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A review of exponential integrators for first order semi-linear problems

by

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Abstract

Recently, there has been a great deal of interest in the construction of exponential integrators. These integrators, as their name suggests, use the exponential function (and related functions) of the Jacobian or an approximation to it, inside the numerical method. However, unlike some of the recent literature suggests, integrators based on this philosophy have been known since at least 1960. The aim of this paper is to review exponential integrators, designed for first order problems, however, we will also briefly discuss some recent research into the construction of exponential integrators, for special problems. Our hope is, that with this article, by reviewing as much of the history of exponential integrators as reasonable possible, we can point interested readers to appropriate references and hopefully reduce the reinvention of known results.

1 Introduction

Even though the theory of numerical methods for time integration is well established for a general class of problems, recently due to improvements in the efficient computation of the exponential function, exponential integrators for the time integration of semi-linear problems

$$y'(t) = f(y(t)) = Ly(t) + N(y(t)), \qquad y(t_{n-1}) = y_{n-1}. \tag{1.1}$$

have emerged as a viable alternative. In [88] it is claimed that the largest performance improvement in the solution of partial differential equations will come from better time integration technology. In the early fifties, the phenomenon of stiffness was first discovered by Curtis and Hirschfelder [18]. Stiffness effectively yields explicit integrators useless, as stability rather than accuracy governs how the integrator performs. It could be said that more integrators have been developed to overcome the phenomenon of stiffness, than any other property that a differential equation may have. Stiffness was also the reason for the introduction of exponential integrators. The recent wave of publications on exponential integrators, have mainly been concerned with the time integration of spatially discretized parabolic and hyperbolic partial differential equations.

Various methods have been developed for the differential equation (1.1). The first paper to construct what are now known as exponential integrators, was by Certaine [15], published in 1960. This paper constructed two exponential integrators based on the Adams–Moulton methods of order two and three. These methods are members of the Exponential Time Differencing (ETD) methods, which find approximations to the integral in the variation of constants formula, using an algebraic polynomial approximation to the nonlinear term. Other papers on this subject include [5, 16, 44, 43, 58, 77]. In 1967, Lawson published [62], which provided a novel approach to solving stiff problems. Integrators were constructed, which solve exactly the linear part of the problem and then used a change of variables to cast the problem in a form, which a traditional explicit method can be used to solve the transformed equation, the approximate solution is then back transformed. These methods are commonly known as Integrating Factor (IF) methods. Further papers on this subject include

[6, 16, 69, 71, 90, 99]. In 1999, Munthe-Kaas published [76], which constructed a class of methods known as the RKMK methods. These methods transform the differential equation to a differential equation evolving on a Lie algebra, which is a linear space. Munthe-Kaas realized that the affine action was very useful in constructing integrators for differential equations of the form (1.1). The affine action was also used in [14] to construct integrators for (1.1) based on the Commutator-Free (CF) Lie group methods. In [58] Krogstad, introduced the Generalized Integrating Factor (GIF) methods, which were shown to exhibit large improvements in accuracy over the IF, ETD and CF methods. In [52, 53] numerical experiments were performed on certain stiff PDEs using the IF, ETD, linearly implicit methods and splitting methods. It was concluded that the ETD methods consistently outperformed all other methods.

The aim of this paper is to try and review the history of exponential integrators tailored for the problem (1.1). The reason being that a significant new interest in developing integrators has lead to many papers in which known integrators have been rediscovered. We aim to represent exponential integrators in a general framework. The paper is organized as follows. Section 2 considers several modifications of the Euler method and motivates our aims. In Section 3 we construct a class of exponential general linear methods, which will provide the framework for various methods. The next four sections discuss the history of the IF, ETD, GIF and the integrators based on Lie group methods respectively and represents these methods as exponential general linear methods. Section 8, then presents an overview of the order conditions of exponential integrators and we follow with a discussion of implementation issues. Exponential integrators which have been constructed for particular problems will be briefly discussed in Section 10. Finally, we conclude with some numerical experiments and several remarks and open questions.

2 Modifications of the Euler method

Before introducing the framework of exponential integrators, we examine several well known extensions of the Euler method. Linearizing the initial value problem (1.1), gives

$$y'(t) = f(y_{n-1}) + f'(y_{n-1})(y - y_{n-1}).$$

The exact solution to this linearized problem is

$$y_n = y_{n-1} + h\varphi_1(hf'(y_{n-1}))f(y_{n-1}), \tag{2.1}$$

where the function φ_1, is defined as

$$\varphi_1(z) = \frac{\mathrm{e}^z - 1}{z}.$$

This method is of order two, for general problems of the form (1.1), and exact for problems, where $f(y) = Ly + N$, it is known as the exponential Euler method. The earliest reference, we can find to this method, is in the paper of Pope [83],

where he calls the method the exponential difference equation. We are unsure if this method had been derived even earlier.

Mainly, due to contributions from Verwer and van der Houwen, the exponential Euler has been generalized in the direction of Runge–Kutta and linear multistep methods and are known as generalized Runge–Kutta and linear multistep methods, [101, 103, 104, 102]. Despite this framework, there does not seem to be (until recently) methods available, which use the exponential or related functions of the exact Jacobian. This is most likely due to the cost involved in recomputing the Jacobian and then computing the exponential or related function of the Jacobian. Given this high cost, most integrators evolved in one of two directions. The first approach is not to use exact representations of the exponential and related functions but approximations, generally Padé approximations. One of the main classes of methods in this direction are the Rosenbrock methods, of which there is a vast literature; we refer only to the papers by Rosenbrock, [85] and the book by Hairer and Wanner, [35]. We also refer to the book of van der Houwen, [101] and the paper by Hairer, Bader and Lubich, [33], where many alternative integrators, in this direction are analyzed. The alternative approach is to compute the exponential and related functions exactly of an approximation to the Jacobian. The first paper in this direction was by Certaine [15] in 1960. Integrators which use exact computations of the exponential and related functions of an approximation to the Jacobian are the main focus of this review. This may seem a rather large restriction class of methods, but in fact a vast array of literature exists, much of which is directed at the efficient time integration of semi-linear problems.

For semi-linear problems, where generally most of the difficulty lies in the operator L and not in the nonlinear term $N(y)$, an approximation to the Jacobian of f, seems reasonable. The natural choice of this approximation, for semi-linear problems is L. Let us assume, that we use L as an approximation to the full Jacobian in the method (2.1) above

$$\begin{aligned} y_n &= y_{n-1} + h\varphi_1(hL)(Ly_{n-1} + N(y_{n-1})) \\ &= \mathrm{e}^{hL}y_{n-1} + h\varphi_1(hL)N(y_{n-1}). \end{aligned} \tag{2.2}$$

What is interesting about this method, is the number of different viewpoints from which it has been derived. It was first introduced by Nørsett [78] in 1969, as the order one method in a class of exponential integrators based on the Adams–Bashforth methods. It is also a special case of the filtered explicit Euler method, see [60, 84]. The method (2.2) is now most commonly called the Exponential Time Differencing (ETD) Euler. Higher order methods based on Adams and Runge–Kutta methods are discussed in more detail in Section 5. Another common name used for (2.2) is the exponentially fitted Euler method. Exponential fitting was introduced by Liniger and Willoughby [63] in 1970. More recently it was derived as the order one Lie group, Runge–Kutta method with affine action (see [76]), and is called the Lie–Euler method. Exponential integrators based on Lie group methods for semi-linear problems are discussed in Section 7. The implicit ETD Euler is

$$y_n = \mathrm{e}^{hL}y_{n-1} + h\varphi_1(hL)N(y_n).$$

We now describe an alternative derivation of the method (2.2). Construct a transformed differential equation by multiplying the original differential equation by $\mathrm{e}^{(t_{n-1}-t)L}$, giving

$$\begin{aligned}\mathrm{e}^{(t_{n-1}-t)L}y'(t) &= \mathrm{e}^{(t_{n-1}-t)L}Ly(t) + \mathrm{e}^{(t_{n-1}-t)L}N(y(t))\\ (\mathrm{e}^{(t_{n-1}-t)L}y(t))' &= \mathrm{e}^{(t_{n-1}-t)L}N(y(t)).\end{aligned}$$

If we find the integral representation of this differential equation and approximate the nonlinear term in the integral by $N(y_{n-1})$, and then solve exactly, we arrive again at the ETD Euler method. Alternatively, if we apply the explicit Euler to the transformed equation and then transformed back into the original variables, we get

$$y_n = \mathrm{e}^{hL}y_{n-1} + \mathrm{e}^{hL}hN(y_{n-1}). \tag{2.3}$$

This is known as the Lawson–Euler, after Lawson [62] who invented it in 1967, as a means of overcoming stiffness, in semi-linear problems. Method (2.3) is most commonly referred to as the Integrating Factor (IF) Euler method, as the differential equation is multiplied by the integrating factor $\mathrm{e}^{(t_{n-1}-t)L}$. However, we choose to call methods based on this idea, Lawson methods, discussed in more detail in Section 4. The implicit Lawson-Euler method is

$$y_n = \mathrm{e}^{hL}y_{n-1} + hN(y_n).$$

We have already introduced three different extensions of the Euler method, all of which are exponential integrators and all have been called the exponential Euler method. It is important to distinguish between these methods, as they often perform quite differently. Recently, Lord and Rougemont [65] extended this idea to the class of semi-linear stochastic PDEs, constructing a first order stochastic Lawson–Euler method. The well-known implicit Euler–Maruyama scheme can be considered an approximation to the stochastic Lawson–Euler.

Following Hochbruck [38] we define an exponential integrator as follows.

Definition 2.1. An exponential integrator is a numerical method which involves an exponential function (or a related function) of the Jacobian or an approximation to it.

Given this definition, the three Euler methods derived in this section are all exponential integrators. However, we will mainly restrict our attention to exponential integrators which use an approximation of the Jacobian. Even so, when appropriate, we will describe how many well-known methods are equivalent to exponential integrators, if the exponential (and related functions) were computed exactly; as the essential difference can be considered as one of computational efficiency. We also mention here, that all exponential integrators considered in this paper are A-stable, which is a direct consequence of using the exponential within the method.

3 Exponential general linear methods

We have chosen to limited the scope of this paper to exponential integrators designed for semi-linear problems, where an approximation to the Jacobian

(rather than the exact Jacobian), is used. The class of exponential integrators we consider, is based on general linear methods, which use the exponential (and related functions) of the approximate Jacobian within the integrator. We require that; if $L = 0$, then the resulting method is a general linear method, which is known as the underlying general linear method; if $N(u) = 0$, then the numerical method will supply the exact solution if the exponential and related functions are evaluated exactly.

Generally, for semi-linear problems, the difficult part (stiff or oscillatory nature) of the differential equation is in the linear part of the problem. By treating the linear part of the problem exactly, using the exponential and related functions, the remaining part of the integrator can be explicit. The tradeoff here is that the exponential and related functions are computed, rather than using an implicit integrator. When a constant stepsize is used throughout the integration, the exponential and related functions can be evaluated before the integration begins, given that storing such information is feasible. These functions can be a significant overhead depending on the dimensionality of the differential equation and the structure of the matrix L. Therefore, exponential integrators are likely to be most competitive when the matrix L is diagonal or cheaply diagonalizable.

If h represents the stepsize and the r quantities

$$y_1^{[n-1]}, y_2^{[n-1]}, \ldots, y_r^{[n-1]},$$

are known, then the computations performed in step number n, of an exponential general linear method, are

$$Y_i = \sum_{j=1}^{s} a_{ij}(hL)hN(Y_j) + \sum_{j=1}^{r} u_{ij}(hL)y_j^{[n-1]} \tag{3.1}$$

$$y_i^{[n]} = \sum_{j=1}^{s} b_{ij}(hL)hN(Y_j) + \sum_{j=1}^{r} v_{ij}(hL)y_j^{[n-1]}. \tag{3.2}$$

The coefficients of the method a_{ij}, b_{ij}, u_{ij} and v_{ij} are function of the exponential and related functions. The quantities which are assumed known at the start of step number n, must be computed using some starting method when the integration begins. We can represent the exponential general linear methods in a more compact notation by introducing the vectors Y, $N(Y)$, $y^{[n-1]}$ and $y^{[n]}$, as

$$Y = \begin{bmatrix} Y_1 \\ Y_2 \\ \vdots \\ Y_s \end{bmatrix} \quad N(Y) = \begin{bmatrix} N(Y_1) \\ N(Y_2) \\ \vdots \\ N(Y_s) \end{bmatrix} \quad y^{[n-1]} = \begin{bmatrix} y_1^{[n-1]} \\ y_2^{[n-1]} \\ \vdots \\ y_r^{[n-1]} \end{bmatrix} \quad y^{[n]} = \begin{bmatrix} y_1^{[n]} \\ y_2^{[n]} \\ \vdots \\ y_r^{[n]} \end{bmatrix}.$$

An exponential general linear method can be represented in matrix form as

$$\begin{aligned} Y &= A(hL)hN(Y) + U(hL)y^{[n-1]}, \\ y^{[n]} &= B(hL)hN(Y) + V(hL)y^{[n-1]}. \end{aligned} \tag{3.3}$$

Often it is convenient to represent the exponential general linear method in the tableau form

$$M(hL) = \left[\begin{array}{c|c} A(hL) & U(hL) \\ \hline B(hL) & V(hL) \end{array}\right].$$

Most of the methods that we will describe in this paper are exponential Runge–Kutta methods or exponential Adams methods.

4 Lawson methods

The generalized Runge–Kutta processes were first discovered by Lawson [62] in 1967 and have been rediscovered many times since. They are more commonly called Integrating Factor (IF) methods, a name used by Boyd [6], Canuto, Hussaini, Quarteroni and Zang [12], Milewski and Tabak, [71], Maday, Patera and Rønquist [69], Smith and Waffle [90], and Trefethen, [99]. They are also known as Linearly Exact Runge–Kutta (LERK) methods a name which seems to have first been used by García-Archilla [27], to describe the single third order method introduced by Jauberteau, Rosier and Temam in [51].

The main idea behind the Lawson methods, is to use a change of variables, often called the Lawson transformation

$$v(t) = \mathrm{e}^{(t_{n-1}-t)L} y(t).$$

Differentiating both sides of this equation yields

$$\begin{aligned} v'(t) &= -L\mathrm{e}^{(t_{n-1}-t)L} y(t) + \mathrm{e}^{(t_{n-1}-t)L} y'(t) \\ &= \mathrm{e}^{(t_{n-1}-t)L} N(y(t)) \\ &= \mathrm{e}^{(t_{n-1}-t)L} N(\mathrm{e}^{(t-t_{n-1})L} v(t)). \end{aligned}$$

The purpose of transforming the differential equation in this way is to remove the explicit dependence in the differential equation on the operator L, except inside the exponential. The exponential function will damp the behaviour of L removing the stiffness or highly oscillatory nature of the problem. The aim is now to use any numerical integrator, (in the case of Lawson, a Runge–Kutta method) on the transformed, hopefully non-stiff, differential equation.

Apply a q-step Adams method to the transformed differential equation and then transform back to the original variable, to obtain the solution approximation. In general, the Lawson–Adams methods are

$$y_n = \mathrm{e}^{hL} y_{n-1} + \sum_{k=0}^{q} \beta_k \mathrm{e}^{khL} N(y_{n-k}),$$

where β_k are the coefficients of the underlying Adams method. Lawson methods based on the q-step BDF methods are

$$y_n = \sum_{k=1}^{q} \alpha_k \mathrm{e}^{khL} y_{n-k} + hN(y_n),$$

where α_k are the coefficients of the underlying BDF method. The general formulation of an s-stage, Lawson–Runge–Kutta method in the original variables is

$$\begin{aligned} Y_i &= \sum_{j=1}^{s} a_{ij} \mathrm{e}^{(c_i - c_j)hL} hN(Y_j) + \mathrm{e}^{c_i hL} y_{n-1}, \quad i = 1, 2, \ldots, s, \\ y_n &= \sum_{j=1}^{s} b_i \mathrm{e}^{(c_i - c_j)hL} hN(Y_j) + \mathrm{e}^{hL} y_{n-1}. \end{aligned} \tag{4.1}$$

This construction requires that the c vector has nondecreasing coefficients. The most computational efficient schemes are when the c vector has uniform abscissae, with as many repetitions as possible.

