NORGES TEKNISK-NATURVITENSKAPELIGE
UNIVERSITET

A review of error analysis for splitting methods and exponential integrators

by

Bård Skaflestad

PREPRINT
NUMERICS NO. 9/2005

NORWEGIAN UNIVERSITY OF
SCIENCE AND TECHNOLOGY
TRONDHEIM, NORWAY

This report has URL
http://www.math.ntnu.no/preprint/numerics/2005/N9-2005.pdf
Address: Department of Mathematical Sciences, Norwegian University of Science and Technology, N-7491 Trondheim, Norway.

A review of error analysis for splitting methods and exponential integrators

Bård Skaflestad

October 17, 2005

We briefly review splitting methods for differential equations and the error analysis of such schemes available in the literature, and present several types of splitting methods. Some of the mathematical tools needed in the analysis are listed for reference. Progressing from splitting methods based on exact flow maps through methods using numerical flow map approximations, we also list some of the splitting methods in common use for time integration of incompressible fluid flow problems. We finally present the class of "exponential integrators" in some detail and give an outline of the concept of stiff order conditions recently introduced by Hochbruck and Ostermann to analyse exponential integrators applied to semi-linear parabolic problems.

1 Introduction

Few numerical techniques for solving differential equations have received more attention than splitting methods. This class of schemes is known under several different names, including fractional step methods. Splitting methods in current form go back to Strang [33] and Marchuk [23], but subsequent developments have proceeded in many different directions, serving a variety of purposes.

Generally, splitting methods assume that the mathematical problem in question can be split into two or more terms, say

$$\dot{u} = X_1(u) + X_2(u), \quad u(0) = u_0. \tag{1}$$

Next one assumes that the flows of each of these two vector fields can be solved—or at least approximated—more easily than the aggregate vector field $X_1 + X_2$. We denote by $u(t) = \operatorname{Exp}(tX)u_0$ the solution at time t of the differential equation $\dot{u} = X(u)$ with initial value $u(0) = u_0$. Thus, in this notation a much used splitting method for the problem (1) is

$$u(h) \approx \operatorname{Exp}(hX_2)\operatorname{Exp}(hX_1)u_0, \tag{2}$$

which composes the separate flows of X_1 and X_2. This celebrated formula is called the Lie–Trotter–Kato (LTK) formula. Using this formula will in general produce an error compared to the exact solution of the original problem (1). By Taylor expansion, the error generally satisfies the relation $\operatorname{Exp}(h(X_1 + X_2))u_0 - \operatorname{Exp}(hX_2)\operatorname{Exp}(hX_1)u_0 = \mathcal{O}(h^2)$. However, under special circumstances, the LTK formula does in fact reproduce the exact solution. Theorem 1.34 of [29] states that this happens if and only if the vector fields X_1 and X_2 commute.

While attractive from a theoretical point of view, the LTK formula and other schemes based on exact flows may not be practically feasible. In particular, the exponential mapping may not be computationally available or too expensive to evaluate exactly. Thus, the flow map Exp is often approximated using some numerical method. Some of the choices studied in the literature are regular ODE-based integration of a single component of the vector field and Krylov subspace approximation of $\mathrm{Exp}(hX)v$ for the important special case of constant linear vector fields X. A feature of numerical approximations to the exponential function is that such approximations usually do not satisfy the composition property experienced by the exact flow. When evaluated exactly, $\mathrm{Exp}((t+s)X) = \mathrm{Exp}(tX)\,\mathrm{Exp}(sX)$ and this does not generally hold whenever Exp is approximated by means of a numerical method. Distinguishing the different approaches, methods based on exact flows are commonly known as "exponential splitting" methods.

Splitting schemes are developed for a multitude of purposes. In partial differential equations, splitting schemes may be the only viable alternative in obtaining a computable numerical solution. As an example we may consider the modelling of unsteady incompressible fluid flow. The governing equations in this case are the Navier–Stokes equations which consists of the linear indefinite Stokes operator, and the non-linear and non-symmetric convection operator. Splitting the equations between the linear and non-linear terms enables explicit treatment of the convection forces while treating the Stokes operator implicitly. Thus, we are left with inverting an expensive linear operator at each viscous time step, but non-linear couplings are eliminated. Examples of such schemes are presented in [22], in which the authors use the framework of integrating factors for decoupling the viscous and convective forces. One of the key advantages of this approach is that it allows taking several convection sub-steps for each viscous time step, thus reducing the computational cost of the viscous terms relative to the convection term.

Additional examples of the necessity of splitting methods may be found in strongly coupled multiphysics problems, such as magneto-hydrodynamics or fluid-structure interaction. Simulating such problems may be too taxing on available computer resources when solved aggregately, but may be tractable if we accept a possible stability time step restriction for the split operator. Another advantage of the operator splitting approach is an inherently modular description of the problem itself. A practical upside of this description is that software components developed separately may be modularly reused in implementing simulation codes for more complex systems.

