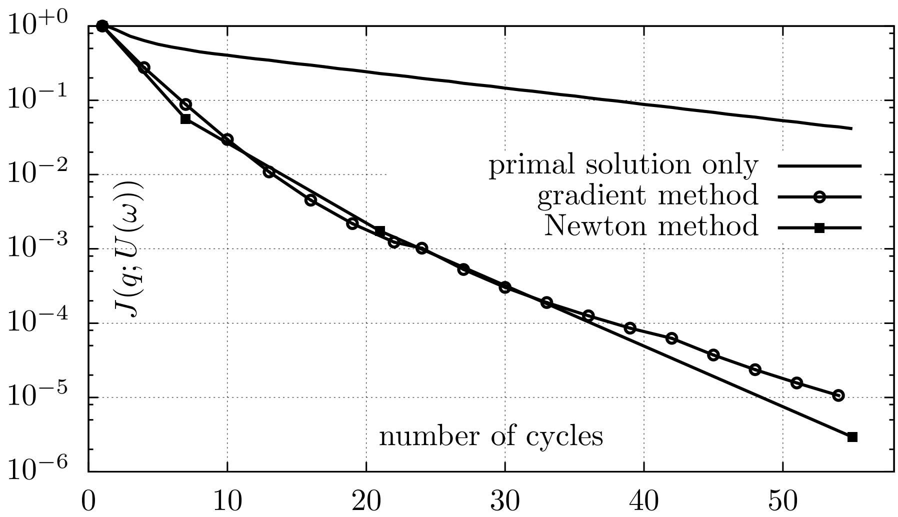

Figure 3: Relative reduction of the function $J(q;U)$ for the solution of the primal problem measured after every cycle and for the gradient method. On the x-axis, we give the number of cycles that have been computed. For the gradient method this is the sum of primal and adjoint cycles.

functional values over the number of cycles (PDE solutions over a time interval of length T) required. In the case of the forward solution, we count all cycles of length $T = 1$; for the gradient scheme, we count all cycles of the forward and the adjoint problem, both in steps 1. and 2. of Algorithm 6 and further necessary cycles within the Armijo rule in step 4. of the algorithm. For the Newton scheme, we also count all steps required for the inexact step calculation as well as the line search. This counting allows for a fair comparison of the computational effort in case of a linear PDE, since all PDE solutions are approximately of equal cost. Considering the gradient scheme and the Newton scheme, we plot the functional values $J(q^{n-1}; U_N^n)$ in the case of the forward problem, we plot $J(U(t_n - T); U(t_n))$ as a measure of periodicity.

While the simple forward simulation reduced the error by only on order of magnitude within the first 50 cycles, both optimization strategies yield a reduction of more then 5 orders in the same total number cycles. We note that the Newton scheme arrives at this low residual in only three steps.

Next, in Figure 4, we show the same comparison of the three different approaches (direct forward simulation, gradient and Newton method) using the $L^2(\Omega) \times H^1(\Omega)$-norm in J that allows us to comply with Assumption 1 according to Theorem 5. Here, we see a greater benefit of using the Newton scheme as compared to the gradient method. Again, both optimization approaches by far outrun the simple forward computation.

