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An exponential time-differencing method for monotonic relaxation systems

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ABSTRACT

We present first- and second-order accurate exponential time differencing methods for a special class of stiff ODEs, denoted as *monotonic relaxation ODEs*. Some desirable accuracy and robustness properties of our methods are established. In particular, we prove a strong form of stability denoted as *monotonic asymptotic stability*, guaranteeing that no overshoots of the equilibrium value are possible. This is motivated by the desire to avoid spurious unphysical values that could crash a large simulation.

We present a simple numerical example, demonstrating the potential for increased accuracy and robustness compared to established Runge–Kutta and exponential methods. Through operator splitting, an application to granular–gas flow is provided.

1. Introduction

We are interested in numerical methods for stiff relaxation systems in the form

$$\frac{\mathrm{d}\boldsymbol{V}}{\mathrm{d}t} = \frac{1}{\epsilon}\boldsymbol{S}(\boldsymbol{V}), \tag{1}$$

to be solved for the unknown vector $\boldsymbol{V}$. Herein, the effect of the *relaxation source term* $\boldsymbol{S}(\boldsymbol{V})$ is to drive the system towards some local equilibrium value $\boldsymbol{V}^{\mathrm{eq}}$. The parameter ϵ represents a characteristic *relaxation time* towards equilibrium.

Our motivation for studying such systems is their relevance for more general hyperbolic relaxation systems in the form

$$\frac{\partial \boldsymbol{U}}{\partial t} + \frac{\partial \boldsymbol{F}(\boldsymbol{U})}{\partial x} = \frac{1}{\epsilon}\boldsymbol{R}(\boldsymbol{U}), \tag{2}$$

as analysed in detail by Chen et al. [4]. The parameter ϵ is typically small, imposing a high degree of stiffness in the system (2).

A popular approach towards solving stiff systems in the form (1) has been the use of *exponential integrators* [5,12,22]. Such methods are motivated in part by computational efficiency considerations [13]; without sacrificing high-order accuracy,

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one gets rid of the severe restriction on the time step commonly associated with explicit methods for stiff problems. The main idea behind such methods consists of splitting the source term into a linear and a nonlinear part as follows:

$$\frac{1}{\epsilon}\boldsymbol{S}(\boldsymbol{V}) = \boldsymbol{L}\boldsymbol{V} + \boldsymbol{N}(\boldsymbol{V}), \tag{3}$$

where $\boldsymbol{L}$ is a constant matrix. Ideally, the stiffness of the system (1) should be associated with the linear part, which may be solved exactly through the matrix exponential. Coupled to this, the nonlinear part $\boldsymbol{N}(\boldsymbol{V})$ is solved by standard Runge–Kutta methods.

In this paper, we wish to emphasize another aspect of methods based on exponential decay; the potential for strong robustness in the sense that the numerical solution is bounded with no restriction on the time step. In particular, one may use such methods to ensure that the relaxation step does not introduce unphysical solutions such as vacuum or negative-density states.

To achieve this, we here present what seems to us a slightly original twist to the idea of exponential integrators. Instead of viewing the exponential integration step as the *exact* solution to a linear sub-problem as given by the splitting (3), we interpret the exponential integration as a *numerical approximation* to the original nonlinear problem, and this approximation is nevertheless accurate to a certain order in the time step. This change of perspective leads to a slightly different formulation, and allows us to construct consistent methods that *by design* guarantee that the equilibrium solution cannot be exceeded. Although this leads to a high degree of robustness and accuracy in the stiff limit, the error of our proposed method nevertheless formally depends on the stiffness of the system.

If the numerical solution is bounded by the equilibrium value, consistency requires the same bound to hold also for the exact mathematical solution. Therefore, we will limit our investigations in this paper to what we denote as *monotonic* equations in the form (1), as defined more precisely in Section 2. This restricts the class of systems where our methods are applicable, but in particular includes many relaxation processes of practical interest within the context of (2).

This paper is organized as follows. In Section 2, we present the exponential integration technique which is the topic of this paper. First and second-order versions are provided. We also prove the following.

(i) The methods are stable in the strong sense that no numerical overshoots of the equilibrium value are possible.
(ii) The error is of second order in perturbations from the equilibrium if the source term decays linearly to zero.

Technical details needed for these proofs are given in Appendix A.

In Section 3, we briefly review hyperbolic relaxation systems in the form (2), and some known challenges associated with developing numerical methods for such systems. In this context, we discuss the potential applicability of the methods derived in Section 2.

In Section 4, some numerical examples are presented. In Section 4.1, we illustrate the main strength of our methods; they respect the monotonicity of the original equation with no restrictions on the time step. This example also demonstrates how standard Runge–Kutta methods and a classical exponential integrator may fail to possess this property.

This high degree of numerical stability would be desirable when solving more general hyperbolic relaxation systems in the form (2). Therefore, in Section 4.2, we present some preliminary investigations on applying our methods to such systems. In particular, we consider a numerical benchmark case known from the literature; a model for *granular–gas flow* as investigated by Serna and Marquina [33]. These initial tests seem to compare satisfactorily to results previously reported in the literature, indicating that our proposed methods may be worthy of further investigation.

Finally, in Section 5 we summarize our results and discuss some directions for further work.

2. Monotonically asymptotic exponential integration

For the purposes of this paper, we make the following definition.

Definition 1. Consider the equation

$$\frac{\mathrm{d}\boldsymbol{V}}{\mathrm{d}t} = \frac{1}{\epsilon}\boldsymbol{S}(\boldsymbol{V}), \qquad \boldsymbol{V} \in \mathcal{D} \subseteq \mathbb{R}^N, \qquad \boldsymbol{V}(0) = \boldsymbol{V}_0 \in \mathcal{D} \tag{4}$$

where $\boldsymbol{S}(\boldsymbol{V})$ is a C^2 function. The system is said to be a **relaxation ODE** provided there exists a unique point $\boldsymbol{V}^{\mathrm{eq}} \in \mathcal{D}$ such that

$$\boldsymbol{S}\big(\boldsymbol{V}^{\mathrm{eq}}\big) = 0, \tag{5}$$

and the solution satisfies

$$\lim_{t\to\infty} \boldsymbol{V}(t) = \boldsymbol{V}^{\mathrm{eq}}. \tag{6}$$