In the context of ordinary differential equations, however, splitting methods are viewed differently than in the PDE case. McLachlan and Quispel, in their 2002 survey paper on splitting methods [25], demonstrate how splitting and composition methods may be employed in the construction of *geometric* integrators for ordinary differential equations with applications to Hamiltonian, Poisson and volume-preserving systems as well as some other kinds of systems. Geometric integration often involves the conservation or near-conservation of various geometric properties of the continuous system. Such properties include the Hamiltonian function, representing the total energy, of a Hamiltonian system or the group structure of a system evolving on a Lie group.

Having constructed splitting methods for ordinary differential equations, the question naturally arises of how to construct accurate schemes which may be used with non-small step sizes. One approach in this direction is the construction of high-order methods, methods for which the numerical flow map φ_h of (1) satisfies

$$\varphi_h = \mathrm{Exp}(h(X_1 + X_2)) + \mathcal{O}(h^{p+1}),$$

with the order p being as high as possible. A standard technique for obtaining such methods is to compose φ_h from more than the two exponentials of the Lie–Trotter–Kato formula.

As such, a typical non-symmetric composition method often used is

$$\varphi_h = \operatorname{Exp}(a_m h X_1) \operatorname{Exp}(b_m h X_2) \cdots \operatorname{Exp}(a_1 h X_1) \operatorname{Exp}(b_1 h X_2) \operatorname{Exp}(a_0 h X_1) \tag{3}$$

and various approaches have been suggested for determining conditions on the free parameters $a_0, a_1, \ldots, a_m$, and $b_1, \ldots, b_m$. Through the "Yoshida approach" of symmetric composition of symmetric methods, one may easily derive methods of any given *even* order p. These methods, however, may not be optimal in terms of accuracy or computational cost when applied to a specific problem. Using symmetrised formulae, any composition method may be used as a basic building block in the Yoshida framework. Such symmetrised formulae resemble the original Strang splitting

$$\varphi(h) = \operatorname{Exp}(\tfrac{1}{2} h X_1) \operatorname{Exp}(h X_2) \operatorname{Exp}(\tfrac{1}{2} h X_1)$$

though possibly extended to vector fields X split into more than two components.

Another approach to determining conditions on the free parameters comes from the so-called BCH formula. This gives order conditions for s-stage methods recursively in terms of the order conditions for $(s-1)$-stage methods. In contrast Murua and Sanz-Serna in [27] use B-series generalised to rooted infinity-trees to derive explicit order conditions for composition methods. The rooted infinity-trees are trees with an unbounded number of different vertex types and with a distinguished root. We note that the cardinality of the set of such trees grows quickly as more nodes are added, and that the complete set of rooted infinity-trees is unmanageble. However, identifying a subset of the trees which procedurally gives all independent order conditions, the authors' main result is an algebraic *lower* bound on the attainable order of a composition method.

As a final introductory example of a class of splitting methods, we also note that the combination of exact and numerical flows yields hybrid methods known as "exponential integrators". Originally introduced as integrating factor methods by Lawson in 1967, these methods were subsequently disregarded due to prohibitive cost in evaluating the exponential function. Recently, however, exponential integrators based on splitting the vector field into a linear and non-linear part have received renewed interest in light of more inexpensive evaluation procedures for the exponential function and related functions.

In [3] we analysed a general class of explicit exponential integrators for systems of the form

$$\dot{u} = Lu + N(u), \quad u(0) = u_0 \tag{4}$$

in which L is a constant linear operator and N is a non-linear function. We note that both ordinary and partial differential equations may be cast in this form. In particular, L may be a linear differential operator such as the Laplacian operator in a non-linear diffusion problem. The class of integrators analysed is abstractly represented as

$$\begin{aligned} N_r &= N(\operatorname{Exp}(c_r h L) u_0 + \sum_{j=1}^{r-1} a_r^j(hL)\, h N_j), \\ u_1 &= \operatorname{Exp}(hL) u_0 + \sum_{r=1}^{s} b^r(hL)\, h N_r \end{aligned} \tag{5}$$

with c_r being free parameters and a_r^j and b^r being analytic functions satisfying $a_r^j(0) = b^r(0) = 1$.

The rest of this paper will be expanding on the introductory comments already given. Section 2 briefly reviews some mathematical tools facilitating the analysis in the literature

on splitting methods. Section 3 then describes various classes of splitting methods—progressing from composition methods through methods based on exact flows to methods based on numerical flow approximations. Order analysis is presented for some of the schemes in this section. Finally, Section 4 presents exponential integrators in more detail than the above introduction. Moreover, this section also presents the order analysis for exponential integrators in both the classical case of bounded linear operators and the case of unbounded linear operators recently studied by Hochbruck and Ostermann [16].

2 Mathematical tools

This section collects some of the tools required to develop the analysis presented in the literature. We refer in particular to the monographs [13, 29, 31] for theoretical development and additional references.

2.1 Basic definitions from Lie group theory

Most pertinent to the following discussion are the concepts of vector fields, flows, Lie brackets and Lie series. We will give a brief introduction to these constructions. We adapt Olver's notation in [29] and repeat some of the definitions in Sections 1.3 and 1.4 of this text.