It is reported in the paper [22] that the Lawson–Runge–Kutta methods only work well on moderately stiff problems in which the solution tends to zero or is periodic. In [22], they tried to overcome this problem by modifying the method (see the next section for details). Numerical tests on the Kuramoto–Sivashinsky equation comparing a variable-order variable-step implementation of the BDF formula and the third order method presented in [51] were given in [27]. These tests showed that the BDF method significantly outperformed the Lawson method.

The main difficulty with Lawson based methods is the overall stiff order achieved is limited to one. This will be discussed further in Section 8, but basically boils down to the fact that Lawson methods only use the exponential function. We also note here that the Lawson methods will not preserve fixed points, which exist in the true solution.

The idea of transforming the differential equation and solving the individual parts separately has lead to great success in convection-dominated PDEs. We refer to the paper by Maday, Patera and Rønquist [69], which has many similarities to the Lawson and generalized Lawson methods discussed in Section 6. Further work in this area by Celledoni, [13] uses the methods reviewed in Section 7.

5 Exponential time differencing

A far more commonly used approach, which also has been rediscovered several times, is the so called Exponential Time Differencing (ETD) methods, a name originally used in computational electrodynamics. These methods also go by the names; generalized linear multistep and generalized Runge–Kutta methods, introduced by van der Houwen and Verwer [102] and Verwer [103]; Exact treatment of the Linear Part (ELP) schemes, introduced by Beylkin, Keiser and Vozovoi [5]; exponential propagation a name used by Friesner et. al. [25] and Edwards et. al. [21]. The ETD methods are very closely related to the W-methods of Steihaug and Wolfbrandt [91] developed in 1979 to overcome the need to use the exact Jacobian in the Rosenbrock methods and the adaptive Runge–Kutta methods constructed as an extension of the W-methods in 1982 by Strehmel and Weiner [92]. The main difference these two classes of methods

is that the ETD methods compute the exponential and related functions exactly, while the W-methods and the adaptive Runge–Kutta methods generally use Padé approximations. This is discussed in more detail later in this section. The ETD methods have been widely used in the physics literature, for example we cite [45, 82, 87, 89, 97].

The ETD methods can be constructed via the variation of constants formulae. To derive the variation of constants formula, take the transformed differential equation

$$(\mathrm{e}^{(t_{n-1}-t)L}y(t))' = \mathrm{e}^{(t_{n-1}-t)L}N(y(t)), \quad y(t_{n-1}) = y_{n-1},$$

and find the corresponding integral representation, which is

$$y(t_{n-1}+h) = \mathrm{e}^{hL}y_{n-1} + \int_0^h \mathrm{e}^{(h-\tau)L}N(y(t_{n-1}+\tau))\,\mathrm{d}\tau. \tag{5.1}$$

The ETD methods are based on approximating the nonlinear term in the variation of constants formulae by an algebraic polynomial. Such ideas in a quadrature setting were first used by Filon [23] in 1928. All ETD methods are designed so that fixed points are preserved.

5.1 ETD linear multistep methods

To construct ETD linear multistep methods, the nonlinear term in the variation of constants formula (5.1) is approximated by an algebraic polynomial, which uses information known from previous steps. When $L = 0$, these methods reduce to the standard linear multistep methods. The first known paper in this direction is that of Certaine [15] from 1960, where order two and order three methods which reduce to the corresponding Adams–Moulton formulae, were derived. What seems to be the next paper in this direction is the 1969 paper of Nørsett [77], where arbitrary order A-stable exponential integrators, which reduce to the Adams–Bashforth methods when $L = 0$, are constructed. There are two main representations of these methods and we believe it is worth giving both here. First, following Nørsett, ETD Adams–Bashforth methods have the form

$$y_n = \mathrm{e}^{hL}y_{n-1} + h\sum_{k=0}^{q-1}\alpha_k(hL)\nabla^k N_{n-1},$$

where $\nabla^0 N_{n-1} = N_{n-1}$ and $\nabla^{k+1}N_{n-1} = \nabla^k N_{n-1} - \nabla^k N_{n-2}$ are the backward differences, and the functions $\alpha_k(x)$, satisfy the following recurrence relations

$$\begin{aligned} x\alpha_0(x) &= \mathrm{e}^x - 1, \\ x\alpha_{k+1}(x) + 1 &= \alpha_k(x) + \tfrac{1}{2}\alpha_{k-1}(x) + \tfrac{1}{3}\alpha_{k-2}(x) + \cdots + \tfrac{1}{k+1}\alpha_0(x). \end{aligned}$$

If appropriate approximations are used to $\alpha_k(x)$, then these methods become a subclass of those introduced in [61]. The above result has been recently rediscovered in the paper by Cox and Matthews [16]. Calvo and Palencia [11] have derived closely related q-step ETD methods and shown that they are convergent and of stiff order q.

It is possible to construct ETD Adams–Moulton formulae using the same philosophy as was used by Nørsett. The most likely reason why Nørsett did not derive these formulas is that the stiffness in the problem is overcome by the use of the exponential function, and therefore, it would seem unnecessary to use an implicit method. However, they could be used as a corrector for an ETD Adams–Bashforth method. The ETD Adams–Moulton methods have the form

$$y_n = \mathrm{e}^{hL} y_{n-1} + h \sum_{k=0}^{q} \beta_k(hL) \nabla^k N_n,$$

where the functions $\beta_k(x)$, satisfy the following recurrence relations

$$\begin{aligned} x\beta_0(x) &= \mathrm{e}^x - 1, \\ x\beta_{k+1}(x) + \tfrac{1}{(k+2)!} &= \left(1 - \tfrac{1}{(k+1)!}x\right)\beta_k(x) + \cdots + (1-x)\beta_0(x). \end{aligned}$$

We have discussed that exponential integrators use the exponential and related functions; the ETD Adams methods use the α and β, as the related functions, however, the most common related functions used in exponential integrators are the so called φ-functions, which are defined as

$$\varphi_\ell(xL) = \frac{1}{x^\ell} \int_0^x \mathrm{e}^{(x-\tau)L} \frac{\tau^{\ell-1}}{(\ell-1)!}\, \mathrm{d}\tau, \qquad \ell \geq 1.$$

The φ-functions are related by the recurrence relation

$$\varphi_{\ell+1}(z) = \frac{\varphi_\ell(z) - \frac{1}{\ell!}}{z}, \quad \varphi_\ell(0) = \frac{1}{\ell!}.$$

For the second representation of the ETD Adams methods we follow the paper of Beylkin, Keiser and Vozovoi [5]. The following lemma provides an expression for the exact solution, which will be used throughout this paper.

Lemma 5.1. *The exact solution of the initial value problem*

$$y'(t) = Ly(t) + N(y(t)), \quad y(t_{n-1}) = y_{n-1},$$

can be represented by the expansion

$$y(t) = \mathrm{e}^{(t-t_{n-1})L} y_{n-1} + \sum_{\ell=1}^{\infty} \varphi_\ell\left((t-t_{n-1})L\right)(t-t_{n-1})^\ell N_{n-1}^{(\ell-1)},$$

where $N_{n-1}^{(\ell-1)} = \frac{\mathrm{d}^{\ell-1}}{\mathrm{d}t^{\ell-1}} N(y(t))\,\big|_{t=t_{n-1}}$.

Proof: Substitute a Taylor series expansion of the nonlinear term into the variation of constants formula and using the expression for the φ-functions, gives

$$\begin{aligned} y(t) &= \mathrm{e}^{(t-t_{n-1})L} y_{n-1} + \int_0^{t-t_{n-1}} \mathrm{e}^{(t-t_{n-1}-\tau)L} N(y(t_{n-1}+\tau))\, \mathrm{d}\tau \\ &= \mathrm{e}^{(t-t_{n-1})L} y_{n-1} + \sum_{\ell=1}^{\infty} \varphi_\ell((t-t_{n-1})L)(t-t_{n-1})^\ell N_{n-1}^{(\ell-1)} \end{aligned} \tag{5.2}$$

The numerical solution approximates the variation of constants formulae (5.1) by

$$y_n = \mathrm{e}^{hL} y_{n-1} + h \sum_{k=0}^{q} \beta_k N_{n-k},$$

where $\beta_0, \beta_1, \ldots, \beta_q$, are the coefficients of the method, computed by expanding the nonlinear terms in a Taylor series, about t_{n-1}

$$h \sum_{k=0}^{q} \beta_k N_{n-k} = \sum_{\ell=1}^{\infty} \frac{h^\ell}{(\ell-1)!} \left(\sum_{k=0}^{q} \beta_k (1-k)^{\ell-1} \right) N_{n-1}^{(\ell-1)}. \tag{5.3}$$

The order conditions for the ETD Adams methods can then be computed by substituting (5.3) into the expression for the numerical solution and comparing with (5.2) evaluated at $t = t_{n-1} + h$,

$$\frac{1}{(\ell-1)!} \sum_{k=0}^{m} \beta_k (1-k)^{\ell-1} = \varphi_\ell(hL),$$

where $\ell = 1, 2, \ldots, m$, with $m = q - 1$ for implicit methods, and $m = q$ for explicit methods. This system of equations is linear and can be represented simply as $A\beta = \varphi$, where the components of the vector φ are φ_ℓ. For the ETD Adams–Bashforth methods $A_{\ell k} = (1-k)^{\ell-1}/(\ell-1)!$, whereas, for the ETD Adams–Moulton methods $A_{\ell k} = (2-k)^{\ell-1}/(\ell-1)!$.

q	β_1	β_2	β_3	β_4
1	φ_1	0	0	0
2	$\varphi_1 + \varphi_2$	$-\varphi_2$	0	0
3	$\varphi_1 + \frac{3}{2}\varphi_2 + \varphi_3$	$-2(\varphi_2 + \varphi_3)$	$\frac{1}{2}\varphi_2 + \varphi_3$	0
4	$\varphi_1 + \frac{11}{6}\varphi_2 + 2\varphi_3 + \varphi_4$	$-3\varphi_2 - 5\varphi_3 - 3\varphi_4$	$\frac{3}{2}\varphi_2 + 4\varphi_3 + 3\varphi_4$	$-\frac{1}{3}\varphi_2 - \varphi_3 - \varphi_4$

Table 1: ETD Adams–Bashforth methods with $q = 1, \ldots, 4$.

q	β_0	β_1	β_2	β_3
0	φ_1	0	0	0
1	φ_2	$\varphi_1 - \varphi_2$	0	0
2	$\frac{1}{2}\varphi_2 + \varphi_3$	$\varphi_1 - 2\varphi_3$	$-\frac{1}{2}\varphi_2 + \varphi_3$	0
3	$\frac{1}{3}\varphi_2 + \varphi_3 + \varphi_4$	$\varphi_1 + \frac{1}{2}\varphi_2 - 2\varphi_3 - 3\varphi_4$	$-\varphi_2 + \varphi_3 + 3\varphi_4$	$\frac{1}{6}\varphi_2 - \varphi_4$

Table 2: ETD Adams–Moulton methods with $q = 0, \ldots, 3$.

We briefly show a connection between the ETD Adams–Bashforth methods and the IMEX schemes of Ascher, Ruuth and Wetton [1]. The order two ETD Adams–Bashforth method is

$$y_n = \mathrm{e}^{hL} y_{n-1} + \varphi_1(hL) N_{n-1} + \varphi_2(hL) h (N_{n-1} - N_{n-2}).$$

Now approximate the exponential using the (1,1) Padé approximation

$$\mathrm{e}^{hL} \approx \left(I - \frac{1}{2}hL\right)^{-1}\left(I - \frac{1}{2}hL\right),$$

and the φ_1 and φ_2, with the (0,1) Padé approximations

$$\varphi_1(hL) \approx \left(I - \frac{1}{2}hL\right)^{-1}, \quad \varphi_2(hL) \approx \frac{1}{2}\left(I - \frac{1}{2}hL\right)^{-1}.$$

Substituting these into the order two ETD Adams–Bashforth method gives the order two IMEX scheme

$$y_n = \left(I - \frac{1}{2}hL\right)^{-1}\left[\left(I - \frac{1}{2}hL\right)y_{n-1} + \left(\frac{3}{2}hN_{n-1} - \frac{1}{2}hN_{n-2}\right)\right].$$

This IMEX method (see [12, 54]) uses the order two Adams–Bashforth method on the nonlinear term and the Crank–Nicolson method on the linear term. The IMEX methods which use an Adams–Moulton method on the linear term can be considered as approximations to the ETD Adams–Bashforth methods. Generally, multistep IMEX methods use a BDF method on the linear term, such methods can not be considered as approximations to ETD multistep methods. This can be seen by trying to find the coefficients α_1, α_2 and β_0 in

$$y_n = \alpha_1 y_{n-1} + \alpha_2 y_{n-2} + \beta_0 N_n,$$

such that when expanded in Taylor series the above expression matches the first few terms of the exact solution given in Lemma 5.1.

An extension to the ETD linear multistep methods was suggested by Jain [50] in 1972. The idea was not to use the Newton interpolation polynomial as was used by Nørsett [77] and Cox and Matthews [16], but a Hermite interpolation polynomial. In this case the first derivate of the differential equation is needed, with this extra information A-stable q-step methods of order $2q$ were derived.

5.2 ETD Runge–Kutta methods

The computations performed in a single step of an ETD Runge–Kutta method are

$$\begin{aligned} Y_i &= \sum_{j=1}^{s} a_{ij}(hL)hN(Y_j) + \mathrm{e}^{c_i hL}y_{n-1}, \quad i = 1, 2, \ldots, s, \\ y_n &= \sum_{i=1}^{s} b_i(hL)hN(Y_i) + \mathrm{e}^{hL}y_{n-1}. \end{aligned} \tag{5.4}$$

In van der Houwen [101] and Verwer, [104] generalized Runge–Kutta methods, which use an approximation to the Jacobian were briefly discussed. These methods could be considered as the first approximations to ETD Runge–Kutta methods, as the exponential and related functions are approximated rather than

exactly computed. The semi-implicit (also known as linearly implicit) methods [33, 94] can also be considered as early approximations to ETD Runge–Kutta methods.