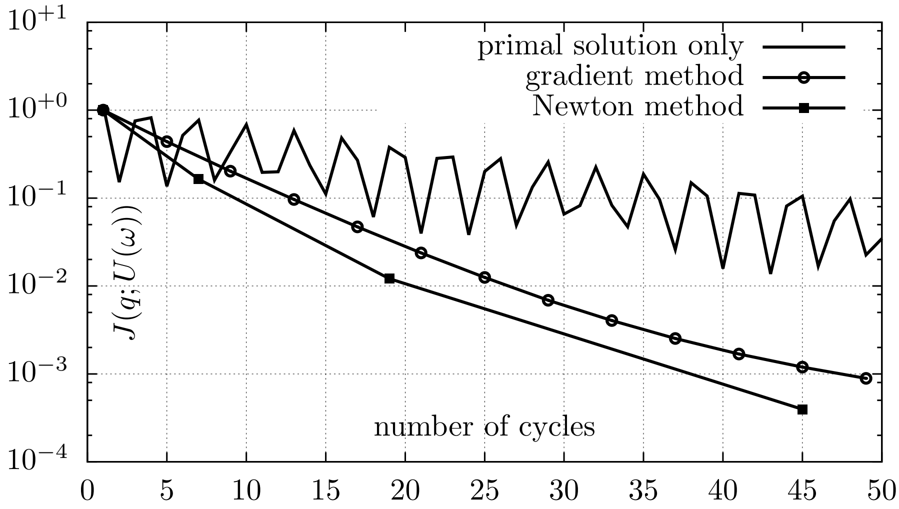

Figure 4: Reduction of the function $J(q;U)$ for the solution of the primal problem measured after every cycle and for the gradient method. In contrast to Figure 3, we now use the correct norm $L^2(\Omega) \times H^1(\Omega)$ for defining the goal functional.

5.2 Nonlinear Problem

As a second test case, we introduce a nonlinearity and solve

$$\begin{aligned} \partial_t v - \mu \Delta u - \lambda \Delta v + u^2 v &= f(t), \\ \partial_t u - v &= 0. \end{aligned}$$

We consider the same oscillatory forcing term $f(t)$ with periodicity $T = 1$ and stick to the parameters $\mu = 0.1$, $\lambda = 0.01$. The boundary data is set as for the linear case. Again, we start by the plotting the functional

$$N\left(U(t)\right) = \int_{\Gamma_l \cup \Gamma_r} \left(\mu \partial_n u(t) + \lambda \partial_n v(t)\right) \,\mathrm{d}s$$

as function of time, see Figure 5, where we show the interval $[0, 50]$. The structure of the solution is similar to the linear test case. The fundamental difference between linear and nonlinear problems is given in the computational effort. While the primal problem might be linear, the dual problem is always a linear problem with potentially lower computational cost.

Finally, in Figure 6, we give a comparison of the forward solution with the gradient method and the Newton scheme. Like in the linear case, we consider the simplified functional based on the $L^2(\Omega)$-norm