Suppose C is a smooth curve on an m-dimensional manifold M. At every point x on C there is a vector $\mathbf{v}|_x$ tangent to the curve itself. The collection of all tangent vectors to all curves on M passing through a given point $x \in M$ is called the *tangent space* to M at x, and is denoted by here T_xM. The tangent space at x is an m-dimensional vector space and, given a suitable set of local coordinates $x = (x^1, \ldots, x^m)$ on M, may be provided with the basis $\{\partial/\partial x^1|_x, \ldots, \partial/\partial x^m|_x\}$.

A *vector field* $\mathbf{v}$ on M assigns a tangent vector $\mathbf{v}|_x \in T_xM$ to each $x \in M$. As such, vector fields generalise derivatives to manifolds. In physics, a typical example of a vector field is the velocity field of a steady fluid flow. That is, at every point $(x, y, z) \in M \subset \mathbf{R}^3$ the vector $\mathbf{v}|_{(x,y,z)}$ is the velocity of fluid particles passing through (x, y, z). From vector fields we may define an *integral curve* as a smooth, parametrised curve $x = \phi(\varepsilon)$ whose tangent vector at any point coincides with the value of $\mathbf{v}$ at the same point:

$$\dot{\phi}(\varepsilon) = \mathbf{v}|_{\phi(\varepsilon)} \tag{6}$$

for all ε. In fluid flow problems, the integral curve thus gives the position at 'time' ε of fluid particles passing through (x, y, z) with velocity $\mathbf{v}|_{(x,y,z)}$.

When the vector field $\mathbf{v}$ is smooth and non-vanishing there exists a unique maximal integral curve, not fully contained in any other integral curve, passing through a given point $x = \phi(0) \in M$. This integral curve is called the *flow* generated by $\mathbf{v}$ and is denoted here by $\mathrm{Exp}(\varepsilon\mathbf{v})\, x$, the same notation also used in the introduction and in the following to denote the exact solution of $\dot{u} = \mathbf{v}(u)$ with initial condtion $u(0) = x$. This is intentional as the construction of integral curves corresponds to solving an autonomous system of differential equations. The defining properties of $\mathrm{Exp}(\varepsilon\mathbf{v})\, x$, detailed in pages 27–28 of [29], mirror those of the traditional exponential function and suggests the above notation.

Underlying the definition of Lie series is the study of how flows act on smooth functions $f : M \to \mathbf{R}$. Following Olver, we investigate how f changes under the flow generated by $\mathbf{v}$. More specifically we study how $f(\mathrm{Exp}(\varepsilon\mathbf{v})x)$ varies as a function of ε. In local coordinates, if the functions $\mathrm{d}x^i/\mathrm{d}\varepsilon = \zeta^i(x), i = 1, \ldots, m$ are smooth, then it follows from (6) and the

basis for T_xM that $\mathbf{v} = \sum_{i=1}^{m} \zeta^i(x)\partial/\partial x^i$. The chain rule then yields

$$\frac{\mathrm{d}}{\mathrm{d}\varepsilon} f(\mathrm{Exp}(\varepsilon\mathbf{v})x) = \sum_{i=1}^{m} \zeta^i(\mathrm{Exp}(\varepsilon\mathbf{v})x) \frac{\partial f}{\partial x^i}(\mathrm{Exp}(\varepsilon\mathbf{v})x) \equiv \mathbf{v}(f)(\mathrm{Exp}(\varepsilon\mathbf{v})x). \tag{7}$$

In particular, at $\varepsilon = 0$, we get

$$\left.\frac{\mathrm{d}}{\mathrm{d}\varepsilon}\right|_{\varepsilon=0} f(\mathrm{Exp}(\varepsilon\mathbf{v})x) = \sum_{i=1}^{m} \zeta^i(x) \frac{\partial f}{\partial x^i}(x) = \mathbf{v}(f)(x)$$

which shows that the vector field $\mathbf{v}$ defines a first order partial differential operator on real-valued functions on M. Now, from repeated differentiation and substitution into the Taylor series we get, assuming convergence of the Taylor series in ε, that

$$f(\mathrm{Exp}(\varepsilon\mathbf{v})x) = \sum_{k=0}^{\infty} \frac{\varepsilon^k}{k!} \mathbf{v}^k(f)(x) \tag{8}$$

in which the powers $\mathbf{v}^k(f)$ are defined recursively as $\mathbf{v}^k(f) = \mathbf{v}(\mathbf{v}^{k-1}(f))$ for all $k > 1$. This defines the *Lie series* for the action of the flow on f. As this definition is applicable to each component of vector-valued functions as well, the Lie series assumes the rôle of the Taylor series when studying functions on manifolds and may be used to construct the Lie series of the flow $\mathrm{Exp}(\varepsilon\mathbf{v})x$ itself. The latter calculation is listed as equation (1.19) of [29].

Lastly in this section we define the *Lie bracket* of two vector fields $\mathbf{v}$ and $\mathbf{w}$. Geometrically, the Lie bracket is the tangent vector at the origin to a specific curve generated from the integral curves of $\mathbf{v}$, $\mathbf{w}$, $-\mathbf{v}$, and $-\mathbf{w}$. The bracket generalises the well-known matrix commutator to vector fields and has a similar algebraic definition.