Another early example of an approximate ETD Runge–Kutta method appeared in the paper by Ehle and Lawson [22] in 1975. The aim of this paper was to overcome the difficulties experienced with the Lawson methods, in which for very stiff problems, they performed poorly. The main difficulty with the Lawson methods, is that they have a maximum stiff order of one. Throughout this section, we will talk about the stiff and non-stiff orders of the ETD Runge–Kutta methods, this will be discussed in more detail in Section 8. Even when the Runge–Kutta–Lawson methods achieve the non-stiff order, their error constants are significantly larger than other exponential integrators. The modification of the Lawson methods proposed in [22] are constructed in a somewhat ad-hoc way, and the conditions that they require the coefficients b_i and a_{ij} to satisfy are insufficient to obtain non-stiff order greater than three and stiff order greater than two. If we replace the rational approximations used in [22] by their exact representations, the resulting method is

$$\left[\begin{array}{cccc|c} 0 & 0 & 0 & 0 & I \\ \frac{1}{2}\varphi_{1,2} & 0 & 0 & 0 & \mathrm{e}^{\frac{1}{2}hL} \\ 0 & \frac{1}{2}\varphi_{1,3} & 0 & 0 & \mathrm{e}^{\frac{1}{2}hL} \\ 0 & 0 & \varphi_{1,4} & 0 & \mathrm{e}^{hL} \\ \hline \varphi_1 - 3\varphi_2 + \varphi_3 & 2\varphi_2 - \varphi_3 & 2\varphi_2 - \varphi_3 & -\varphi_2 + \varphi_3 & \mathrm{e}^{hL} \end{array}\right],$$

where, for stylistic reasons we define $\varphi_{i,j} = \varphi_i(c_j hL)$. As we will see in Section 7 it is not possible to multiply each of the internal stages by φ_1 and retain the correct order. In 1978, an article in German was published by Friedli [24], where the coefficients a_{ij} and b_i, are

$$a_{ij}(hL) = \sum_{k=1}^{i-1} \alpha_{ijk}\varphi_k(c_i hL), \quad b_i(hL) = \sum_{k=1}^{s} \beta_{ik}\varphi_k(hL), \tag{5.5}$$

It is worth noting here that the φ_k functions need not be evaluated at $c_i hL$, see Section 8, for more details. The non-stiff order conditions, for methods up to order five were derived and examples of methods up to non-stiff order four were included. Below we give a method of Friedli, which is based on the order four Runge–Kutta method of England, with stiff order three, not four as Friedli had thought

$$\left[\begin{array}{cccc|c} 0 & 0 & 0 & 0 & I \\ \frac{1}{2}\varphi_{1,2} & 0 & 0 & 0 & \mathrm{e}^{\frac{1}{2}hL} \\ \frac{1}{2}\varphi_{1,3} - \frac{1}{2}\varphi_{2,3} & \frac{1}{2}\varphi_{2,3} & 0 & 0 & \mathrm{e}^{\frac{1}{2}hL} \\ \varphi_{1,4} - 2\varphi_{2,4} & -\frac{26}{25}\varphi_{1,4} + \frac{2}{25}\varphi_{2,4} & \frac{26}{25}\varphi_{1,4} + \frac{24}{25}\varphi_{2,4} & 0 & \mathrm{e}^{hL} \\ \hline \varphi_1 - 3\varphi_2 + 4\varphi_3 & 0 & 4\varphi_2 - 8\varphi_3 & -\varphi_2 + 4\varphi_3 & \mathrm{e}^{hL} \end{array}\right].$$

The next class of methods, we consider, are the W-methods developed by Wolfbrandt in his PhD thesis [107] to avoid the use of the exact Jacobian in the

Rosenbrock methods. The general non-stiff order conditions for these methods were constructed by Steihaug and Wolfbrandt [91] in 1979. To keep consistency with the rest of this paper we assume that the approximation to the Jacobian is given by the matrix L. In this case, the W-methods can be expressed as

$$k_i = L\left(y_{n-1} + \sum_{j=1}^{i-1} a_{ij} h k_j\right) + N\left(y_{n-1} + \sum_{j=1}^{i-1} a_{ij} h k_j\right) + L\sum_{j=1}^{i} \gamma_{ij} h k_j,$$
$$y_n = y_{n-1} + \sum_{j=1}^{s} b_j h k_j.$$

This formulation does not provide much insight into the potential connections with the ETD methods, but by making the substitution

$$Y_i = y_{n-1} + \sum_{j=1}^{i-1} a_{ij} h k_j,$$

the matrices $A(hL)$ and $B(hL)$, can be expressed as

$$A(hL) = (a \otimes I_m)(I_s \otimes I_m - h(\gamma + a) \otimes L)^{-1},$$
$$B(hL) = (b \otimes I_m)(I_s \otimes I_m - h(\gamma + a) \otimes L)^{-1},$$

where the components of a, b and γ are a_{ij}, b_i and γ_{ij}, and

$$U(hL) = I_m \otimes e_s + hA(hL)(L \otimes e_s), \quad V(hL) = I_m + hB(hL)(L \otimes e_s).$$

This representation of the W-methods was realized by Strehmel and Weiner [94]. What this shows, is that the W-methods are not ETD Runge–Kutta methods, as the exponential (and related functions) are not computed exactly. However, they can be considered as approximations to ETD Runge–Kutta methods. In 1982, Strehmel and Weiner [92] constructed the adaptive Runge–Kutta methods, which are linearly implicit Runge–Kutta methods where the coefficient matrices a_{ij} and b_j are defined as in (5.5), but rational approximations are used for the exponential and related functions. Strehmel and Weiner constructed in general the non-stiff order conditions for the adaptive Runge–Kutta methods in [92] and discussed B-convergence results when rational approximations are used in [94]. We give one fourth order method of Strehmel and Weiner, which is based on the order four Runge–Kutta method of England, we assume that the functions are computed exactly

$$\left[\begin{array}{cccc|c} 0 & 0 & 0 & 0 & I \\ \frac{1}{2}\varphi_{1,2} & 0 & 0 & 0 & \mathrm{e}^{\frac{1}{2}hL} \\ \frac{1}{2}\varphi_{1,3} - \frac{1}{2}\varphi_{2,3} & \frac{1}{2}\varphi_{2,3} & 0 & 0 & \mathrm{e}^{\frac{1}{2}hL} \\ \varphi_{1,4} - 2\varphi_{2,4} & -2\varphi_{2,4} & 4\varphi_{2,4} & 0 & \mathrm{e}^{hL} \\ \hline \varphi_1 - 3\varphi_2 + 4\varphi_3 & 0 & 4\varphi_2 - 8\varphi_3 & -\varphi_2 + 4\varphi_3 & \mathrm{e}^{hL} \end{array}\right].$$

A significant body of work by researchers in Halle, have extend the adaptive Runge–Kutta methods and W-methods to partitioned systems, implemented

these methods in both sequential and parallel environments, constructed two step variations and considered B-convergence. A small selection of references from this work includes [7, 93, 95, 106]. Do connections exist between the B-convergence order and the stiff order of exponential integrators? This question is discussed in Section 8.

As was mentioned previously, there has been renewed interest in developing exponential integrators recently. One of the main reasons for this renewed interest is that the exponential and related functions can now be evaluated to high precision, much more efficiently, than in the past. This overcomes the order reduction apparent when Padé approximations are used. In the paper by Cox and Matthews [16] apart from the ETD Adams–Bashforth methods they included three ETD Runge–Kutta methods with two, three and four, stages. The methods with two and three stages can be written as above, where the coefficients of the method are linear combinations of the φ-functions, but this is not the case for the four stage method. It has some important differences from the three example methods given above. Representing the Cox and Matthews method, which is based on the classical order four Runge–Kutta method, in tableau form reads

$$\left[\begin{array}{cccc|c} 0 & 0 & 0 & 0 & I \\ \frac{1}{2}\varphi_{1,2} & 0 & 0 & 0 & \mathrm{e}^{\frac{1}{2}hL} \\ 0 & \frac{1}{2}\varphi_{1,2} & 0 & 0 & \mathrm{e}^{\frac{1}{2}hL} \\ \frac{1}{2}(\mathrm{e}^{\frac{1}{2}hL}-I)\varphi_{1,2} & 0 & \varphi_{1,2} & 0 & \mathrm{e}^{hL} \\ \hline \varphi_1-3\varphi_2+4\varphi_3 & 2\varphi_2-4\varphi_3 & 2\varphi_2-4\varphi_3 & -\varphi_2+4\varphi_3 & \mathrm{e}^{hL} \end{array}\right].$$

There are two interesting points with this method of Cox and Matthews. The first, pointed out by Krogstad [58] is that the internal stages have the same structure as the commutator-free Lie group method, based on the classical order four Runge–Kutta method, constructed by Celledoni, Martinsen and Owren [14] with affine Lie group action (see Section 7). The second is that the coefficients defining the method are not linear combinations of the φ-functions. As long as the coefficients of the method satisfy the stiff order conditions given in Section 8 and the coefficients remain bounded, there is no reason why the coefficients need to be linear combinations of the φ-functions. The four stage method of Cox and Matthews motivated Krogstad [58] to develop a method which did not require a product of functions, which is very similar to the methods of Friedli, and Strehmel and Weiner.

Finally, in this section, we will briefly discuss some of the isolated examples of ETD methods appearing in various areas of science. In the integration of chemical reactions many integrators have been proposed. For example, the Pseudo-Steady-State Approximation (PSSA) scheme, which reduces to the ETD Runge–Kutta method

$$\left[\begin{array}{cc|c} 0 & 0 & I \\ \varphi_1 & 0 & \mathrm{e}^{hL} \\ \hline \frac{1}{2}\varphi_1 & \frac{1}{2}\varphi_1 & \mathrm{e}^{hL} \end{array}\right],$$

for semi-linear problems and has stiff order one. In a recent article, Mott, Oran and van Leer [75] proposed the α-Quasi-Steady-State (α-QSS) integrator. This

integrator works also when the linear part is a function of t. However, when the linear part is constant, the α-QSS integrator reduces to the ETD Runge–Kutta method, with stiff order two

$$\left[\begin{array}{cc|c} 0 & 0 & I \\ \varphi_1 & 0 & \mathrm{e}^{hL} \\ \hline \varphi_1 - \varphi_2 & \varphi_2 & \mathrm{e}^{hL} \end{array}\right].$$

Several numerical experiments were performed in [105], comparing these low order ETD methods with standard stiff solvers RADU5 and DASSAL. Friesner et. al. [25] and Edwards et. al. [21] constructed a class of integrators called exponential propagation. These methods are derived from the variation of constants formula using an iteration scheme until convergence is reached

$$y^{(m)}(t_{n-1}+h) = \mathrm{e}^{hL} y_{n-1} + \int_0^h \mathrm{e}^{(h-\tau)L} N(y^{(m-1)}(t_{n-1}+\tau))\,\mathrm{d}\tau,$$

where $y^{(0)}(t_{n-1}+\tau) = y(t_{n-1})$. If past values of the solution were used then the resulting method would be an exponential Adams method. However, they calculate $N(y^{(m-1)}(t_{n-1}+\tau))$ at several values of τ within the interval $[0,h]$, in order to fit an algebraic polynomial of the form

$$N(y^{(m-1)}(t_{n-1}+\tau)) \approx \sum_{j=0}^{m} n_j \tau^j.$$

The exponential propagation methods can be written as ETD Runge–Kutta methods, where the number of stages depends on the number of iterations and the number of points used to construct an algebraic polynomial. In the computations performed in [21, 25] the exponential propagation integrators use Krylov subspace methods to evaluate the exponential and related functions.

In [43], Hockbruck and Ostermann, constructed a class of implicit exponential Runge–Kutta methods based on collocation. The methods are constructed by choosing the collocation nodes $c_1, \ldots, c_s$ and a collocation polynomial to approximate the nonlinear term in the variation of constants formulae. An example method of order four, which reduces to the Lobatto IIIC when $L = 0$, is

$$\left[\begin{array}{ccc|c} 0 & 0 & 0 & I \\ \frac{1}{2}\varphi_1 - \frac{3}{4}\varphi_2 + \frac{1}{2}\varphi_3 & \varphi_2 - \varphi_3 & -\frac{1}{4}\varphi_2 + \frac{1}{2}\varphi_3 & \mathrm{e}^{\frac{1}{2}hL} \\ \varphi_1 - 3\varphi_2 + 4\varphi_3 & 4\varphi_2 - 8\varphi_3 & -\varphi_2 + 4\varphi_3 & \mathrm{e}^{hL} \\ \hline \varphi_1 - 3\varphi_2 + 4\varphi_3 & 4\varphi_2 - 8\varphi_3 & -\varphi_2 + 4\varphi_3 & \mathrm{e}^{hL} \end{array}\right].$$

The advantage of these methods is that the high stage order ensures there is no order reduction even in the stiff case. The problem is that the method is implicit, however fixed point iteration can be used to evaluate the stages. As long as only a few iterations are needed for convergence, these methods may be competitive. An early method constructed in 1978, by Palusinski and Wait [81] is the first and only known example of a partitioned ETD method.

6 Generalized Lawson methods

In Section 4 we discussed the Lawson methods and showed how the Lawson transformation was used to rewrite the differential equation in a more appropriate form, in which L only appeared inside an exponential. Recently Krogstad [58] proposed a way of generalizing the Lawson methods. Krogstad called these methods Generalized Integrating Factor (GIF) methods, as he was unaware of the original paper by Lawson. We suggest that they should be known as the Generalized Lawson (GL) methods. In order to solve the original problem, Krogstad proposed to represent the solution of (1.1) as the exact solution of a differential equation which approximates the original problem with a modified initial condition. We then obtain a differential equation for the initial condition. Let $P(t)$ be an algebraic polynomial of degree $q-1$ through the points $\{(t_{n-\ell}, N_{n-\ell})\}_{\ell=1,\ldots,q}$,

$$P(t) = \sum_{\ell=1}^{q} \frac{(t-t_{n-1})^{\ell-1}}{(\ell-1)!} p_{\ell-1}, \tag{6.1}$$

where we are assuming that a fixed stepsize h is used throughout the integration, that is $h = t_\ell - t_{\ell-1}$, and

$$p_{\ell-1} = \frac{1}{h^{\ell-1}} \sum_{k=1}^{q} \gamma_{k\ell} N_{n-k},$$

with the elements $\gamma_{k\ell} = (A^{-1})_{\ell k}$, where A is defined as for the ETD Adams–Bashforth methods. We use the polynomial $P(t)$ to approximate the nonlinear term; the GL methods solve exactly the modified initial value problem

$$y'(t) = Ly(t) + P(t), \quad y(t_{n-1}) = v(t).$$

The exact solution (which can be seen immediately from Lemma 5.1) is

$$y(t) = \mathrm{e}^{(t-t_{n-1})L} v(t) + \sum_{\ell=1}^{q} (t-t_{n-1})^{\ell} \varphi_\ell((t-t_{n-1})L) p_{\ell-1}. \tag{6.2}$$

We will denote this as the Krogstad transformation. Differentiating the above solution with respect to t, and simplifying yields

$$y'(t) = \mathrm{e}^{(t-t_{n-1})L} v'(t) + Ly(t) + P(t),$$

which is equivalent to the differential equation

$$v'(t) = \mathrm{e}^{(t_{n-1}-t)L} \left(N(y(t)) - P(t) \right), \quad v(t_{n-1}) = y_{n-1}. \tag{6.3}$$

Now we can numerically solve this transformed equation to approximate the initial condition $v(t)$. At first sight this seems a rather strange approach for solving the original problem, but preprocessing dates back to the late sixties when Butcher [9] used a similar idea to overcome the barrier which states no five stage Runge–Kutta methods exist with fifth order.

As a first example, we approximate the nonlinear term with a zeroth order polynomial $P(t) = N_{n-1}$. Applying the classical fourth order Runge–Kutta method to estimate the modified initial condition and then back transforming using the Krogstad transformation, results in the GL1/cRK4 method

$$\left[\begin{array}{ccccc} 0 & 0 & 0 & 0 & I \\ \frac{1}{2}\varphi_{1,2} & 0 & 0 & 0 & \mathrm{e}^{\frac{1}{2}hL} \\ \frac{1}{2}\varphi_{1,3} - \frac{1}{2}I & \frac{1}{2}I & 0 & 0 & \mathrm{e}^{\frac{1}{2}hL} \\ \varphi_{1,4} - \mathrm{e}^{\frac{1}{2}hL} & 0 & \mathrm{e}^{\frac{1}{2}hL} & 0 & \mathrm{e}^{hL} \\ \hline \varphi_1 - \frac{2}{3}\mathrm{e}^{\frac{1}{2}hL} - \frac{1}{6}I & \frac{1}{3}\mathrm{e}^{\frac{1}{2}hL} & \frac{1}{3}\mathrm{e}^{\frac{1}{2}hL} & \frac{1}{6}I & \mathrm{e}^{hL} \end{array}\right].$$

There are three interesting properties to observe about the method GL1/cRK4. The first, is that when $L = 0$, this method reduces to the classical fourth order Runge–Kutta method. Secondly, the only difference with the traditional Lawson method is the first (block) column of the matrix $A(hL)$ and the first (block) element of the matrix $b(hL)$. Thirdly, fixed points are preserved, this is true for all GL methods.

