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Splitting methods for constrained diffusion–reaction systems

R. Altmann [a], A. Ostermann [b,*]

[a] *Institut für Mathematik MA4-5, Technische Universität Berlin, Straße des 17. Juni 136, 10623 Berlin, Germany*

[b] *Department of Mathematics, University of Innsbruck, Technikerstraße 13, 6020 Innsbruck, Austria*

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ABSTRACT

We consider Lie and Strang splitting for the time integration of constrained partial differential equations with a nonlinear reaction term. Since such systems are known to be sensitive with respect to perturbations, the splitting procedure seems promising as we can treat the nonlinearity separately. This has some computational advantages, since we only have to solve a linear constrained system and a nonlinear ordinary differential equation. However, Strang splitting suffers from order reduction which limits its efficiency. This reduction is caused by the fact that the nonlinear subsystem produces inconsistent initial values for the constrained subsystem. The incorporation of an additional correction term resolves this problem without increasing the computational cost significantly. Numerical examples including a coupled mechanical system illustrate the proved convergence results.

1. Introduction

Splitting methods for evolution equations have been studied extensively in the past years. The use of such methods for time integration allows one to split the problem into subsystems which can be integrated more efficiently or sometimes even exactly [1–3]. Moreover, splitting methods perform well in the preservation of geometric properties, which is one of the requirements of numerical integration [4]. For reaction–diffusion equations with a linear elliptic diffusion operator, several contributions to splitting methods can be found in the literature, e.g., [5–7].

In this paper, we consider nonlinear evolution equations of diffusion–reaction type which have an additional constraint. The diffusion is modelled with a linear elliptic differential operator, whereas the reaction term is nonlinear but smooth. Because of the constraint, we deal with so-called *partial differential–algebraic equations* (PDAEs) which generalize the concept of differential–algebraic equations (DAEs) [8,9] to the infinite dimensional case. Since these systems are known to be very sensitive (e.g. with respect to perturbations), we propose to apply splitting methods that reduce the given system to a linear PDAE and a nonlinear ordinary differential equation (ODE). With this, we only need to solve a nonlinear system in every spatial discretization point instead of a high-dimensional nonlinear PDAE.

It has been observed in various situations that splitting methods suffer from order reduction, e.g., if non-trivial boundary conditions are prescribed [10,7,11]. Since boundary conditions can be seen as a constraint on the dynamics, similar effects must be expected for general constraints. This can also be observed in numerical experiments. To overcome this kind of order reduction, we introduce a modification similar as in [11].

In this paper, we consider constrained systems of the form

$$\begin{aligned} \dot{u} \;-\; \mathcal{A}u - f(u) + \mathcal{D}^{-}\lambda &= F, \\ \mathcal{D}u \qquad\qquad\qquad &= G \end{aligned}$$

* Corresponding author.
E-mail addresses: raltmann@math.tu-berlin.de (R. Altmann), alexander.ostermann@uibk.ac.at (A. Ostermann).

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on a time interval $[0, T]$ with consistent initial condition $u(0) = u_0$, i.e., $\mathcal{D}u_0 = G(0)$. To enforce the constraint we employ the Lagrange multiplier λ. As mentioned before, we use a splitting approach in order to eliminate the nonlinearity from the PDAE. More precisely, we split the problem into a nonlinear unconstrained ODE and a linear PDAE of similar structure as the original problem. On the time interval $[t_n, t_{n+1}]$ the two subsystems have the form

$$\dot{w}_n = f(w_n) - q_n, \qquad w_n(0) = u_n,$$

which is a nonlinear ODE (the reaction part only), and the linear system

$$\dot{v}_n - \mathcal{A}v_n + \mathcal{D}^-\lambda_n = F_n + q_n, \qquad \mathcal{D}v_n = G_n, \qquad v_n(0) = w_n(\tau).$$

Note that u_n denotes the approximation to the solution $u(t_n)$, whereas v_n, w_n, and λ_n denote the exact solutions of the two subsystems, and $F_n(s) := F(t_n + s)$, $G_n(s) := G(t_n + s)$. We introduce a correction term q_n which is zero for the classical Lie and Strang splittings but aims to maintain the expected convergence orders of those methods. With a suitable correction we are able to obtain second-order convergence of Strang splitting. Such a correction is necessary, since the outcome of the ODE is, in general, not consistent with the given constraint.

