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A Fast Compact Exponential Time Differencing Runge-Kutta Method for Time-Dependent Advection-Diffusion-Reaction Equations

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Abstract. A fast and accurate exponential Runge-Kutta method for a class of time-dependent advection-diffusion-reaction equations is developed. To discretise the convection term, a modified upwind difference scheme is used. This allows to avoid numerical oscillation and achieve second order spatial accuracy. The method demonstrates good stability and numerical examples show the applicability of the method to advection-diffusion-reaction problems with stiff nonlinearities.

AMS subject classifications: 65M06, 65M22, 65Y20

Key words: Advection-diffusion-reaction, exponential time differencing, linear splitting, discrete Fourier transforms, Runge-Kutta approximations.

1. Introduction

Advection-diffusion-reaction equations are widely used in diverse applications, including atmospheric air and groundwater pollution and bacterial and tumour growth [9]. In this paper, we consider advection-diffusion-reaction equations of the form

$$\frac{\partial u}{\partial t} = Lu - f(u), \quad \mathbf{x} \in \Omega, \quad t \in [t_0, t_0 + T], \tag{1.1}$$

where $\Omega \subset \mathbb{R}^d$ is an open rectangular domain, $f(u)$ a reaction function, $T > 0$ the duration time, and operator L is defined by

$$Lu = \nabla \cdot (D\nabla u) - \mathbf{b} \cdot \nabla u$$

with a diffusion diagonal matrix $D > 0$ having constant leading diagonal entries $(d_1, d_2, \cdots, d_d)$ and a convective velocity $\mathbf{b} = (b_1, b_2, \cdots, b_d)^T$.

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The Eq. (1.1) is often accompanied by an initial condition $u|_{t=t_0} = u_0$ for $\mathbf{x} \in \Omega$ and certain boundary conditions.

Numerical methods for the model equation (1.1) attracted considerable attention in the past decades — cf. [9]. The use of exponential integrators in time discretisation turned out to be very efficient, especially in advection-diffusion-reaction problems involving stiff nonlinearities. The family of exponential integrators are based on the approximation of the respective integral formulation of nonlinear terms in the differential equation, finding the exact solution of the linear part and computing the exponential of a matrix. Caliari *et al.* [1] proposed a second-order exponential integrator for semi-discretised advection-diffusion-reaction equations by coupling exponential like Euler and midpoint integrators. Nie *et al.* [17] used the compact form of the integration factor methods to develop an implicit integration factor method that serves as an efficient class of time-stepping methods for reaction diffusion systems with both stiff reaction and diffusion terms in high spatial dimensions. Later on, Zhao *et al.* [21] combined the integration factor method with WENO to solve advection-diffusion-reaction equation. Tambue *et al.* [18] applied the real Leja points technique to obtain an exponential time integrator for advection-dominated reactive transport in highly heterogeneous porous media. Jiang and Zhang [10] studied the Krylov implicit integration factor WENO methods for semi-linear and fully nonlinear advection-diffusion-reaction equations. Recently, Ju and Wang [12] considered a compact exponential time differencing Gauge method for incompressible viscous flows.

Although exponential integrators can solve the linear part exactly in time, matrix exponentials have to be involved and this is a notoriously difficult problem in numerical analysis [16]. Recently, an efficient exponential time differencing method has been presented in [14]. It uses a compact representation of the central difference scheme for spatial discretisation and allows to use FFT-based fast calculation of matrix exponentials. The method utilises a high order multi-step integration factor in time scheme along with usual splitting technique for treating stiff nonlinearities incorporated into the resulting scheme. It improves stability and does not require solving nonlinear systems. The method was extended to the Cahn-Hilliard equation and successfully used in computing material coarsening rates under constant and variable mobilities — cf. [13]. We also note efficient and stable exponential Runge-Kutta methods for parabolic equations developed in [22] and fast high-order compact exponential time differencing Runge-Kutta methods for second-order semi-linear parabolic equations proposed in [23]. However, to the best of authors' knowledge, so far this fast compact exponential time differencing Runge-Kutta method has been not applied to advection-diffusion-reaction equations.

Here, we develop a fast compact exponential time differencing Runge-Kutta method for the advection-diffusion-reaction equation (1.1). It uses the modified upwind difference scheme from [24] in order to discretise the convection term. As the result, there is no numerical oscillation and the method has second order accuracy in space direction. Combining the stabilised compact explicit exponential time differencing Runge-Kutta method from [22] and a modified upwind difference scheme, we establish a novel compact exponential time differencing Runge-Kutta method for the Eq. (1.1). This method has second order spacial accuracy and good stability, while the FFT-based fast calculation techniques