The performance improvement of the method above can be significantly improved by allowing $P(t)$ to be a higher order approximation of $N(y(t))$. This requires the use of approximations from the past, thus providing a multistep flavour to the method. As a second example, we include the GL2/cRK4, which uses the classical order four Runge–Kutta method to approximate the modified initial value and back transforms using the Krogstad transformation. The resulting method, where $y^{[n-1]} = [y_{n-1}, hN_{n-2}]^T$, is

$$\left[\begin{array}{ccccc|cc} 0 & 0 & 0 & 0 & I & 0 \\ \frac{1}{2}\varphi_{1,2} + \frac{1}{4}\varphi_{2,2} & 0 & 0 & 0 & \mathrm{e}^{\frac{1}{2}hL} & -\frac{1}{4}\varphi_{2,2} \\ \frac{1}{2}\varphi_{1,3} + \frac{1}{4}\varphi_{2,3} - \frac{3}{4}I & \frac{1}{2}I & 0 & 0 & \mathrm{e}^{\frac{1}{2}hL} & -\frac{1}{4}\varphi_{2,3} + \frac{1}{4}I \\ \varphi_{1,4} + \varphi_{2,4} - \frac{3}{2}\mathrm{e}^{\frac{1}{2}hL} & 0 & \mathrm{e}^{\frac{1}{2}hL} & 0 & \mathrm{e}^{hL} & -\varphi_{2,4} + \frac{1}{2}\mathrm{e}^{\frac{1}{2}hL} \\ \hline \varphi_1 + \varphi_2 - \mathrm{e}^{\frac{1}{2}hL} - \frac{1}{3}I & \frac{1}{3}\mathrm{e}^{\frac{1}{2}hL} & \frac{1}{3}\mathrm{e}^{\frac{1}{2}hL} & \frac{1}{6}I & \mathrm{e}^{hL} & -\varphi_2 + \frac{1}{3}\mathrm{e}^{\frac{1}{2}hL} + \frac{1}{6}I \\ I & 0 & 0 & 0 & 0 & 0 \end{array}\right].$$

There are several interesting properties of this method. First of all, it is an exponential general linear method which passes two quantities from step to step. Secondly, only the first (block) column of the matrix A and the first (block) element of the first row of the matrix B, differ from the Lawson method. This property holds for all GL methods, which use a Runge–Kutta method to approximate the modified initial condition. This method is the unique method, with stage order two, which passes the quantities y_n and N_{n-1} from step to step. Finally, we mention that when $L = 0$, the underlying general linear method was constructed by Butcher [8] in the first paper on general linear methods. The main difficulty with these methods as Krogstad pointed out in [58] is the improved accuracy comes to some extent at the price of stability. GL methods, which use trigonometric instead of algebraic polynomials to approximate the nonlinear term in the original problem, were constructed in [72]. In [79], a general formulation of the GLq/RKp, is given and a modification of the GL methods is proposed, which significantly improves accuracy and overcomes the problems of stability.

We now turn our attention to the situation when the initial condition is approximated using an Adams–Bashforth method of order p. If $P(t)$, is of order k, then the modified initial condition is approximated by

$$v_n = v_{n-1} + \sum_{i=1}^{p} \alpha_i \mathrm{e}^{(i-1)hL} h \left[N_{n-i} - \sum_{k=1}^{q} N_{n-k} \sum_{\substack{\ell=1 \\ \ell \neq k}}^{q} \frac{\ell - i}{\ell - k} \right].$$

Using the Krogstad transformation, the resulting approximation in the original variable is

$$y_n = y_{n-1} + \sum_{k=1}^{q} \left[\sum_{\ell=1}^{q} \gamma_{\ell k} \varphi_\ell(hL) + \sum_{i=q+1}^{p} \alpha_i \mathrm{e}^{ihL} \prod_{\substack{\ell=1 \\ \ell \neq k}}^{q} \frac{\ell - i}{\ell - k} \right] h N_{n-k} + \sum_{k=q+1}^{p} \alpha_k \mathrm{e}^{khL} h N_{n-k}.$$

If $q = 0$, then we recover the Lawson–Adams–Bashforth methods; if $p \leq q$, then the GLq/ABp, reduces to the ETD Adams–Bashforth method; if $p > q$, then the GLq/ABp, extends the class of ETD methods. Therefore, all exponential Adams–Bashforth methods can be constructed using this approach. In [79], it is shown that in general a GLq method is convergent and has at least stiff order $q + 1$.

7 Lie group methods

Lie group methods were originally designed to ensure that the exact and numerical solutions, evolve on the same manifold. To achieve this, Lie group methods advance from one point on the manifold to another by following the flow of some simple vector fields, called *frozen vector fields*. The flow of a frozen vector field defines a map which is often called the *exponential* map. We use the notation Exp when we refer to it. An alternative (and often used in the literature) definition of the basic motions on the manifold can also be given in terms of Lie groups, Lie algebras and their *actions* upon the manifold. To avoid unnecessary complications and heavy notation, we introduce just some of the basic concepts of Lie group methods, particularly adopted to the special type of semi-linear problems which we have in mind. For readers which are unfamiliar with the theory of Lie groups and Lie algebras, for the numerical solution of differential equations, we suggest [46, 72].

In recent years, there has been a significant amount of work in the field of Lie group methods. Maybe the first paper to construct such methods was by Crouch and Grossman [17] in 1993. The Crouch–Grossman (CG) methods were later extended to the Commutator-Free (CF) methods, see [14]. The construction of Lie group integrators for the solution of semi-discretized partial differential equations started with the paper by Munthe-Kaas [76] and further

investigated for the heat equation in [14, 64, 96], parabolic problems in [57, 58, 72], convection-diffusion problems in [13] and for the nonlinear Schrödinger equation in [3].

The manifold in which the solution of the initial value problem (1.1) evolves is $\mathcal{M} \equiv \mathbf{R}^m$. Therefore, it is not difficult to construct a numerical integrator which stays on $\mathcal{M}$. However, the framework of Lie group methods provides, through the freedom in the choice of the basic motions, a powerful tool for constructing new exponential integrators. The question is, how to define the basic motions on the manifold $\mathcal{M}$ so that they capture the key features of the original vector field? For example, choosing the basic motions on $\mathcal{M}$ to be given by translations, leads to the standard numerical schemes. For the semi-linear problem (1.1) a natural choice, is to define the basic motions on $\mathcal{M}$, to be the flow of the following differential equation

$$y' = \alpha L y + N, \quad y(t_{n-1}) = y_{n-1},$$

where $\alpha \in \mathbf{R}$ and $N \in \mathbf{R}^m$. The frozen vector field $\mathcal{F}_{(\alpha L, N)}(y) = \alpha L y + N$ can be seen as a local approximation to the original vector field, for appropriate α and N. The exact solution of the above equation is given by

$$y(t) = e^{(t-t_{n-1})\alpha L} y_{n-1} + \varphi_1\big((t-t_{n-1})\alpha L\big)(t-t_{n-1})N.$$

The set $\mathfrak{g} = \{(\alpha L, N) \,|\, \alpha \in \mathbf{R}, N \in \mathbf{R}^m\}$ defines an algebra with zero element (O, o), where the first element is interpreted as a matrix. It is also closed under the bilinear bracket $[\cdot,\cdot] : \mathfrak{g} \times \mathfrak{g} \to \mathfrak{g}$, given by

$$\big[(\alpha_1 L, N_1), (\alpha_2 L, N_2)\big] = (\mathsf{O}, \alpha_1 L N_2 - \alpha_2 L N_1), \tag{7.1}$$

and thus $\mathfrak{g}$ is a Lie algebra. If $\mathcal{G}$ denotes the Lie group corresponding to $\mathfrak{g}$, we can define the exponential map Exp: $\mathfrak{g} \to \mathcal{G}$, as

$$\mathrm{Exp}(\alpha L, N) = (\mathrm{e}^{\alpha L}, \varphi_1(\alpha L)N).$$

Therefore, the basic motions on $\mathcal{M}$ can be written in the following compact form

$$\begin{aligned} y(t) &= \mathrm{e}^{(t-t_{n-1})\alpha L} y_{n-1} + \varphi_1\big((t-t_{n-1})\alpha L\big)(t-t_{n-1})N \\ &= \mathrm{Exp}\big((t-t_{n-1})(\alpha L, N)\big) \cdot y_{n-1}, \end{aligned}$$

where the map $\cdot : \mathcal{G} \times \mathcal{M} \to \mathcal{M}$ is the *affine* group action

$$(G, g) \cdot y = Gy + g. \tag{7.2}$$

The use of the affine action for solving semi-discretized semi-linear problems was first suggested by Munthe-Kaas [76] and later studied in [3, 14, 57, 58, 96]. In [72], it is proposed how this idea can be generalized so that better approximations to the original vector field can be used.

We will not discuss the CG methods with affine action, as these are considered an inefficient subclass of the CF methods. So, we now turn our attention

to the Runge–Kutta–Munthe-Kaas (RKMK) Lie group methods. The RKMK methods were introduced to avoid the high number of Exp evaluations needed in the CG methods. The main idea is to transform the original differential equation evolving on a manifold $\mathcal{M}$ to a corresponding differential equation evolving on a Lie algebra $\mathfrak{g}$. Since $\mathfrak{g}$ is a linear space, a standard Runge–Kutta method can be used on the transformed equation. The result is then transformed back to the manifold. For the semi-linear problems (1.1) this idea applies as follows, search for a curve $v(t) = (tL, z(t))$ in $\mathfrak{g}$, such that $v(0) = (\mathsf{O}, \mathsf{o})$ and the solution of (1.1) can be expressed as

$$y(t_{n-1} + t) = \mathrm{Exp}(v(t)) \cdot y_{n-1} = \mathrm{e}^{tL} y_{n-1} + \varphi_1(tL) z(t). \tag{7.3}$$

Differentiating both sides of (7.3) leads to the following differential equation in the Lie algebra $\mathfrak{g}$

$$v'(t) = \mathrm{dExp}^{-1}_{v(t)}\big(L, N(\mathrm{Exp}(v(t)) \cdot y_{n-1})\big), \quad v(0) = (\mathsf{O}, \mathsf{o}), \tag{7.4}$$

where the map $\mathrm{dExp}^{-1}_{v(t)} : \mathfrak{g} \to \mathfrak{g}$ is defined as

$$\mathrm{dExp}^{-1}_{(\alpha_1 L,\, N_1)}(\alpha_2 L, N_2) = \sum_{k=0}^{\infty} \frac{B_k}{k!} \mathrm{ad}^k_{(\alpha_1 L, N_1)}(\alpha_2 L, N_2).$$

The coefficients B_k are the Bernoulli numbers $\{1, -\frac{1}{2}, \frac{1}{6}, 0, -\frac{1}{30}, 0, \frac{1}{42}, \ldots\}$. Powers of the adjoint operator ad are recursively defined by the following relation $\mathrm{ad}^k_{(\alpha_1 L, N_1)}(\alpha_2 L, N_2) = \mathrm{ad}_{(\alpha_1 L, N_1)} \mathrm{ad}^{k-1}_{(\alpha_1 L, N_1)}(\alpha_2 L, N_2)$ with $\mathrm{ad}_{(\alpha_1 L, N_1)}(\alpha_2 L, N_2)$ given by (7.1). Therefore,

$$\mathrm{ad}^k_{(\alpha_1 L, N_1)}(\alpha_2 L, N_2) = (\mathsf{O}, \alpha_1^{k-1} L^k (\alpha_1 N_2 - \alpha_2 N_1)).$$

Substituting this expression into the dExp^{-1} operator and simplifying gives

$$\mathrm{dExp}^{-1}_{(\alpha_1 L, N_1)}(\alpha_2 L, N_2) = \left(\alpha_2 L, \varphi_1^{-1}(\alpha_1 L)\left(N_2 - \tfrac{\alpha_2}{\alpha_1} N_1\right) + \tfrac{\alpha_2}{\alpha_1} N_1\right).$$

Using the above expression for the dExp^{-1} operator, and keeping in mind that $v(t) = (tL, z(t))$, the transformed differential equation (7.4) can be rewritten as

$$z'(t) = \varphi_1^{-1}(tL)\left(N(\mathrm{Exp}(tL, z(t)) \cdot y_{n-1}) - \tfrac{z(t)}{t}\right) + \tfrac{z(t)}{t}, \quad z(0) = \mathsf{o}. \tag{7.5}$$

The same result can be alternatively obtained by differentiating (7.3), with respect to t and using the obvious equality $\varphi_1^{-1}(tL) e^{tL} - tL = \varphi_1^{-1}(tL)$.

The computations performed by a RKMK Lie group method, applied to the semi-linear problem (1.1), are given in the following algorithm.

Algorithm 7.1. (Runge–Kutta–Munthe-Kaas Lie group methods)
for $i = 1, 2, \ldots, s$ **do**

$$Z_i = h \sum_{j=1}^{s} a_{ij} \left(\varphi_1^{-1}(c_j h L)\left(N(Y_j) - \tfrac{1}{c_j h} Z_j\right) + \tfrac{1}{c_j h} Z_j\right)$$

$$Y_i = \mathrm{e}^{c_i hL} y_{n-1} + \varphi_1(c_i hL) Z_i$$

end

$$z_n = h \sum_{j=1}^{s} b_j \left(\varphi_1^{-1}(c_j hL) \left(N(Y_j) - \tfrac{1}{c_j h} Z_j \right) + \tfrac{1}{c_j h} Z_j \right)$$

$$y_n = \mathrm{e}^{hL} y_{n-1} + \varphi_1(hL) z_n$$

Here the coefficients a_{ij} and b_j are the classical Runge–Kutta coefficients, therefore RKMK methods do not require a new order theory. As an example, we apply the classical fourth order Runge–Kutta method to the transformed differential equation (7.5). The resulting method denoted as RKMK4e represented in the original variables is

$$\left[\begin{array}{ccccc} 0 & 0 & 0 & 0 & I \\ \frac{1}{2}\varphi_{1,2} & 0 & 0 & 0 & \mathrm{e}^{\frac{1}{2}hL} \\ \frac{1}{2}\varphi_{1,2} - \frac{1}{2}I & \frac{1}{2}I & 0 & 0 & \mathrm{e}^{\frac{1}{2}hL} \\ \varphi_{1,2}^{-2} - 2\varphi_{1,2}^{-1} + I & \varphi_1(-\varphi_{1,2}^{-2} + \varphi_{1,2}^{-1}) & \varphi_1 \varphi_{1,2}^{-1} & 0 & \mathrm{e}^{hL} \\ \hline b_1(z) & b_2(z) & b_3(z) & \frac{1}{6}I & \mathrm{e}^{hL} \end{array}\right],$$

where the coefficients b_1, b_2 and b_3 are

$$\begin{aligned} b_1(z) &= \varphi_1\left(\tfrac{1}{2}\varphi_{1,2}^{-2} - \tfrac{4}{3}\varphi_{1,2}^{-1} + I\right) - \tfrac{1}{6}\varphi_{1,2}^{-2} + \tfrac{1}{3}\varphi_{1,2}^{-1} - \tfrac{1}{6}I, \\ b_2(z) &= \varphi_1\left(-\tfrac{1}{2}\varphi_{1,2}^{-2} + \tfrac{5}{6}\varphi_{1,2}^{-1}\right) + \tfrac{1}{6}\varphi_{1,2}^{-2} - \tfrac{1}{6}\varphi_{1,2}^{-1}, \\ b_3(z) &= \tfrac{1}{2}\varphi_1\varphi_{1,2}^{-1} - \tfrac{1}{6}\varphi_{1,2}^{-1}. \end{aligned}$$

This shows again that the coefficients of the method need not only be linear combinations of φ-functions. Unfortunately, the RKMK methods do not work well for problems where L represents the stiff term, the reason being that $\|L\|$ is typically much larger than $\|\varphi_1(L)\|$, and to evaluate the dExp^{-1} operator commutators need to be evaluated, which involve products of the form $LN(u)$. As was pointed out by Krogstad [57] certain stepsize restrictions are present due to singularities of the function φ_1^{-1} at the points $2\pi k$ for $k = \pm 1, \pm 2, \ldots$. In [76], it was mentioned that it is not necessary to compute the dExp^{-1} operator exactly as was done in the previous example. It is possible to truncate the series to the order of the method or one less. The following example gives the RKMK4t with a truncation of the dExp^{-1} operator

$$\left[\begin{array}{cccc|c} 0 & 0 & 0 & 0 & I \\ \frac{1}{2}\varphi_{1,2} & 0 & 0 & 0 & \mathrm{e}^{\frac{1}{2}hL} \\ \frac{1}{8}hL\varphi_{1,2} & \frac{1}{2}(I - \frac{1}{4}hL)\varphi_{1,2} & 0 & 0 & \mathrm{e}^{\frac{1}{2}hL} \\ 0 & 0 & \varphi_1 & 0 & \mathrm{e}^{hL} \\ \hline \frac{1}{6}(I + \frac{1}{2}hL)\varphi_1 & \frac{1}{3}\varphi_1 & \frac{1}{3}\varphi_1 & \frac{1}{6}(I - \frac{1}{2}hL)\varphi_1 & \mathrm{e}^{hL} \end{array}\right]. \tag{7.6}$$

We finish our discussion on RKMK methods by pointing out that the Lawson methods, discussed in Section 4, and the GL methods, discussed in Section 6, can also be seen as RKMK methods, with appropriate approximations to the Exp map, see [72].