Algebraically, if $\mathbf{v}$ and $\mathbf{w}$ are vector fields on M their Lie bracket $[\mathbf{v}, \mathbf{w}]$ is the unique vector field satisfying

$$[\mathbf{v}, \mathbf{w}](f) = \mathbf{v}(\mathbf{w}(f)) - \mathbf{w}(\mathbf{v}(f)) \tag{9}$$

for all smooth functions $f : M \to \mathbf{R}$. Proposition 1.32 of [29] states that the Lie bracket is bilinear, skew symmetric, and satisfies the Jacobi identity

$$[\mathbf{u}, [\mathbf{v}, \mathbf{w}]] + [\mathbf{w}, [\mathbf{u}, \mathbf{v}]] + [\mathbf{v}, [\mathbf{w}, \mathbf{u}]] = 0$$

for all vector fields $\mathbf{u}$, $\mathbf{v}$, and $\mathbf{w}$.

The Lie bracket may be used to define a linear operator, ad, on vector fields. In particular, we define $\mathrm{ad}_{\mathbf{v}}(\mathbf{w}) = [\mathbf{v}, \mathbf{w}]$. Moreover, powers of this operator is recursively defined as

$$\mathrm{ad}_{\mathbf{v}}^k(\mathbf{w}) = \begin{cases} \mathbf{w}, & k = 0 \\ \left[\mathbf{v}, \mathrm{ad}_{\mathbf{v}}^{k-1}(\mathbf{w})\right], & k > 0 \end{cases}, \tag{10}$$

for all integral $k \geq 0$. This operator is needed to construct the Baker–Campbell–Hausdorff formula in Section 2.3.

2.2 Adjoint and symmetric methods

For completeness we briefly review the concept of adjoint and symmetric methods. This review closely follows section II.3 of [13]. A numerical method $\varphi(h)$ for the autonomous initial value problem

$$\dot{u} = f(u), \quad u(t_0) = u_0$$

generates the numerical approximation $u_1 = \varphi(h)u_0$ to the exact solution $u(h) = \mathrm{Exp}(hf)u_0$. The *adjoint* method, $\varphi(h)^*$, of $\varphi(h)$ is then implicitly defined by the relation

$$\varphi(-h)u_1 = u_0, \tag{11}$$

that is $\varphi(h)^* = \varphi(-h)^{-1}$. In the case of Runge–Kutta methods, theorem II.8.3 of [14] gives explicit formulae for the coefficients of the adjoint method in terms of the coefficients of the original method.

A numerical method for which $\varphi(h)^* = \varphi(h)$ is called *symmetric* or self-adjoint. Symmetric methods therefore satisfy the relation

$$\varphi(h) \circ \varphi(-h) = I$$

and have error expansions in even powers of h. This property simplifies order conditions considerably. Composing any method with its adjoint method yields a symmetric method of the form

$$\psi(h) = \varphi(h/2) \circ \varphi(h/2)^*.$$

This method may then subsequently be employed as a basic building for constructing more involved schemes by means of composition techniques as demonstrated in Section 3 below. Moreover, the principle of composing methods is applicable if the method is a numerical approximation to $\mathrm{Exp}(hf)$ or even the exact flow map.

2.3 The BCH formula

Proposed initially by J.E. Campbell in 1898 and subsequently proved independently by Baker in 1905 [1] and Hausdorff in 1906, the so-called Baker–Campbell–Hausdorff (BCH) formula is a procedure for constructing a vector field $C(A, B)$ such that

$$\mathrm{Exp}(A)\,\mathrm{Exp}(B) = \mathrm{Exp}\big(C(A, B)\big) \tag{12}$$

when A and B are general vector fields. It is well known that in the case of commuting vector fields, $[A, B] = 0$, equation (12) reduces to $\mathrm{Exp}(A)\,\mathrm{Exp}(B) = \mathrm{Exp}(A + B)$. In the general case of non-commuting vector fields however, this relation does not hold. A detailed derivation in sections 2.14 and 2.15 of Varadarajan's monograph [34] and paraphrased in section III.4 of [13] leads to a differential equation for $C(A, B)$ given by

$$\frac{\mathrm{d}C}{\mathrm{d}t} = A + B + \frac{1}{2}\,\mathrm{ad}_{A-B}\,(C) + \sum_{k\geq 2} \frac{B_k}{k!}\,\mathrm{ad}_C^k\,(A + B), \tag{13}$$

in which B_k are the Bernoulli numbers and the ad operator is defined in (10). The series converges whenever A and B are chosen sufficiently close to the origin. Equation (13) allows computation of the Taylor coefficients of the function $Y(t) = \sum_{k=1}^{\infty} Y_k t^k$ defined by $\mathrm{Exp}(tX_1)\,\mathrm{Exp}(tX_2) = \mathrm{Exp}(Y(t))$ for general vector fields X_1 and X_2.

The first few of these are given in [13] and repeated here for reference

$$\begin{aligned} Y_1 &= X_1 + X_2, \quad & Y_3 &= \tfrac{1}{12}\big([X_1, [X_1, X_2]] + [X_2, [X_2, X_1]]\big), \\ Y_2 &= \tfrac{1}{2}[X_1, X_2], \quad & Y_4 &= \tfrac{1}{24}\big[X_1, [X_2, [X_2, X_1]]\big]. \end{aligned}$$

Unfortunately, the expressions involved soon become very complicated, thus somewhat limiting the practical use of the BCH formula. On the other hand, we note that whenever X_1 and X_2 actually *do* commute, these Taylor coefficients are all zero apart from Y_1. As

such, the BCH formula reduces to the well known relation for commuting vector fields in this case.