The paper is structured as follows. In Section 2 we provide the required assumptions on the considered PDAE system and present a number of examples with different kinds of constraints which fit into the given framework. Moreover, we derive a variation-of-constants formula for linear PDAEs of the given structure which is the basis for the subsequent analysis. The convergence analysis for Lie and Strang splitting is then given in Sections 3 and 4, respectively. There we show that Lie splitting converges also without a correction term (as long as the boundary conditions are not affected by f), whereas Strang splitting requires a correction to guarantee second-order convergence. Throughout the paper we assume homogeneous Dirichlet boundary conditions. The extension to more general boundary conditions, however, will be discussed in Section 5. In Section 6 we consider three numerical examples. These include a coupled system of an elastic string and a nonlinear spring-damper system. Finally, we conclude in Section 7.

2. Preliminaries

Let X and Q be two Banach spaces and consider a partial differential equation (PDE) of the form

$$\dot{u} - \mathcal{A}u - f(u) = F$$

with a densely defined closed linear operator $\mathcal{A}$ on X and a smooth nonlinearity f. Typically, $\mathcal{A}$ is a differential operator, defined on a subspace $Z \subset X$. It is continuous from Z to X if Z is equipped with the graph norm. The system is constrained by

$$\mathcal{D}u = G.$$

Here, $\mathcal{D}\colon X \to Q$ is the linear constraint operator which is assumed to have a right-inverse $\mathcal{D}^-\colon Q \to X$. The right-hand sides are given functions $F\colon [0, T] \to X$ and $G\colon [0, T] \to Q$. We formulate the constrained PDE using the Lagrangian method, i.e., we add a Lagrange multiplier $\lambda\colon [0, T] \to Q$ which enforces the constraint and consider the system

$$\dot{u} - \mathcal{A}u - f(u) + \mathcal{D}^-\lambda = F, \tag{2.1a}$$
$$\mathcal{D}u = G. \tag{2.1b}$$

Note that the first equation is given in X while the second one is formulated in the Banach space Q. Eq. (2.1a) includes the right-inverse of $\mathcal{D}$ which enables the formulation of the dynamics in X although it is constrained to a subspace. Note that we consider here the right-inverse in place of the dual operator of $\mathcal{D}$, which is used when working in the weak setting.

We call such a system a partial differential–algebraic equation, since it generalizes both the concept of a classical DAE and of a PDE. However, we consider here the semigroup setting in contrast to the weak setting used, e.g., in [12,9,13] that corresponds to the weak formulation of the underlying PDE. We assume that $\mathcal{A}$ generates an analytic semigroup on the kernel of $\mathcal{D}$, cf. Section 2.1 for the precise assumptions. Thus we restrict our attention for the moment to homogeneous boundary conditions. However, we will discuss the required extensions for the non-homogeneous case in Section 5.

The given setting includes the following example. Further examples with more details are given in Section 2.2.

Example 2.1 (*Weighted Integral Mean*). Consider the semilinear heat equation, i.e., a parabolic PDE with a polynomial nonlinearity, subject to an additional constraint on the integral of the solution. On the domain $\Omega = (0, 1)$ the constraint operator $\mathcal{D}$ is given by

$$\mathcal{D}\colon X = L^2(\Omega) \to Q = \mathbb{R}, \qquad \mathcal{D}v = \int_0^1 v(x)\sin(\pi x)\,\mathrm{d}x.$$

The right-hand side $G\colon [0, T] \to \mathbb{R}$ defines the prescribed mean value. The overall system may have the form

$$\dot{u} - \Delta u - u^2 + \mathcal{D}^-\lambda = 0, \qquad \mathcal{D}u = G.$$

In this case, the operator $\mathcal{A}$ corresponds to the Laplacian with spaces $Z = H^2(\Omega)$, $D(\mathcal{A}) = H^2(\Omega) \cap H_0^1(\Omega)$, and $f(u) = u^2$ is a polynomial nonlinearity.

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