We now consider the CF Lie group methods originally designed in [14]. These methods were introduced to overcome the high costs of the CG methods and the need for commutators in the RKMK methods. The computations performed by the method are given in the following algorithm.

Algorithm 7.2. (Commutator-Free Lie group method)

for $i = 1, 2, \ldots, s$ **do**

$$Y_i = \operatorname{Exp}\left(h\sum_{j=1}^{s}\alpha_{ij}^{J}(L, N_j)\right)\cdots\operatorname{Exp}\left(h\sum_{j=1}^{s}\alpha_{ij}^{1}(L, N_j)\right)\cdot y_{n-1}$$

$$N_i = N(Y_i)$$

end

$$y_n = \operatorname{Exp}\left(h\sum_{j=1}^{s}\beta_{j}^{J}(L, N_j)\right)\cdots\operatorname{Exp}\left(h\sum_{j=1}^{s}\beta_{j}^{1}(L, N_j)\right)\cdot y_{n-1}$$

The coefficients α_{ij}^{k} and β_{j}^{k} are parameters of the method. They are determined from order theory which can be adapted from the order theory presented in [80]. In general the method is implicit unless $\alpha_{ij}^{k} = 0$ for $i \leq j$, in which case, it is explicit. The parameter J counts the number of Exp evaluations at each stage and it is equal to the number of sub-stages included in the stage.

As an example, we consider the CF Lie group method of order four proposed in [14]. It is based on the classical fourth order Runge–Kutta method and imposes splitting on the last stage and the output approximation. When the affine action (7.2) is used to obtain an exponential integrator, it is sufficient to multiply the coefficients of the CF Lie group method by $\varphi_1(c_i hL)$ and the incoming quantities by $\mathrm{e}^{c_i hL}$. Note that this procedure works only if the underlying method is a CF Lie group method. Otherwise this will be insufficient to guarantee the required order. This was the mistake made by Ehle and Lawson [22]. As we have already mentioned, the internal stages of the order four CF Lie group method, based on the classical Runge–Kutta method of order four, are the same as the internal stages of Cox and Matthews method, we therefore consider only the output approximation

$$\begin{aligned}
y_n &= \mathrm{e}^{\frac{1}{2}hL}\left(\varphi_{1,2}\left(\tfrac{1}{4}hN(Y_1) + \tfrac{1}{6}hN(Y_2) + \tfrac{1}{6}hN(Y_3) - \tfrac{1}{12}hN(Y_4)\right) + \mathrm{e}^{\frac{1}{2}hL}y_{n-1}\right)\\
&\quad + \varphi_{1,2}\left(-\tfrac{1}{12}hN(Y_1) + \tfrac{1}{6}hN(Y_2) + \tfrac{1}{6}hN(Y_3) + \tfrac{1}{4}hN(Y_4)\right)\\
&= \tfrac{1}{12}\varphi_{1,2}(3\mathrm{e}^{\frac{1}{2}hL} - I)hN(Y_1) + \tfrac{1}{6}\varphi_{1,2}(\mathrm{e}^{\frac{1}{2}hL} + I)hN(Y_2)\\
&\quad + \tfrac{1}{6}\varphi_{1,2}(\mathrm{e}^{\frac{1}{2}hL} + I)hN(Y_3) + \tfrac{1}{12}\varphi_{1,2}(3I - \mathrm{e}^{\frac{1}{2}hL})hN(Y_4) + \mathrm{e}^{hL}y_{n-1}.
\end{aligned}$$

When implementing a CF method one would not expand the last stage and the output approximation as the resulting formulation is more expensive to implement. However, we represent the CF method in this way to show that it can indeed be represented as an exponential Runge–Kutta method

$$\left[\begin{array}{cccc|c}
0 & 0 & 0 & 0 & I\\
\frac{1}{2}\varphi_{1,2} & 0 & 0 & 0 & \mathrm{e}^{\frac{1}{2}hL}\\
0 & \frac{1}{2}\varphi_{1,2} & 0 & 0 & \mathrm{e}^{\frac{1}{2}hL}\\
\frac{1}{2}(\mathrm{e}^{\frac{1}{2}hL} - I)\varphi_{1,2} & 0 & \varphi_{1,2} & 0 & \mathrm{e}^{hL}\\
\hline
\frac{1}{2}\varphi_1 - \frac{1}{3}\varphi_{1,2} & \frac{1}{3}\varphi_1 & \frac{1}{3}\varphi_1 & -\frac{1}{6}\varphi_1 + \frac{1}{3}\varphi_{1,2} & \mathrm{e}^{hL}
\end{array}\right]. \tag{7.7}$$

This gives another example of how the coefficients of the method can have a more general nature than just linear combinations of certain φ-functions.

8 Order conditions

The order conditions for generalized Runge–Kutta methods were first studied by van der Houwen [101]. The case when an inexact Jacobian is used was also briefly discussed, but order conditions for this situation were not derived. The Rosenbrock methods are a special case of the generalized Runge–Kutta methods, when low order Padé approximations are used. We limit our discussion, in this section, to exponential integrators which use an approximate Jacobian.

8.1 Non-Stiff order conditions

The first major contributions to constructing a non-stiff order theory, came in three independent papers [24, 91, 92]. In the first paper, Friedli considered ETD Runge–Kutta methods; although a general theory was not given, the non-stiff order conditions up to order five were derived. In the following year, Steihaug and Wolfbrandt constructed the order conditions for the W-methods, which use an approximation to the Jacobian. As we saw in Section 5, these methods can be considered as approximations to ETD Runge–Kutta methods. Strehmel and Weiner [92] constructed in 1982 the general non-stiff order conditions for the ETD Runge–Kutta methods.

In this section, we extend the non-stiff order theory to exponential general linear methods (3.3). It should be noted, that the order theory constructed here, and in all the papers referenced above, assume that powers of the matrix L, exist and thus the method coefficients can be expanded into a power series. As was first pointed out in [91] it is useful to use bi-coloured (white and black) rooted trees, with the extra requirement that the white nodes only have one child, in the analysis of the non-stiff order conditions. Let $2\mathrm{T}^*$, denote this set of rooted trees. The restriction on the white nodes comes directly from the linear term in the differential equation (1.1). We use B-series to analyze the non-stiff order conditions. For an elementary weight function $a : 2\mathrm{T}^* \to \mathbf{R}$, the B-series is defined as

$$\mathrm{B}(a,u) = a(\emptyset)u + \sum_{\tau\in 2\mathrm{T}^*} h^{|\tau|}\frac{a(\tau)}{\sigma(\tau)}F(\tau)(u).$$

For those not familiar with these concepts we suggest the monographs [10, 36] for a complete treatment. Each tree τ can be decomposed as $\tau = [\tau_1,\ldots,\tau_\ell]_{\mathrm{tp}(\tau)}$, where $\mathrm{tp}(\tau) = \{\ ,\ \}$ represents the colour of the root node and $\tau_1,\ldots,\tau_\ell$ is the forest remaining after the root node has been removed. The order $|\tau|$, symmetry $\sigma(\tau)$ and density $\gamma(\tau)$ are defined in the same way as for Runge–Kutta methods. A one to one correspondence between the rooted bi-coloured trees and the elementary differentials exists, where $F(\tau)(\ ) = Lu$ and $F(\tau)(\ ) = N(u)$, and

$$F(\tau)(u) = \begin{cases} LF(\tau_1)(u), & \text{if } \tau = [\tau_1]\ , \\ N^{(\ell)}(u)(F(\tau_1)(u),\ldots,F(\tau_\ell))(u)), & \text{if } \tau = [\tau_1,\ldots,\tau_\ell]\ . \end{cases} \tag{8.1}$$

The exact solution of (1.1) can be represented by the following B-series $u(t+h) = \mathrm{B}(\gamma^{-1}, u)$, which is exactly the same as for Runge–Kutta methods. We are now interested in finding the elementary weight function which describes the operations of the numerical method. Before we do this, it is convenient to expand a_{ij}, b_{ij}, u_{ij} and v_{ij} into power series, which gives

$$\begin{aligned} Y_i &= \sum_{j=1}^{s} \sum_{l\geq 0} a_{ij}^{[l]} (hL)^l hN(Y_j) + \sum_{j=1}^{r} \sum_{l\geq 0} u_{ij}^{[l]} (hL)^l y_j^{[n-1]}, \quad i = 1, \ldots, s, \\ y_i^{[n-1]} &= \sum_{j=1}^{s} \sum_{l\geq 0} b_{ij}^{[l]} (hL)^l hN(Y_j) + \sum_{j=1}^{r} \sum_{l\geq 0} v_{ij}^{[l]} (hL)^l y_j^{[n-1]}, \quad i = 1, \ldots, r. \end{aligned} \tag{8.2}$$

To obtain B-series expansions of the numerical solution we need the following two lemmas. These are extensions of well known results, and we therefore, do not include proofs.

Lemma 8.1. *Let $a : 2\mathrm{T}^* \to \mathbf{R}$ be a mapping satisfying $a(\emptyset) = 1$, then*

$$hN(B(a(\tau), u)) = B(a'(\tau), u),$$

where the derivative of the elementary weight function satisfies $a'(\emptyset) = 0$, and

$$a'(\tau) = \begin{cases} 0, & \text{if } \tau = [\tau_1] \ , \\ a(\tau_1) \ldots a(\tau_\ell), & \text{if } \tau = [\tau_1, \ldots, \tau_\ell] \ . \end{cases}$$

Lemma 8.2. *Let $\psi_x(z)$ be a power series in z, $\psi_x(z) = \sum_{l\geq 0} x^{[l]} z^l$, and let $a : 2\mathrm{T}^* \to \mathbf{R}$ be a mapping, then*

$$\psi_x(hL) B(a(\tau), u) = B((\psi_x(\mathcal{L})a)(\tau), u),$$

where the elementary weight function satisfies $(\psi_x(\mathcal{L})a)(\tau) = \sum_{l\geq 0} x^{[l]} (\mathcal{L}^l a)(\tau)$, with $(\mathcal{L}^l a)(\emptyset) = 0$, and

$$(\mathcal{L}^l a)(\tau) = \begin{cases} (\mathcal{L}^{l-1} a)(\tau_1), & \text{if } \tau = [\tau_1] \ , \\ 0, & \text{if } \tau = [\tau_1, \ldots, \tau_\ell] \ . \end{cases}$$

We now have everything we need to represent the numerical method denoted by (8.2) using B-series. From Lemmas 8.1 and 8.2, it follows

$$\sum_{l\geq 0} a_{ij}^{[l]} (hL)^l hN(Y_j) = \psi_{a_{ij}}(hL) B(\xi_j'(\tau), y_{n-1}) = B((\psi_{a_{ij}}(\mathcal{L})\xi_j')(\tau), y_{n-1}).$$

Let α denote the generating function of the starting method $S(hL)$, that is $y_i^{[n-1]} = \mathrm{B}(\alpha_i, y_{n-1})$, then for all $\tau \in 2\mathrm{T}^*$ and $|\tau| \leq p$, the generating functions for the order conditions satisfy

$$\begin{aligned} \xi_i(\tau) &= \sum_{j=1}^{s} (\psi_{a_{ij}}(\mathcal{L})\xi_j')(\tau) + \sum_{j=1}^{r} (\psi_{u_{ij}}(\mathcal{L})\alpha_j)(\tau), \\ E\alpha_i(\tau) &= \sum_{j=1}^{s} (\psi_{b_{ij}}(\mathcal{L})\xi_j')(\tau) + \sum_{j=1}^{r} (\psi_{v_{ij}}(\mathcal{L})\alpha_j)(\tau), \end{aligned}$$

where E is the elementary weight function of the exact solution. The matrix representation of the elementary weight functions interpreted in the natural way are

$$\xi(t) = (\psi_A(\mathcal{L})\xi')(\tau) + (\psi_U(\mathcal{L})\alpha)(\tau),$$
$$E\alpha(\tau) = (\psi_B(\mathcal{L})\xi')(\tau) + (\psi_V(\mathcal{L})\alpha)(\tau).$$

Given that we have B-series expansions for both the exact and the numerical solutions, we can now define order in a similar way as for general linear methods.

Definition 8.3. An exponential general linear method $M(hL)$, with elementary weight function $m : 2\mathrm{T}^* \to \mathbf{R}$, has non-stiff order p, if, for all $\tau \in 2\mathrm{T}^*$ such that $|\tau| \leq p$,

$$m(\tau) = E\alpha(\tau).$$

This shows that it is not possible, in general, to obtain order by simply using a general linear method for the nonlinear part N of the problem. There are coupling conditions between the nonlinear and linear parts of the problem despite the fact that the linear part has been solved exactly. Note that if $L = 0$, the order conditions simply reduce to the order conditions corresponding to the black trees. In this case the method (3.3) is equivalent to a general linear method for the nonlinear part N.

Along with the recent resurgence in constructing exponential integrators, there has been a resurgence in developing the order conditions for these methods, we cite the papers [2, 44, 55, 56]. In all of these papers except [44] the non-stiff order conditions have been rederived.

8.2 Stiff order conditions

The main problem with the non-stiff order conditions, is that they assume the exponential and related function can be expanded in a power series. However, for the problems that we are interested in solving; parabolic and hyperbolic PDEs, the operator or matrix L, is unbounded. The φ-functions are bounded, but because L is unbounded it is not possible to expand the φ-functions in power series. What is interesting is that even though methods are constructed using the non-stiff order conditions, that is the exponential and related functions are expanded in power series, they are implemented so that these functions are computed exactly. For almost all problems, which are used to test exponential integrators, the method implemented in this way will perform at its non-stiff order. Recently, Hochbruck and Ostermann constructed a problem in which, most exponential integrators performed significantly worse than their non-stiff order, see problems 3 and 4 in Section 11. To overcome this, Hochbruck and Ostermann, [43] introduced a class of implicit collocation ETD Runge–Kutta methods. The high stage order makes it possible to analyze the order without expanding the coefficients of the method in power series. The problem now is, how do we treat the implicit nature of the method, given that the exponential integrators are designed to overcome the need for implicit computations. It is sufficient for these methods to use a fixed point iteration scheme instead of a

modified Newton type iteration scheme. The resulting explicit method, given a suitable number of iterations, will be of the appropriate stiff order. The overall process would involve a significant number of stages, around sp, where s is the number of stages and p is the stiff order required.