$$J(q; U_N) = \frac{1}{2}\|v_N - q_v\|^2 + \frac{1}{2}\|u_N - q_u\|^2.$$

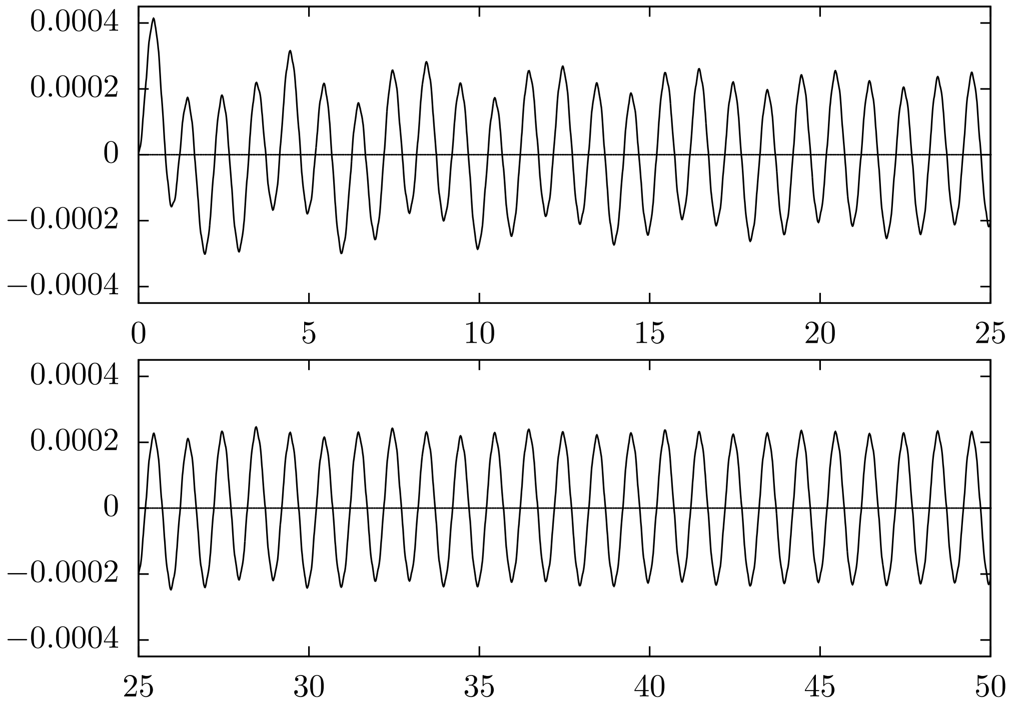

Figure 5: First 50 cycles of the nonlinear test case. Showing the functional $N(U(t))$.

We compare the reduction in $J(\cdot)$ over the number of required solution cycled relative to the initial value. Again, we observe a significant decrease in computational effort by using a systematic optimization approach in running to the cyclic state. In about 60 cycles, gradient and Newton scheme are able to reduce the goal functional by more than 3 orders of magnitude compared to a reduction between 1 and 2 orders of magnitude obtained with the simple forward simulation.

In contrast to the linear case, the Newton method is a bit more favorable here, since nonlinear PDEs need to be solved only once in each iteration and eventually during line search - which here only occurred for the gradient method.

6 Conclusion

We have introduced a new numerical approach for the efficient simulation of cyclic states with partial differential equations. In contrast to space-time techniques or approaches based on the shooting method, we only require the simulation of standard primal and dual solutions. There are various possibilities for enhancing the efficiency of the proposed scheme:

- The optimization loops can be run in a hierarchical configuration similar to [16] using coarse temporal and spatial meshes. This approach is promising as the dual

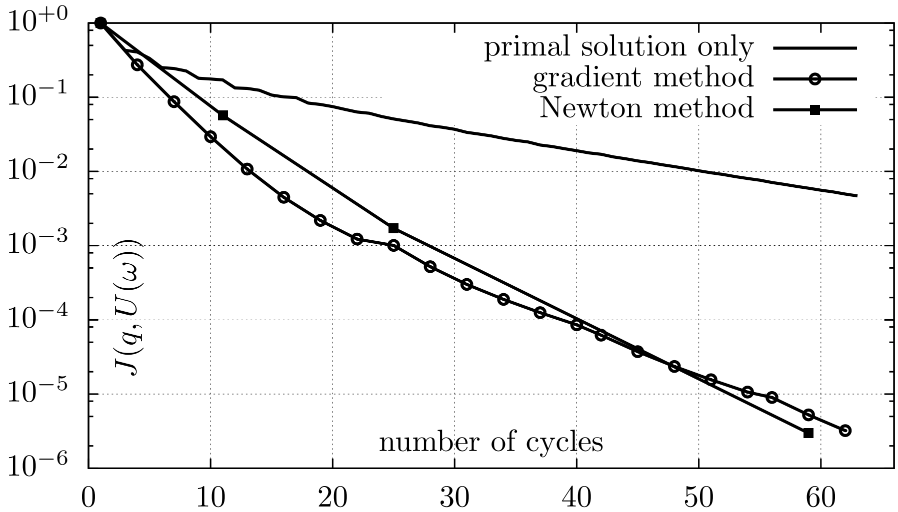

Figure 6: Reduction of in the function $J(q;U)$ for the solution of the primal problem measured after every cycle and for the gradient method. On the x-axis, we give the number of cycles that have been computed. For the gradient method this is the sum of primal and adjoint cycles.

solutions that are already available can be used to guide adaptive schemes for a control of optimization error in $q - u_N$ as well as spatial and temporal discretization error.

- The Newton scheme is highly effective in terms of Newton iterations. For both problems the desired residual of 10^{-8} is reached in only three steps. Still a large number of linear PDE solutions is required within to find a good line search parameter.

A next step is the application of the optimization schemes to problems where the periodicity T is not known a priori. Such situations frequently appear in fluid dynamics regarding the self-excited oscillatory flow around obstacles. The interval length T must be added as unknowns to the optimization problem, e.g.,

$$J(q,T;U) := \frac{1}{2}\|q - U(T)\|^2 \quad \mapsto \quad \min.$$

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