Symmetric flow compositions such as $\mathrm{Exp}(\frac{t}{2}X_1)\,\mathrm{Exp}(tX_2)\,\mathrm{Exp}(\frac{t}{2}X_1)$ may be similarly analysed. It is interesting to note that in this case only odd powers of t enter into the Taylor series expansion of $Y(t)$. The first few Taylor coefficients of this series is similarly listed in [13].

3 Classes of splitting schemes

Order analysis for splitting and composition methods produces order conditions for numerical methods of the form (3). Methods based on composing a basic numerical method with itself using different step sizes is analysed as well. Such composition methods employ the general format

$$\psi(h) = \varphi(\alpha_s h) \circ \varphi(\beta_s h)^* \circ \cdots \circ \varphi(\alpha_1 h) \circ \varphi(\beta_1 h)^* \tag{14}$$

and are known as s-stage composition methods. It is assumed that $\varphi(h)$, commonly known as the *basic method*, is a consistent numerical method when applied to an autonomous initial value problem $\dot{u} = X(u)$, $u(0) = u_0$. Order conditions for composition methods (14) constitute a set of algebraic constraints on the free parameters α_i and β_i. This set may be classified according to which order each constraint belong. Determining α_i and β_i such that the constraints are satisfied up to and including order p guarantees that the composition method $\psi(h)$ is of overall order p.

At least four approaches have been proposed to determine order conditions for the coefficients of methods of high order. McLachlan and Quispel [25] summarise these approaches as

- A direct method of Suzuki and Yoshida [35] which gives methods of arbitrary even order.
- Series expansion of the flow map composition by means of the BCH formula. The resulting order conditions describe constraints on an s-stage method in terms of the conditions of an $(s-1)$-stage method. This approach is presented in several places, among which Section III.5 of [13] may be the most accessible.
- Murua and Sanz-Serna's extension of the theory of rooted trees [27], which gives the order conditions explicitly. In complete detail, this extension requires some technical tools and definitions which we do not describe in the following. We will however outline the extension of B-series to rooted infinity-trees in Section 3.1 below.
- A method due to Tsuboi and Suzuki based on time-ordered symmetrised products of non-commuting operators, which also gives the order conditions explicitly.

Two results due to McLachlan in the context of Lie algebras [24] show that there is a link between splitting methods and composition methods. In particular, a splitting method of order p for the special case of integrable splittings may be viewed as a specially construced composition method. More detailed, for split systems of the form (1), the basic Lie–Trotter–Kato method $\varphi(h) = \mathrm{Exp}(hX_1)\,\mathrm{Exp}(hX_2)$ and its adjoint method $\varphi(h)^* = \mathrm{Exp}(hX_2)\,\mathrm{Exp}(hX_1)$ may be used as building blocks in the composition method (14) as

$$\psi(h) = \mathrm{Exp}(a_{s+1}hX_1)\,\mathrm{Exp}(b_s hX_2)\cdots\mathrm{Exp}(b_1 hX_2)\,\mathrm{Exp}(a_1 hX_1)$$

in which $b_i = \alpha_i + \beta_i$ and $a_i = \alpha_{i-1} + \beta_i$. The reciprocal result, that a p-th order splitting method has a corresponding p-th order composition method, at least under some conditions on the vector fields X_1 and X_2, is proved as theorem III.3.17 in [13].

3.1 Composition methods

Murua and Sanz-Serna in 1999 published a rigorous order analysis [27] for composition methods (14) applied to the standard initial value problem $\dot{u} = X(u)$, $u(0) = u_0$. Underlying their analysis is a formal series expansion of the basic method in terms of unknown quantities d_i according to

$$\varphi(h) = I + \sum_{i=1}^{\infty} h^i d_i. \tag{15}$$

As the basic method is assumed to be consistent, we conclude that $d_1 = X$. However, no prior conditions are placed on the vector fields d_i for $i > 1$. Repeated insertion of (15) into itself using different step sizes $(\alpha_1 h, \ldots, \alpha_s h)$ then gives rise to series expansions of the quantities

$$v_k = \varphi(\alpha_k h)\, v_{k-1}, \quad k = 1, \ldots, s$$

for some initial condition v_0. These expansions have similar structure to the standard series expansion of Runge–Kutta methods for ordinary differential equations. However, the resulting series is notably different from the standard expansion in that each elementary differential itself is composed of infinitely many terms rather than just a single function.