To overcome the need for so many stages, Hochbruck and Ostermann, [43] constructed the stiff order conditions up to order four, for an ETD explicit Runge–Kutta method. We refer to that paper for details, but we give the order four conditions below, where we interpret them in a component by component sense

$$\begin{aligned}
A(hL)e &= c\varphi_1(chL),\\
b(hL)e &= \varphi_1(hL),\\
b(hL)c &= \varphi_2(hL),\\
b(hL)\frac{c^2}{2!} &= \varphi_3(hL),\\
b(hL)J\left(\varphi_2(chL) - A(hL)c\right) &= 0,\\
b(hL)\frac{c^3}{3!} &= \varphi_4(hL),\\
b(hL)J\left(c^3\varphi_3(chL) - A(hL)\frac{c^2}{2!}\right) &= 0,\\
b(hL)JA(hL)J\left(c^2\varphi_2(chL) - A(hL)c\right) &= 0,\\
b(hL)cK\left(c^2\varphi_2(chL) - A(hL)c\right) &= 0,
\end{aligned}$$

both J and K are certain problem dependent operators. The first condition is a generalization of the $C(1)$ condition satisfied by most Runge–Kutta methods. It also, along with the second condition, ensures that the method preserves fixed points. The second, third, fourth and sixth conditions are generalizations of the bushy tree conditions. The remaining conditions contain either a generalization of the $C(2)$ or $C(3)$ conditions. As it is well known that a Runge–Kutta method can not have stage order greater than one, it is not possible to satisfy the generalizations of the $C(2)$ and $C(3)$ conditions. So ETD Runge–Kutta methods with high stiff order must have some of the $b(hL)$ coefficients equal to zero. This is evident in the stiff order four method derived in [44],

$$\left[\begin{array}{ccccc|c}
0 & 0 & 0 & 0 & 0 & I\\
\frac{1}{2}\varphi_{1,2} & 0 & 0 & 0 & 0 & \mathrm{e}^{\frac{1}{2}hL}\\
\frac{1}{2}\varphi_{1,3} - \varphi_{2,3} & \varphi_{2,3} & 0 & 0 & 0 & \mathrm{e}^{\frac{1}{2}hL}\\
\varphi_{1,4} - 2\varphi_{2,4} & \varphi_{2,4} & \varphi_{2,4} & 0 & 0 & \mathrm{e}^{hL}\\
\frac{1}{2}\varphi_{1,5} - 2a_{5,2} - a_{5,4} & a_{5,2} & a_{5,2} & \frac{1}{4}\varphi_{2,5} - a_{5,2} & 0 & \mathrm{e}^{\frac{1}{2}hL}\\
\hline
\varphi_1 - 3\varphi_2 + 4\varphi_3 & 0 & 0 & -2\varphi_2 + 4\varphi_3 & 4\varphi_2 - 8\varphi_3 & \mathrm{e}^{hL}
\end{array}\right], \quad (8.3)$$

where

$$a_{5,2} = \frac{1}{4}\varphi_{2,5} - \varphi_{3,4} + \frac{1}{4}\varphi_{2,4} - \frac{1}{2}\varphi_{3,5}.$$

It is even more evident for the implicit ETD Runge–Kutta methods with fixed point iteration. In [44], the authors proved the following lemma.

Lemma 8.4. *For an exponential integrator to have stiff order p, it is sufficient to satisfy the stiff order $p-1$ conditions and order p conditions with $b(0)$.*

What the stiff order conditions and the lemma tell us, is that to achieve order p, we must have at least φ_ℓ, for $\ell = 1, \ldots, p-1$, within the method. This means that the Lawson methods discussed in Section 4, can have in general, at most stiff order one. But for some particular applications, it can be shown that they perform to their full non-stiff order. In [3], it is shown, that for the nonlinear Schrödinger equation with smooth potential, the Lawson methods exhibit the full non-stiff order. Kværnø, [59] has derived the stiff order conditions using a B-series approach for scalar equations. In this case, the elementary differentials commute so it is possible to overcome the need to expand in power series. Whether it is possible to use a B-series approach on non-scalar equations is still unclear.

In this subsection we have only discussed the stiff order conditions for exponential Runge–Kutta methods, the reason being that the q-step ETD Adams methods derived in Section 5 have stiff order q. This was recently proved by Calvo and Palencia in [11]. Also recently in [79] it is proved that the Generalized Lawson methods discussed in Section 6 have stiff order $q+1$, for a GLq method. Explicit exponential general linear methods, with high stage order, seem to be the most promising class of methods for semi-linear problems. High stiff stage order overcomes the problems of obtaining high stiff order, without requiring the method to be implicit.

9 Implementation issues

In this section, we briefly address some practical issues regarding the implementation of the exponential integrators. The main computational challenge in the implementation of any exponential integrator is the need for fast and computationally stable evaluations of the exponential and the related φ-functions. There are many methods available in the literature for computing the exponential function, we refer to [73] and references within. Almost all exponential integrators, with the exception of the integrators derived from the Lie group framework, explicitly use linear combinations of the functions

$$\varphi_0(z) = \mathrm{e}^z, \quad \varphi_{\ell+1} = \frac{\varphi_\ell(z) - \frac{1}{\ell!}}{z}, \quad \ell = 0, 1, \ldots, \tag{9.1}$$

as previously defined in Section 5. A straightforward implementation, based on the above formulas, suffers for small z, from cancellation errors [37, 53]. As ℓ increases, the cancellation errors become even more extreme. A way to avoid this problem is to approximate each φ-functions by its truncated Taylor series expansion. This approach, however, fails to produce correct results for large z. Thus, a natural idea, first used by Cox and Matthews [16] is to introduce a cutoff point and to compute the φ-functions directly by (9.1) when z is large, and by truncated Taylor series expansions, when z is small. The problem with this approach, is that there may exist a region, in the z variables, in which neither

approximation is accurate. To avoid this drawback, Kassam and Trefethen [53] proposed to approximate the φ-functions by the Cauchy integral formula

$$\varphi_\ell(z) = \frac{1}{2\pi i} \int_\Gamma \varphi_\ell(\lambda)(\lambda - z)^{-1} \mathrm{d}\lambda, \tag{9.2}$$

where Γ is a contour in the complex plane that encloses z and is well separated from 0. In [53], it is suggested that the contour Γ, can be chosen to be a circle centered on the real axis. In this case, due to symmetry, one can evaluate the integral only on the upper half of the circle and then double the real part of the result. However, we mention that depending on the type of the problem we have to solve, other contours, different from circles, can also be used. For example, for parabolic problems, it seems preferable to choose the contour Γ to be a parabola also centered on the real axis. The integral in (9.2) can be easily approximated by the trapezoid rule [99]. The main disadvantages of the Cauchy integral approach are: Unless the matrix L has a very special structure, computing approximations to the φ-functions, is simply too expensive to implement; In general the contour varies for each problem, making it difficult to obtain general algorithms.

Another approach for approximating the φ-functions, is to use high order Padé approximations, combined with a scaling and squaring technique, which can be adopted from the approach proposed in [5]. Obtaining general formulae for the elements of the Padé table is more difficult than for the exponential function. Unique expressions of order $d + n$, where d and n are the degrees of the denominator and numerator respectively, exist for $\ell \geq 2$. This is not possible for the φ_1 function. An example, is the Padé (1,3) approximation to the φ_1 function, which is actually only a third order approximation.

Using the similarity transformation

$$z = SyS^{-1},$$

where y is such that $\varphi_\ell(y)$ is cheap and easy to compute. Then

$$\varphi_\ell(z) = S\varphi_\ell(y)S^{-1}.$$

The choices of S and y involve two conflicting tasks. Try to make y as close to diagonal as possible while requiring S to be well conditioned. Therefore, it is natural to choose S to be an unitary matrix. Two algorithms, based on this decomposition idea are of practical interest. These are the block Schur–Parlett algorithm [19], and the tridiagonal reduction algorithm, first proposed for the φ_1 function in [67] and latter generalized to all φ-functions in [72]. As for the Cauchy integral approach, except in some special cases, these methods are also too expensive to implement. This is even worse if a variable-stepsize strategy is used, in which case, we need to recompute the φ-functions, every time the stepsize is changed.

A way to overcome the higher computational cost arising from the change of the stepsize, is to take advantage of the fact that when implementing any exponential integrator, we do not really need to compute the φ-functions. What we

need, is just their action to a given state vector v. Krylov subspace approximations to the exponential and some related functions, have been studied by many authors, see for example [26, 39, 74, 86]. The main idea is to approximately project the action of the function $\varphi_\ell(z)$ on a state vector v, to a smaller Krylov subspace

$$K_m \equiv \text{span}\{v, zv, \ldots, z^{m-1}v\}.$$

The dimensionality m of the Krylov subspace is usually much smaller than the dimensionality of z. If $V_m = [v_1, v_2, \ldots, v_m]$ is an orthogonal basis of K_m and z_m is the orthogonal projection of z to the subspace K_m with respect to the basis V_m, then we can approximate the action of $\varphi_\ell(z)$, on the vector v by

$$\varphi_\ell(z)v \approx ||v||\, V_m\, \varphi_\ell(z_m)e_1,$$

where e_1 is the identity vector in $\mathbf{R}^m$. The main advantage of the above formula, is that, instead of working with the original large space, we work with its orthogonal approximation, which has much smaller dimension. Thus, the cost of computing the expression $||v||\, V_m\, \varphi_\ell(z_m)e_1$ is usually much smaller than the cost needed to compute $\varphi_\ell(z)v$. In addition, when the linear part L of the equation (1.1) arises from a spatial discretization of an elliptic operator, it is possible to speed up the iterative process by using a preconditioned operation see [100].

10 Special methods

In this section, we aim to briefly mention (and direct the reader to the appropriate references) exponential integrators, which are not our primary concern in this article, but have played an important role in providing efficient numerical solutions.

Much of the recent effort into the construction of exponential integrators, has been for the numerical solution of highly oscillatory problems. There has been several recent papers for second order problems of the form

$$y''(t) = -Ly(t) + N(y(t)), \quad y(t_{n-1}) = y_{n-1}, \quad y'(t_{n-1}) = y'_{n-1},$$

where L is a symmetric and positive semi-definite real matrix with arbitrary large norm. Such problems, produce oscillatory solutions and the aim of the exponential integrators, in this situation, is to evaluate the right hand side of the differential equation only a few times for several periods of the fastest oscillation. Such methods can be effectively used for the numerical solution of problems from astrophysics and molecular dynamics among others.

The variation of constants formula, is again, the starting point for construction of exponential integrators for second order problems. To use the variation of constants formula (5.1) we express the second order problem as a system of two first order problems, with $\Omega = L^{1/2}$,

$$\begin{bmatrix} y(t) \\ y'(t) \end{bmatrix} = \begin{bmatrix} \cos(t-t_{n-1})\Omega & \Omega^{-1}\sin(t-t_{n-1})\Omega \\ -\Omega\sin(t-t_{n-1})\Omega & \cos(t_{n-1})\Omega \end{bmatrix} \begin{bmatrix} y_{n-1} \\ y'_{n-1} \end{bmatrix}$$
$$+ \int_{t_{n-1}}^{t} \begin{bmatrix} \Omega^{-1}\sin(t-\tau)\Omega \\ \cos(t-\tau)\Omega \end{bmatrix} N(y(\tau))\mathrm{d}\tau.$$

If we approximate the nonlinear term $N(y(\tau))$ by N_{n-1}, and compute the exact solution, the resulting method, once the velocity components have been eliminated, reads

$$y_{n+1} - 2\cos(h\Omega)y_n + y_{n-1} = h^2\mathrm{sinc}^2(\tfrac{1}{2}h\Omega)N_n. \tag{10.1}$$

This method (for scalar equations) was discovered by Gautschi [28] in 1961. In this paper multistep type methods were constructed, which produce the exact solution if the problem emits a sufficiently low degree, trigonometric polynomial solution. Note that the method of Gautschi reduces to the well known Störmer–Verlet method when $L = 0$. The starting values y_n and y'_n are computed by replacing the $N(y(\tau))$ by $N(y_{n-1})$, from which one can conclude that both the solution and derivative are exact when $N(y(t))$ is a constant. Deuflhard [20] constructed a similar method by approximating, using the trapezoidal rule, the integral term in the variation of constants formulae, which leads to

$$y_{n+1} - 2\cos(h\Omega)y_n + y_{n-1} = h^2\mathrm{sinc}(h\Omega)N_n.$$

Both the methods of Gautschi and Deuflhard, suffer from resonant problems, when the eigenvalues of $h\Omega$, are integer multiples of π. To overcome this problem, Hochbruck and Lubich [41] use a filter function ψ, such that $\psi(0) = 1$ and $\psi(k^2\pi^2) = 0$, for $k = 1, 2, \ldots$, that is

$$N_{n-1} = N(\psi(h^2L)y_{n-1}). \tag{10.2}$$

Hochbruck and Lubich [41] and Grimm, [31, 32], (for the situation when L is a function of t and y), prove that (10.1) with N_{n-1} defined as (10.2), is a second order integrator, independent of the product of the stepsize with the frequencies. A method with two force evaluations was proposed by Hairer and Lubich, [34], which provided the correct slow energy exchange between stiff components for the Fermi–Pasta–Ulam problem. We refer to the book by Hairer, Lubich and Wanner [36] for a thorough review of integrators for highly oscillatory differential equations, providing the various filter functions used, and which methods preserve geometric properties of the differential equation.

Another important application, where exponential integrators have proven to be extremely competitive is for Schrödinger equations, with time dependent Hamiltonian

$$\psi'(t) = -iH(t)\psi(t), \quad H(t) = U + V(t). \tag{10.3}$$

We have already discussed integrators, which use the fact that the Hamiltonian can be split in this way, and only use the exponential and related functions of U. Several methods exist, which exponentiate the full Hamiltonian. For example, the so-called exponential midpoint scheme

$$\psi_n = \exp(-ihH(t_{n-1/2}))\psi_{n-1},$$

which is proved by Hochbruck and Lubich [40] to have second order behaviour independent of the smoothness of the solution. The exponential midpoint rule relies on the fact that the exponential of a large matrix can be computed efficiently. We cite the review article of Lubich [68] (and references within), which

addresses this issue for various methods for problems of the form (10.3). Jahnke and Lubich in a series of papers [47, 48, 49], construct numerical methods for a singularly perturbed Schrödinger equation

$$\psi'(t) = -\frac{i}{\epsilon}H(t)\psi(t), \quad H(t) = U + V(t), \quad (0 < \epsilon \ll 1),$$

allowing stepsizes $h > \epsilon$, which is not possible due to accuracy constraints for the exponential midpoint rule. The method of construction relies on the transformation to adiabatic variables

$$Q(t)^T\psi(t) = \exp\left(-\frac{i}{\epsilon}\varphi(t)\right)\nu(t), \quad \varphi(t) = \int_{t_{n-1}}^{t} \Lambda(\tau)\,\mathrm{d}\tau.$$

where, the Hamiltonian is diagonalized as $H(t) = Q(t)\Lambda(t)Q(t)^T$. The integrator is applied to the transformed differential equation in the adiabatic variables. We do not give the numerical methods here due to excess notation, but refer directly to [47] for a complete treatment. This transformation to adiabatic variables was also used by Lorenz, Jahnke and Lubich [66], where the adiabatic midpoint and adiabatic Magnus method is developed for the problem

$$y''(t) = -\frac{1}{\epsilon^2}L(t)y(t) + \frac{1}{\epsilon^2}N(t), \quad y(t_{n-1}) = y_{n-1}, \quad y'(t_{n-1}) = y'_{n-1}.$$

Both the adiabatic midpoint and adiabatic Magnus method are of order two, independent of ϵ and the stepsize h used by the integrators.

Recently, in [29, 98], the exponential mid-point rule was also combined with a second-order Magnus method [70] to find the solution of the following non-autonomous semi-linear parabolic problem

$$y'(t) = L(t)y(t) + N(y(t)), \quad y(t_{n-1}) = y_{n-1}.$$

The stability and convergence properties of the resulting exponential integrator

$$y_n = \mathrm{e}^{hL(t_{n-1}+\frac{1}{2}h)}y_{n-1} + h\varphi_1\big(hL(t_{n-1}+\tfrac{1}{2}h)\big)N\left(y(t_{n-1}+\tfrac{1}{2}h)\right),$$

were studied using the framework of sectorial operators and analytic semi-groups. It was found that under reasonable smoothness assumptions on the data and the exact solution, this method achieves the desired order, without imposing unnatural restrictions on the stepsize. It is worth mentioning that the above exponential integrator can be also derived from the framework of Lie group methods, with affine algebra action, by choosing to freeze the vector field at the point $t_{n-1} + \frac{1}{2}h$. In the Lie group methods literature, this method is often called the exponential Lie-Euler method. A similar type of analysis for the same method applied to quasi-linear parabolic problems was performed in [30].

Finally, in this section, we mention the Matlab code `exp4`, which is described in [42]. This code is the first actual implementation of an exponential integrator, as before this all implementations used low order approximations to the exponential and related functions. The method used in the code `exp4`,

is of fourth order and can be regarded as a Rosenbrock-like exponential integrator. Only the $\varphi_1(\gamma h f'(y_{n-1}))$ function is used in the method and its action on a vector is evaluated using a Krylov subspace approximation. A Padé (6,6) approximation using a scaling and squaring technique, is used to evaluate the resulting φ_1 function. The implementation used variable-stepsizes and was compared against well known standard solvers such as a matlab implementation of `radau5`, and `ode45` and `ode15s`, from the Matlab ODE suite. The code `exp4` performed very well on stiff and highly oscillatory problems, despite the lack of a preconditioner.