In order to analyse this structure, Murua and Sanz-Serna introduce the *infinity trees*, T_∞, which consist of all rooted trees where each vertex is associated to a positive integer without any further restriction. In other words, T_∞ is the set of all rooted trees with an unbounded number of vertex types. These trees, and their associated elementary differentials are defined as (definition III.3.1 of [13])

$$\begin{aligned}
\text{①},\text{②},\text{③},\ldots &= \text{the trees with a single vertex,}\\
\tau = [\tau_1, \ldots, \tau_m]_i &= \text{tree formed by grafting } \tau_1, \ldots, \tau_m \text{ onto a common root } \textcircled{i}\\
F(\textcircled{i})(u) &= d_i\, u\\
F(\tau)(u) &= d_i^{(m)}(F(\tau_1), \ldots, F(\tau_m))(u).
\end{aligned}$$

Extended B-series, known as B_∞-series, may be defined for these trees by the relation

$$B_\infty(a, u) = a(\emptyset)u + \sum_{\tau \in T_\infty} \frac{h^{\|\tau\|}}{\sigma(\tau)} a(\tau) F(\tau)(u) \tag{16}$$

for an arbitrary map $a : T_\infty \cup \emptyset \to \mathbf{R}$. Here, $\|\tau\|$ is the sum of the labels of τ, and $\sigma(\tau)$ denotes the symmetry coefficient of τ.

Using these tools lemma III.3.4 of [13] gives recurrence relations establishing B_∞-series expansions of the intermediate mappings

$$\varphi^{(k-1/2)}(h) = \varphi(\beta_k h)^* \circ \varphi^{(k-1)}(h), \quad \varphi^{(k)}(h) = \varphi(\alpha_k h) \circ \varphi^{(k-1/2)}(h) \tag{17}$$

for $k = 1, \ldots, s$, assuming $\varphi^{(0)}(h) = I$. In particular,

$$\begin{aligned}
\varphi^{(k-1/2)}(h)u = B_\infty(b_k, u), \quad b_k(\tau) = a_{k-1}(\tau) - (-\beta_k)^{i(\tau)} b_k'(\tau)\\
\varphi^{(k)}(h)u = B_\infty(a_k, u), \quad a_k(\tau) = b_k(\tau) + \alpha_k^{i(\tau)} b_k'(\tau)
\end{aligned} \tag{18}$$

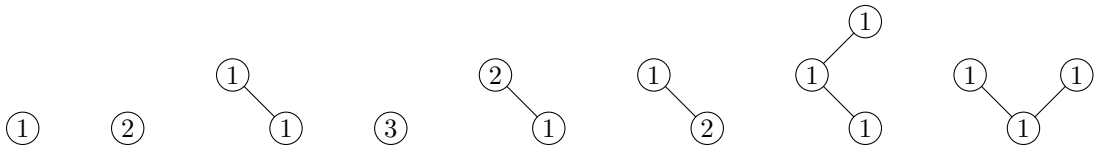

Figure 1: T_∞ trees of orders up to and including 3

with $b'_k(\tau) = b_k(\tau_1) \cdot \ldots \cdot b_k(\tau_m)$ for $\tau = [\tau_1, \ldots, \tau_m]_i$, and $i(\tau)$ denoting the label of the root of τ.

The exact solution to $\dot{u} = X(u)$ can be represented as a B_∞-series, $B_\infty(\mathbf{e}, u_0)$ for which $\mathbf{e}(\tau) = 0$ for all $\tau \in T_\infty$ having at least one label different from 1. This, then, means that the order conditions for composition methods can be extracted from the B_∞-series expansion $B_\infty(a_s, u)$ of the complete composition method by matching the coefficients $a_s(\tau)$ and $\mathbf{e}(\tau)$ up to the desired order.

However, not all order conditions arising from direct application of the Murua–Sanz-Serna analysis are independent. Specifically, some of the order conditions are automatically satisfied whenever other conditions are fulfilled. Examples of this phenomenon occur even for very low order. The conditions for orders up to and including 3 are given in equation (19). We note that starred indices, such as $k*$, present in the conditions modify the last term of their corresponding sum. Specifically, for $\ell = k*$ we use only the term α_ℓ rather than $\alpha_\ell + \beta_\ell$.

$$
\begin{aligned}
\sum_{k=1}^{s}(\alpha_k+\beta_k) &= 1, & \sum_{k=1}^{s}(\alpha_k^2-\beta_k^2) &= 0,\\
\sum_{k=1}^{s}(\alpha_k+\beta_k)\sum_{\ell=1}^{k*}(\alpha_\ell+\beta_\ell) &= \tfrac{1}{2}, & \sum_{k=1}^{s}(\alpha_k^3+\beta_k^3) &= 0,\\
\sum_{k=1}^{s}(\alpha_k^2-\beta_k^2)\sum_{\ell=1}^{k*}(\alpha_\ell+\beta_\ell) &= 0, & \sum_{k=1}^{s}(\alpha_k+\beta_k)\sum_{\ell=1}^{k*}(\alpha_\ell^2-\beta_\ell^2) &= 0,\\
\sum_{k=1}^{s}(\alpha_k+\beta_k)\sum_{\ell=1}^{k*}(\alpha_\ell+\beta_\ell)\sum_{m=1}^{\ell*}(\alpha_m+\beta_m) &= \tfrac{1}{6}, & \sum_{k=1}^{s}(\alpha_k+\beta_k)\Big(\sum_{\ell=1}^{k*}(\alpha_\ell+\beta_\ell)\Big)^2 &= \tfrac{1}{3}.
\end{aligned}
\tag{19}
$$

These conditions are derived by transcribing the structure of the corresponding T_∞ tree of figure 1 and introducing a summation for each vertex in the tree, and translating tree type into powers of the method parameters α_k and β_k. Moreover, even powers of β_k must be accompanied by a negative sign.

However, not all order conditions arising from mechanically applying the above procedure to all rooted inifinty-trees are independent. It is a routine check to verify that

$$
\Big(\sum_{k=1}^{s}(\alpha_k+\beta_k)\Big)^2 = 2\sum_{k=1}^{s}(\alpha_k+\beta_k)\sum_{\ell=1}^{k*}(\alpha_\ell+\beta_\ell) + \sum_{k=1}^{s}(\alpha_k^2-\beta_k^2),
$$

and, consequently, that the order conditions derived from the trees in figure 2 are interdependent. To eliminate such order conditions, the authors construct a subset of T_∞ which contains only those trees carrying independent order conditions. This construction is somewhat technical, and we refer the interested reader to the original paper [27] for detailed description of the process and tools involved. Additional explanation may be found in section III.3 of [13].

Figure 2: First inter-dependent T_∞ trees

An immediate consequence of the order condition $\sum_{k=1}^{s}(\alpha_k^3 + \beta_k^3) = 0$ which must be satisfied to attain an order 3 method is that some of the coefficients α_k or β_k must be negative. This fact has important implications for the possibility of constructing higher order schemes for partial differential equations. Such equations often evolve only on a semigroup [31] and hence cannot be integrated in the reverse direction without adversely affecting the stability of the numerical solution. Blanes and Casas, in an as yet unpublished work [5], prove, in a slightly different fashion, the non-existence of purely positive method parameters for methods of orders $p \geq 3$. The authors also study composition methods of *effective* order $p \geq 3$. The notion of effective order concerns order behaviour of integrators of the form

$$\hat{\psi}(h) = \pi(h) \circ \psi(h) \circ \pi(h)^{-1}$$

in which $\pi(h)$ is known as a *post-processor* method which is only evaluated for the sake of outputting data. A numerical method is of effective order p if $\hat{\psi}(h)u_0 = \mathrm{Exp}(hX)u_0 + \mathcal{O}(h^{p+1})$. The map $\pi(h)$ is usually taken as a flow map close to the identity $\pi(h) = I + \mathcal{O}(h)$. Effective order is less restrictive than 'regular' order as a method of order p will exhibit effective order of at least p, while the converse is not true in general.

On the other hand, the paper constructs an order $p = 4$ pure positive coefficient splitting method for the second order autonomous differential equation $\ddot{y} = g(y)$ by incorporating the flow of an iterated commutator vector field into the integrator. Further research into processed methods and their effective orders is presented in recent papers by Blanes, Casas and Murua [7, 6].

3.2 Methods based on exact flows

McLachlan and Quispel in [25] trace the history of splitting methods to the product formula

$$\lim_{n\to\infty} \left(\mathrm{Exp}(tX_1/n)\,\mathrm{Exp}(tX_2/n) \right)^n = \mathrm{Exp}(t(X_1 + X_2)), \tag{20}$$

presented in Trotter's 1959 paper on semi-group operators. The formula holds under certain conditions on X_1 and X_2 and admissible values of the parameter t. Schemes based on exact flows exploit this relationship in its simplest form in the LTK formula (2), but more advanced alternatives have been developed, notably the more general scheme (3).

Several important physical problems exist for which the exact flow map is readily availble. Hamiltonian systems

$$\dot{q} = \partial H/\partial p, \qquad \dot{p} = -\partial H/\partial q$$

occur for instance in problems involving the dynamics of multiple rigid bodies, and can often be split into a sum of simpler Hamiltonian systems for which the flow map is both known and easily computable. Examples of such problems may be found in pages 363–368 of [25]. An integrator may then be constructed by composing the flows of the individual, integrable parts. Such integrators may also possess attractive geometric properties, e.g. preservation or near-preservation of the system's total energy. We refer the reader to the above mentioned survey paper for a much expanded treatment of this theory and focus in the following on the error analysis of a few exact flow map integrators.

3.2.1 Local error in stiff/non-stiff splitting

In their recent paper [20] Kozlov, Kværnø and Owren study the behaviour of the local error of several splitting methods applied to problems of the form (1). The vector field X_2 is assumed to be stiff, typically in terms of a small parameter $\varepsilon > 0$, such as $X_2(u) = \tilde{X}_2(u)/\varepsilon$. A very popular model problem in this form, and the problem used in [20], is the Van der Pol equation

$$x'' + \tfrac{1}{\varepsilon}(x^2 - 1)x' + x = 0, \quad x(0) = x_0, \quad x'(0) = \dot{x}_0,$$

which, rewritten as a first order system, becomes

$$\begin{bmatrix} u_1 \\ u_2 \end{bmatrix}' = \begin{bmatrix} u_2 \\ -u_1 \end{bmatrix} + \frac{1}{\varepsilon}\begin{bmatrix} 0 \\ (1-u_1^2)u_2 \end{bmatrix} = X_1(u) + \tfrac{1}{\varepsilon}\tilde{X}_2(u). \tag{21}$$

Here, the vector field X_1 is a rotation in the u_1u_2-plane and $X_2 = \tilde{X}_2/\varepsilon$ is stiff near the initial point for small values of ε.