11 Numerical experiments

In this section, we compare six exponential integrators on five well known PDEs. The methods under consideration are: `lawson4`, the Runge–Kutta–Lawson method (4.1), with classical order four Runge–Kutta coefficients; `hochost4`, the stiff order four ETD method of Hochbruck and Ostermann, (8.3); `abnorsett4`, the order four Adams–Bashforth–Nørsett method see Table 5.1, `genlawson43`, the GL method GL3/cRK4; `rkmk4t`, the RKMK method given in (7.6); `cfree4`, the CF method given in (7.7). We also include `cranknicolson`, the Crank–Nicolson scheme which is the most commonly used integrator for such problems. We believe these methods to be a fair representation of the methods available.

The φ-functions are evaluated using (6,6) Padé approximations, with a scaling and squaring technique. All experiments use a matlab package described in [4], which can be downloaded from `http://www.math.ntnu.no/num/expint/`. For the sake of convenience we briefly include a description of each of the five PDEs under consideration.

Problem 1. The Kuramoto–Sivashinsky equation with periodic boundary conditions (see [53])

$$\begin{aligned} y_t &= -y_{xx} - y_{xxxx} - y y_x, \quad x \in [0, 32\pi], \\ y(x,0) &= \cos\left(\tfrac{x}{16}\right)\left(1 + \sin\left(\tfrac{x}{16}\right)\right). \end{aligned}$$

This is a semi-linear parabolic problem and we discretized in space using a 128-point Fourier spectral discretization. The resulting ODE is integrated over the interval $t = 0$ to $t = 65$. Due to the periodic boundary conditions the matrix L is diagonal. The fourth order term makes this problem extremely stiff, with rapid linear decay of high wave number modes.

Problem 2. The Burgers equation with periodic boundary conditions (see [53])

$$\begin{aligned} y_t &= \lambda y_{xx} - \tfrac{1}{2}(y^2)_x, \quad x \in [-\pi, \pi], \\ y(x,0) &= \exp(-10\sin^2(x/2)), \end{aligned}$$

where $\lambda = 0.03$. We use a 128-point Fourier spectral discretization and the resulting ODE is integrated over one period $t = [0, 1]$. The stiffness in this problem comes from the term λy_{xx}, which results in rapid oscillations of the high wave number modes.

Problem 3. The Allen–Cahn equation with constant Dirichlet boundary conditions (see [53])

$$\begin{aligned} y_t &= \lambda y_{xx} + y - y^3, \quad x \in [-1, 1], \\ y(x, 0) &= 0.53x + 0.47 \sin(-1.5\pi x), \quad u(-1, t) = -1, \quad u(1, t) = 1, \end{aligned}$$

where $\lambda = 0.001$. A 50-point Chebyshev spectral discretization is used and the ODE is then integrated from $t = 0$ to $t = 3$. To satisfy the boundary conditions, define $y = w + x$ and work with homogeneous boundary conditions in the w variable. In this problem the matrix L, is full and the computations are more demanding.

Problem 4. A semi-linear parabolic problem of Hochbruck and Ostermann with homogeneous Dirichlet boundary conditions (see [44])

$$y_t = y_{xx} + \frac{1}{1 + y^2} + \Phi, \quad x \in [0, 1],$$

where Φ is chosen so that the exact solution is $y(x, t) = x(1-x)\mathrm{e}^t$. The problem is discretized in space using a 64-point standard finite difference scheme. The resulting ODE is integrated from $t = 0$ to $t = 1$.

Problem 5. The nonlinear Schrödinger equation with periodic boundary conditions (see [3])

$$\begin{aligned} i y_t &= -y_{xx} + \left(V(x) + \lambda |u|^2\right) y, \\ y(x, 0) &= \exp(\sin(2x)), \end{aligned}$$

where the nonlinear constant $\lambda = 1$ and the potential V has a regularity of two. We use a 256-point Fourier spectral discretization and integrate in time from $t = 0$ to $t = 1$. The stiffness in this problem comes from the term y_{xx}, which results in rapid oscillations of the high wave number modes.

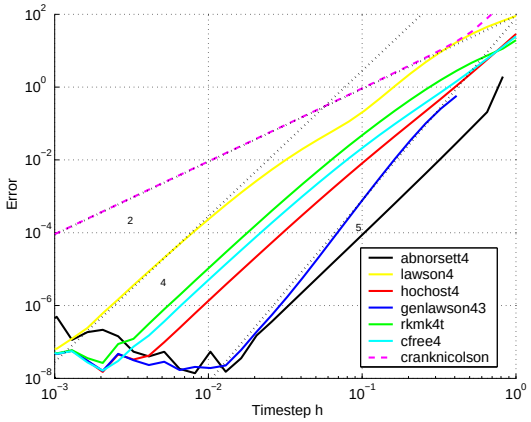

Figure 1: Relative stepsize vs global error for Kuramoto–Sivashinsky equation.

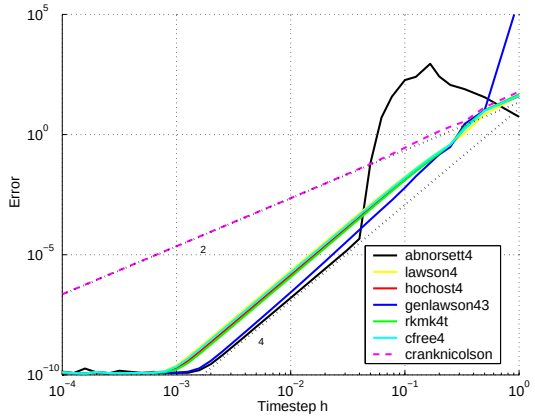

Figure 2: Relative stepsize vs global error for Burgers equation.

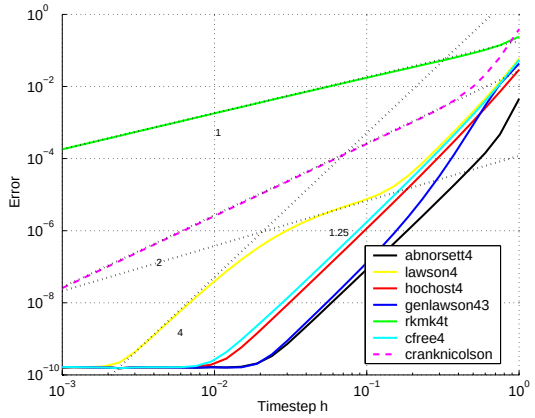

Figure 3: Relative stepsize vs global error for Allen–Cahn equation.

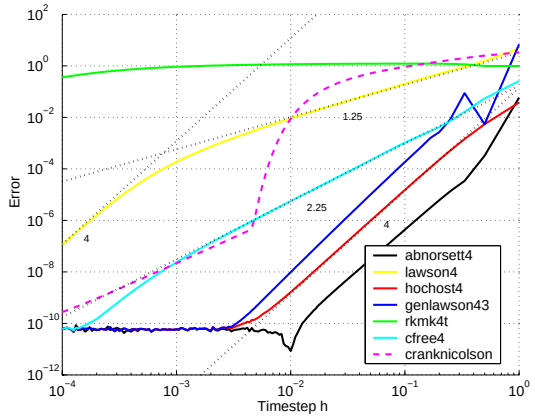

Figure 4: Relative stepsize vs global error for Hochbruck–Ostermann equation.

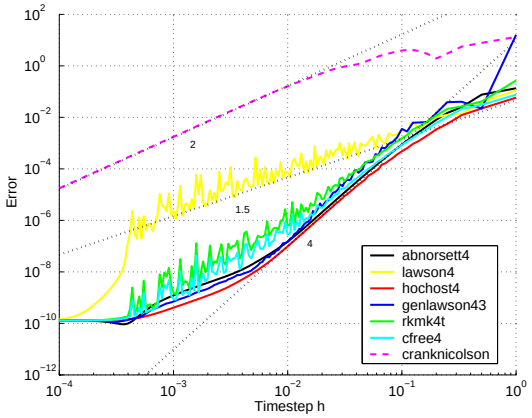

Figure 5: Relative stepsize vs global error for nonlinear Schrödinger equation.

The Kuramoto–Sivashinsky, Allen–Cahn and Hochbruck–Ostermann problems are all parabolic and therefore, the stiff order theory briefly discussed in Section 8 applies. The observed error in the Hochbruck–Ostermann problem is exactly as the theory predicts. We see that `abnorsett4` has six orders of magnitude improvement over the `lawson4` method. The Kuramoto–Sivashinsky problem is implemented using periodic boundary conditions and we see that all methods achieve their non-stiff order. What is surprising, is that for the Allen–Cahn equation which does not have periodic boundary conditions, all methods except `lawson4` and `rkmk4t` achieve the non-stiff order. The `rkmk4t` performs badly on all problems, which do not have periodic boundary conditions. The Burgers and nonlinear Schrödinger equations are hyperbolic problems. The Burgers equation is implemented with periodic boundary conditions and all methods perform similarly and achieve the non-stiff order. On the other hand the nonlinear Schrödinger, which has a non-smooth potential, has a significant effect on the order achieved. The `lawson4` method produces large oscillations in the numerical approximation, but achieves an order around 1.5. The lie group solvers also produce erratic behaviour of order around 2.25. The three stiff order four methods `abnorsett4`, `genlawson43` and `hochost4` seem to achieve order four for most of the computation. This reduces as the stepsize reduces, whether this is caused by roundoff is unclear. It has been shown that for the nonlinear Schrödinger equation the Lawson methods are much less sensitive to non-smooth initial conditions, see [3]. Understanding exactly why the Lawson methods perform better in this situation is worth further investigation. We note that the integrator used in most computations of this sort is the Crank–Nicolson scheme, we point out that in all experiments the exponential integrators perform significantly better.

Over all problems we see that the leading contenders are the methods `abnorsett4`, `genlawson43` and `hochost4`, which are the only methods with full stiff order four. The first two methods have stiff stage order equal to stiff order. This can only be achieved by passing more than the approximation from step to step, but methods of this type are likely to be the best contenders for an efficient implementation. The loss of stability observed for the `genlawson43` method on

the Kuramoto–Sivashinsky equation can be rectified but a slight modification of the output approximation. This modification is described in [79], where it is shown that the modified methods have improved stability and a significant improvement in accuracy. Even though we have not included these methods in our experiments, we promote the modified generalized Lawson methods as the integrator of choice. We note that in all the experiments roundoff errors start affecting accuracy generally around the $1e^{-10}$ accuracy level. It is likely that this loss of accuracy can be overcome using compensated summation.

12 Discussion

In this article we have attempted to provide a partial history of the exponential integrators, for the numerical solution of first order semi-linear problems. These methods, date back to around the early sixties and have been developed not only by numerical analysts but by mathematicians studying, for example, pattern formation, which end up with an systems of equations of the form (1.1) to solve. Also chemists and physicists, among others, have independently developed exponential integrators. One of the major difficulties we found when working on this paper, is trying to find the appropriate references, searching databases is difficult when a particular method has almost ten different names, as has the exponential time differencing methods. It is for this reason that we do not claim we have a complete list of references and we see why these methods, which are very natural, have been reproduced so often.

Exponential integrators or approximations to them, encompasses a huge variety of methods, we have therefore, restricted the focus of this paper, mainly to semi-linear problems of first order. Traditionally such problems have been the focus of most of the research. In doing so we have constructed a unified framework for representing the methods, known as exponential general linear methods, which facilitates a clearer understanding of the similarities and differences between methods. The Lawson, exponential time differencing, generalized Lawson and the Lie group methods with affine action all fit into this class of methods. The non-stiff order theory for these problems has been generalized to the class of exponential general linear methods using B-series. We have chosen to include this not because it gives the correct order conditions for problems when L has arbitrary large norm, but rather because such conditions have been constructed by several authors in the last few years, just to find in the review process that they were first derived for Runge–Kutta methods in the late seventies and early eighties.

The research into this paper has lead us to various areas in which we believe future research would be useful. Developing convergence results for semi-linear hyperbolic problems, as was done for semi-linear parabolic problems by Hochbruck and Ostermann, [44], is essential. In many numerical experiments the order achieved by certain methods is greater than the stiff order of the method and often equal to the non-stiff order. Well-known examples include the Allen–Cahn, Kuramoto–Sivashinsky, KdV and nonlinear Schrödinger equations. Determining exactly when one can expect a higher order of convergence,

than the stiff order predicts, would make constructing methods for particular problems easier. Most exponential integrators are implemented in a fixed stepsize regime, this allows an explicit implementation once the appropriate preprocessing has been done before the integration begins. A major concern with exponential integrators is whether they will be efficient when variable-stepsizes are allowed as this requires the exponential and related functions to be recomputed each time the stepsize is changed. This is likely not to be a problem when the matrix L is diagonal, generally the result of a Fourier spectral discretization, but more evident in the the case when L is a full matrix, resulting from a Chebyshev or finite difference discretization. In such situations Krylov approximations are likely to provide the most efficient methods. The functions which arise naturally from the variation of constants formula, the so-called φ-functions, are needed to satisfy the stiff order conditions. Is it possible to construct integrators with high stiff stage order which also use other functions? If so, what are the properties these functions need to satisfy. What is evident throughout the literature is that the observed order is closely related to high stage order, the situation is no different for exponential integrators. This motivates the need to look for exponential integrators with high stage order. Are there traditional integrators with high stage order, which can be generalized to the exponential setting? Another interesting question, which needs further investigation, is how to construct higher order exponential integrators, for non-autonomous semi-linear and quasi-linear problems, which are different from those arising from the framework of Lie group methods.

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References

[1] U. M. Ascher, S. J. Ruuth, and B. T. R. Wetton. Implicit-explicit methods for time dependent partial differential equations. *SIAM J. Numer. Anal.*, 32(3):797–823, 1995.

[2] H. Berland, B. Owren, and B. Skaflestad. B-series and order conditions for exponential integrators. Technical Report 5/04, The Norwegian Institute of Science and Technology, 2004. http://www.math.ntnu.no/preprint/.

[3] H. Berland and B. Skaflestad. Solving the nonlinear Schrödinger equation using exponential integrators. Technical Report 3/05, The Norwegian Institute of Science and Technology, 2005. http://www.math.ntnu.no/preprint/.

[4] H. Berland, B. Skaflestad, and W. Wright. Expint - a Matlab package for exponential integrators. Technical Report 4/05, The Norwegian Institute of Science and Technology, 2005. http://www.math.ntnu.no/preprint/.

[5] G. Beylkin, J. M. Keiser, and L. Vozovoi. A new class of time discretization schemes for the solution of nonlinear PDEs. *J. of Comp. Phys.*, 147:362–387, 1998.

[6] J. P. Boyd. *Chebyshev and Fourier spectral methods*. Dover, New York, 2001.

[7] J. Bruder, K. Strehmel, and R. Weiner. Partitioned adaptive Runge–Kutta methods for the solution of non-stiff and stiff systems. *Numer. Math.*, 52:621–638, 1988.

[8] J. C. Butcher. On the convergence of numerical solutions to ordinary differential equations. *Math. Comp.*, 20:1–10, 1966.

[9] J. C. Butcher. The effective order of Runge-Kutta methods. *Lecture Notes Math.*, 109:133–139, 1969.

[10] J. C. Butcher. *Numerical methods for ordinary differential equations*. John Wiley & Sons, 2003.

[11] M. P. Calvo and C. Palencia. A class of multistep exponential integrators for semilinear problems. Submitted, 2005.

[12] C. Canuto, M. Y. Hussaini, A. Quateroni, and T. A. Zang. *Spectral methods in fluid dynamics*. Springer Verlag, 1988.

[13] E. Celledoni. Eulerian and semi-Lagrangian schemes based on commutator free exponential integators. To appear, 2005.

[14] E. Celledoni, A. Marthinsen, and B. Owren. Commutator-free Lie group methods. *FGCS*, 19(3):341–352, 2003.

[15] J. Certaine. The solution of ordinary differential equations with large time constants. In *Mathematical methods for digital computers*, pages 128–132. Wiley, New York, 1960.

[16] S. M. Cox and P. C. Matthews. Exponential time differencing for stiff systems. *J. Comput. Phys.*, 176(2):430–455, 2002.

[17] P. E. Crouch and R. Grossman. Numerical integration of ordinary differential equations on manifolds. *J. Nonlinear Sci.*, 3:1–33, 1993.

[18] C. F. Curtiss and J. O. Hirschfelder. Integration of stiff equations. *Proc. Nat. Acad. Sci.*, 38:235–243, 1952.

[19] P. Davies and N. Higham. A Schur–Parlett algorithm for computing matrix functions. *SIAM J. Matrix Anal. Applic.*, 25(2):464–485, 2003.

[20] P. Deuflhard. A study of extrapolation methods based on multistep schemes without parasitic solutions. *Z. Angew. Math. Phys.*, 30:177–189, 1979.

[21] W. S. Edwards, L. S. Tuckerman, R. A. Friesner, and D. C. Sorensen. Krylov methods for the incompressible Navier–Stokes equations. *J. of Comp. Phys.*, 110:82–102, 1994.

[22] B. L. Ehle and J. D. Lawson. Generalized Runge–Kutta processes for stiff initial-value problems. *J. Inst. Maths. Applics.*, 16:11–21, 1975.

[23] L. N. G. Filon. On a quadrature formulae for trigonometric polynomials. *Proc. Roy. Soc. Edinburgh*, 49:38–47, 1928–1929.

[24] A. Friedli. Verallgemeinerte Runge–Kutta Verfahren zur Lösung steifer Differentialgleichungssysteme. In *Numerical treatment of differential equations*, pages 35–50. Lecture Notes in Math., Vol. 631. Springer, Berlin, 1978.

[25] R. A. Friesner, L. S. Tuckerman, B. C. Dornblaser, and T. V. Russo. A method for the exponential propagation of large stiff nonlinear differential equations. *J. Sci. Comput.*, 4(4):327–354, 1989.

[26] E. Gallopoulos and Y. Saad. Efficient solution of parabolic equations by Krylov approximation methods. *SIAM J. Sci. Statist. Comput.*, 13:1236–1264, 1992.

[27] B. García-Archilla. Some practical experience with the time integration of dissipative equations. *J. of Comp. Phys.*, 122:25–29, 1995.

[28] W. Gautschi. Numerical integration of ordinary differential equations based on trigonometric polynomials. *Numer. Math.*, 3:381–397, 1961.

[29] C. González, A. Ostermann, and M. Thalhammer. A second-order Magnus integrator for non-autonomous parabolic problems. To appear in J. Comp. Appl. Math, 2005.

[30] C. González and M. Thalhammer. A second-order Magnus type integrator for quasilinear parabolic problems. Submitted to Math. Comp., 2004.

[31] V. Grimm. On error bounds for Gautschi-type exponential integrators applied to oscillatory second-order differential equations. *Numer. Math.*, 100(1):71–89, 1995.

[32] V. Grimm. *Exponentielle integratoren als lange-Zeitschritt-Verfahren für oszillatorische Differentialgleichungen zweiter Ordnung.* PhD thesis, University of Düsseldorf, 2002.

[33] E. Hairer, G. Bader, and C. Lubich. On the stability of semi-implicit methods for ordinary differential equation. *BIT*, 22:211–232, 1982.

[34] E. Hairer and Ch. Lubich. Long-time energy conservation of numerical methods for oscillatory differential equations. *SIAM J. Numer. Anal.*, 38(2):414–441, 2000.

[35] E. Hairer and G. Wanner. *Solving Ordinary Differential Equations. II*, volume 14 of *Springer Series in Computational Mathematics*. Springer-Verlag, Berlin, second edition, 1996. Stiff and differential-algebraic problems.

[36] Ernst Hairer, Christian Lubich, and Gerhard Wanner. *Geometric Numerical Integration*, volume 31 of *Springer Series in Computational Mathematics*. Springer-Verlag, Berlin, 2002. Structure-preserving algorithms for ordinary differential equations.

[37] N. J. Higham. *Accuracy and Stability of Numerical Algorithms*. SIAM, Philadelphia, 1996.

[38] M. Hochbruck. Exponential integrators. Workshop on Exponential Integrators, Innsbruck, October 20-23, 2004.

[39] M. Hochbruck and C. Lubich. On Krylov subspace approximations to the matrix exponential operator. *SIAM J. Numer. Anal.*, 34(5):1911–1925, 1997.

[40] M. Hochbruck and C. Lubich. Exponential integrators for quantum-classical molecular dynamics. *BIT*, 39(4):620–645, 1999.

[41] M. Hochbruck and C. Lubich. A Gautschi-type method for oscillatory second order differential equations. *Numer. Math.*, 83:403–426, 1999.

[42] M. Hochbruck, C. Lubich, and H Selhofer. Exponential integrators for large systems of differential equations. *SIAM J. Sci. Comput.*, 19(5):1552–1574, 1998.

[43] M. Hochbruck and A. Ostermann. Exponential Runge–Kutta methods for parabolic problems. *Appl. Numer. Math.*, 53:323–339, 2005.

[44] M. Hochbruck and A. Ostermann. Explicit exponential Runge–Kutta methods for semilinear parabolic problems. *SIAM J. Numer. Anal.*, To appear 2005.

[45] R. Holland. Finite-difference time-domain (FDTD) analysis of magnetic diffusion. *IEEE Trans. Elect. Comp.*, 36(1):32–39, 1994.

[46] A. Iserles, H. Z. Munthe-Kaas, S. P. Nørsett, and A. Zanna. Lie-group methods. *Acta Numerica*, 9:215–365, 2000.

[47] T. Jahnke. *Numerische VVerfahren für fast adiabatische Quantendynamik*. PhD thesis, University of Tübingen, 2003. In German.

[48] T. Jahnke. Long-time-step integrators for almost adiabatic quantum dynamics. *SIAM J. Sci. Comput.*, 25(6):2145–2164, 2004.

[49] T. Jahnke and C. Lubich. Numerical integrators for quantum dynamics close to the adiabatic limit. *Numer. Math.*, 94:289–314, 2003.

[50] R. K. Jain. Some A-stable methods for stiff ordinary differential equations. *Math. Comp.*, 26:71–77, 1972.

[51] F. Jauberteau, C. Rosier, and R. Temam. A nonlinear galerkin method for the Navier–Stokes equations. *Comput. Methods Appl. Mech. Engrg.*, 80:245–260, 1990.

[52] A.-K. Kassam. *High Order Timestepping for Stiff Semilinear Partial Differential Equations*. PhD thesis, University of Oxford, 2004.

[53] A.-K. Kassam and L. N. Trefethen. Fourth-order time-stepping for stiff PDEs. *SIAM J. Sci. Comput.*, 26(4):1214–1233, 2005.

[54] J. Kim and P. Moin. Application of a fractional-step method to incompressible Navier–Stokes equations. *J. of Comp. Phys.*, 59:308–325, 1985.

[55] S. Koikari. Bicolored tree analysis and order conditions of ETD Runge–Kutta methods. http://www16.ocn.ne.jp/˜koikari/, 2005.

[56] S. Koikari. Rooted tree analysis of Runge–Kutta methods with exact treatment of linear terms. *J. Comput. Appl. Math*, 177:427–453, 2005.

[57] S. Krogstad. RKMK-related methods for stiff PDEs. Technical report, University of Bergen, 2003. http://www.ii.uib.no/∼stein/.

[58] S. Krogstad. Generalized integrating factor methods for stiff PDEs. *J. of Comp. Phys.*, 203(1):72–88, 2005.

[59] A. Kværnø. Error behaviour of exponential Runge–Kutta methods. Technical Report 7/04, The Norwegian Institute of Science and Technology, 2004. http://www.math.ntnu.no/preprint/.

[60] J. D. Lambert. *Computational methods in ordinary differential equations*. John Wiley & Sons, 1973.

[61] J. D. Lambert and S. T. Sigurdsson. Multistep methods with variable matrix coefficients. *SIAM J. Numer. Anal.*, 9:715–733, 1972.

[62] D. J. Lawson. Generalized Runge–Kutta processes for stable systems with large lipschitz constants. *SIAM J. Numer. Anal.*, 4:372–380, 1967.

[63] W. Liniger and R. A. Willoughby. Efficient integration methods for stiff systems of ordinary differential equations. *SIAM J. Numer. Anal.*, 7:47–66, 1970.

[64] E. Lodden. Geometric integration of the heat equation. Master's thesis, University of Bergen, 2000.

[65] G. Lord and J. Rougemont. A numerical scheme for stochastic PDEs with Gevrey regularity. *IMA J. Numer. Anal.*, 24(4):587–604, 2004.

[66] K. Lorenz, T. Jahnke, and C. Lubich. Adiabatic integrators for highly oscillatory second order linear differential equations with time-varying eigendecomposition. Technical report, University of Tübingen, 2005.

[67] Y. Y. Lu. Computing a matrix function for exponential integrators. *J. Comput. Appl. Math*, 161(1):203–216, 2003.

[68] C. Lubich. Integrators for quantum dynamics: a numerical analyst's brief review. In *Quantum Simulations of Many-Body Systems: From Theory to Algorithms*, pages 459–466. NIC series, 2002.

[69] Y. Maday, A. T. Patera, and E. M. Rønquist. An operator-integration-factor splitting method for time-dependent problems: application to incompressible fluid flow. *SIAM J. Sci. Comput.*, 5(4):263–292, 1990.

[70] W. Magnus. On the exponential solution of differential equations for a linear operator. *Comm. Pure and Appl. Math.*, VII:649–673, 1954.

[71] P. A. Milewski and E. G. Tabak. A pseudospectral procedure for the solution of nonlinear wave equations with examples from free surface flows. *SIAM J. Sci. Comput.*, 21(3):1002–1114, 1999.

[72] B. Minchev. *Exponential integration for semi-linear problems*. PhD thesis, University of Bergen, 2004.

[73] C. B. Moler and C. F. van Loan. Nineteen dubious ways to compute the exponential of a matrix, twenty five years later. *SIAM Review*, 45(1):3–49, 2003.

[74] I. Moret and P. Novati. A rational Krylov method for solving time-periodic differential equations. Preprint http://univaq.it/~novati/, 2004.

[75] D. R. Mott, E. S. Oran, and B. van Leer. A quasi-steady-state solver for stiff ordinary differential equations of reaction kinetics. *J. of Comp. Phys.*, 164:407–428, 2000.

[76] Hans Munthe-Kaas. High order Runge–Kutta methods on manifolds. In *Proceedings of the NSF/CBMS Regional Conference on Numerical Analysis of Hamiltonian Differential Equations (Golden, CO, 1997)*, volume 29,1, pages 115–127, 1999.

[77] S. P. Nørsett. An A-stable modification of the Adams–Bashforth methods. In *Conf. on Numerical Solution of Differential Equations (Dundee, 1969)*, pages 214–219. Springer, Berlin, 1969.

[78] S. P. Nørsett. Numerisk integrasjon av stive likninger. Master's thesis, University of Oslo, 1969.

[79] A. Ostermann, M. Thalhammer, and W. Wright. More on generalized Lawson methods. In preperation, 2005.

[80] B. Owren and A. Marthinsen. Runge–Kutta methods adapted to manifolds and based on rigid frames. *BIT*, 39(1):116–142, 1999.

[81] O. A. Palusinski and J. V. Wait. Simulation methods for combined linear and nonlinear systems. *Simulation*, pages 85–94, 1978.

[82] P. G. Petropoulus. Analysis of exponential time-differencing for FDTD in lossy dielectrics. *IEEE Trans. Antennas Propagation*, 45:1054–1057, 1997.

[83] D. A. Pope. An exponential method of numerical integration of ordinary differential equations. *Comm. AGM*, 6:491–493, 1963.

[84] David T. Pratt. Exponential-fitted methods for stiff ordinary differential equations. In *Numerical mathematics and applications (Oslo, 1985)*, IMACS Trans. Sci. Comput.—85, I, pages 145–151. North-Holland, Amsterdam, 1986.

[85] H. H. Rosenbrock. Some general implicit processes for the numerical solution of differential equations. *Comput. J.*, 5:329–330, 1962/1963.

[86] Y. Saad. Krylov subspace methods for solving large unsymmetric linear systems. *Math. Comp.*, 37:105–126, 1981.

[87] M. Sato, K. Kawabata, and J. E. Hansen. A fast invariant imbedding method for multiple scattering calculations and an application to equivalent widths of CO_2 lines of venus. *Astro. J.*, 216:947–962, 1977.

[88] M. Schatzman. Toward non-commutative numerical analysis: high order integration in time. *J. Sci. Comp.*, 17(1–4):99–116, 2002.

[89] C. Schuster, A. Christ, and W. Fichtner. Review of FDTD time-stepping for efficient simulation of electric conductive media. *Microwave Optical Technol. Lett.*, 25:16–21, 2000.

[90] L. M. Smith and F. Waleffe. Generation of slow large scales in forced in forced rotating stratified turbulence. *J. Fluid Mech.*, 451:145–169, 2002.

[91] T. Steihaug and A. Wolfbrandt. An attempt to avoid exact Jacobian and nonlinear equations in the numerical solution of stiff differential equations. *Math. Comp.*, 33(146):521–534, 1979.

[92] K. Strehmel and R. Weiner. Behandlung steifer Anfangswertprobleme gewöhnlicher Differentialgleichungen mit adaptiven Runge-Kutta-Methoden. *Computing*, 29(2):153–165, 1982.

[93] K. Strehmel and R. Weiner. Partitioned adaptive Runge-Kutta methods and their stability. *Numer. Math.*, 45(2):283–300, 1984.

[94] K. Strehmel and R. Weiner. B-convergence results for linearly implicit one step methods. *BIT*, 27:264–281, 1987.

[95] K. Strehmel, R. Weiner, and I. Dannehl. A study of B-convergence of linearly implicit Runge-Kutta methods. *Computing*, 40(3):241–253, 1988.

[96] A. Suslowicz. Application of numerical Lie group integrators to parabolic PDEs. Technical Report 13/01, University of Bergen, 2001.

[97] A. Taflove. *Computational electrodynamics: The finite-difference time-domain model*. Artech House, 1995.

[98] M. Thalhammer. A second-order Magnus type integrator for non-autonomous semilinear parabolic problems. Submitted to IMA J. Numer. Anal., 2004.

[99] L. N. Trefethen. *Spectral methods in matlab*. Soc. Industr. Appl. Math., 2000.

[100] J. van den Eshof and M. Hochbruck. Preconditioning Lanczos approximations to the matrix exponential. Technical report, University of Düsseldorf, 2004. http://www.am.uni-duesseldorf.de/ marlis/.

[101] P. J. van der Houwen. *Construction of integration formulas for initial value problems*. North-Holland Publishing Co., Amsterdam, 1977. North-Holland Series in Applied Mathematics and Mechanics, Vol. 19.

[102] P. J. van der Houwen and J. G. Verwer. *Generalized linear multistep methods. I. Development of algorithms with zero-parasitic roots*. Mathematisch Centrum, Amsterdam, 1974. Mathematisch Centrum, Afdeling Numerieke Wiskunde NW 10/74.

[103] J. G. Verwer. On generalized linear multistep methods with zero-parasitic roots and an adaptive principal root. *Numer. Math.*, 27:143–155, 1976.

[104] J. G. Verwer. S-stability properties for generalized Runge–Kutta methods. *Numer. Math.*, 27:359–370, 1976.

[105] J. G. Verwer and M. van Loon. An evaluation of explicit pseudo-steady-state approximation schemes for stiff ODE systems from chemical kinetics. *J. of Comp. Phys.*, 113:347–352, 1994.

[106] R. Weiner, B. A. Schmitt, and H. Podhaisky. ROWMAP—a ROW-code with Krylov techniques for large stiff ODEs. *Appl. Numer. Math.*, 25(2-3):303–319, 1997.

[107] A. Wolfbrandt. *A study of Rosenbrock processes with respect to order conditions and stiff stability*. PhD thesis, University of Technology Gotenburg, 1977.