The authors consider the schemes

$$\begin{aligned} u_1 &= \operatorname{Exp}(hX_1)\operatorname{Exp}(hX_2)\,u_0, \quad u_1 = \operatorname{Exp}(\tfrac{h}{2}X_1)\operatorname{Exp}(hX_2)\operatorname{Exp}(\tfrac{h}{2}X_1)\,u_0 \\ u_1 &= \operatorname{Exp}(hX_2)\operatorname{Exp}(hX_1)\,u_0, \quad u_1 = \operatorname{Exp}(\tfrac{h}{2}X_2)\operatorname{Exp}(hX_1)\operatorname{Exp}(\tfrac{h}{2}X_2)\,u_0 \end{aligned} \tag{22}$$

and analyse their respective local error from the point of view of both formal Lie series computations and singular perturbation analysis. Of particular interest are step sizes in the region $\varepsilon \lessapprox h \lessapprox \sqrt{\varepsilon}$. Numerical experiments show that the local error for schemes following the flow of the X_2 vector field as their final substep remain constant in this region. In other words, these schemes reduce to order zero. We do remark, however, that this does not necessarily imply an inherent disadvantage of the schemes, but rather relates to properties of the specific problem being solved. On the other hand, the existence of an order zero region implies that one should be careful when using variable step methods employing traditional step size controllers based on local error estimates.

The Lie series analysis is further substantiated in Section 4 of [20] which applies singular perturbation theory to the local error. The singular perturbation approach assumes u_1 and u_2 are smoothly varying functions perturbed by fast transients. Expanding the smooth parts in formal series of the parameter ε and collecting terms of equal power of this parameter, a sequence of differential-algebraic equations may be formulated. Analysing these systems reveal that the schemes concluding the step with the flow of X_2 will tend to a manifold $\mathcal{O}(\varepsilon)$ away from the correct manifold of $X_1 + X_2$. This translates to an $\mathcal{O}(\varepsilon)$ error for these schemes while a similar analysis shows that schemes ending with the flow of X_1 will exhibit an error of $\mathcal{O}(h)$.

3.2.2 Commutator bounds for Strang splitting

Restricting their attention to the linear evolution problem

$$\dot{u} = (X_1 + X_2)\,u, \quad u(0) = u_0, \tag{23}$$

Jahnke and Lubich in [17] develop error analysis for Strang splitting scheme

$$u_1 = S_h(X_1, X_2)\,u_0 = \operatorname{Exp}(\tfrac{h}{2}X_2)\operatorname{Exp}(hX_1)\operatorname{Exp}(\tfrac{h}{2}X_2)\,u_0. \tag{24}$$

This paper is interesting because the analysis is developed purely in terms of commutator bounds, rather than explict use of specific properties of the operators X_1 and X_2 themselves.

We may assume, without loss of generality, that the fractional powers $(-X_1)^\gamma$ are well defined for all $\gamma \geq 0$. Then, the commutator bounds in question assert the existence of constants c_1 and c_2 as well as non-negative numbers α and β such that

$$\|[X_1, X_2]\, v\| \leq c_1 \|(-X_1)^\alpha v\|, \tag{25}$$

$$\|[X_1, [X_1, X_2]]\, v\| \leq c_2 \|(-X_1)^\beta v\| \tag{26}$$

hold for all functions v in the domain of $[X_1, X_2]$ and $[X_1, [X_1, X_2]]$ respectively. Commutator terms of the form (25) and (26) occur in the expansion of the local error of the Strang splitting scheme when applied to (23). This error expansion is facilitated through repeated application the variation of constants formula representation of the exact solution and subsequently writing the local error in Peano form.

We illustrate the validity of the approach by recounting the example from Section 3 of [17]. Here, the authors consider a Cauchy problem for the linear Schrödinger equation

$$\mathrm{i}\frac{\partial u}{\partial t} = -\Delta u + Vu, \quad u(0) = u_0. \tag{27}$$

Assuming V is sufficiently differentiable and defining $-X_1 = \Delta$ and $X_2 = V$, this is a problem for which the bounds (25) and (26) hold with $\alpha = \frac{1}{2}$ and $\beta = 1$ respectively.

The general error analysis for (24) applied to (23) is settled in two theorems which, through the above assumptions, establish the local error bounds

$$\left\|S_h(X_1, X_2)\, v - \mathrm{Exp}(h(X_1 + X_2))\, v\right\| \leq C_1 h^2 \|(-X_1)^\alpha v\|$$
$$\left\|S_h(X_1, X_2)\, v - \mathrm{Exp}(h(X_1 + X_2))\, v\right\| \leq C_2 h^3 \|(-X_1)^\beta v\|$$

in which C_1 depends only on c_1 and $\|X_2\|$ and C_2 depends only on c_1, c_2, and $\|X_2\|$. The first bound is valid if (25) is satisfied while the second bound addtionally requires (26). First and second order global error bounds then follow through standard means. We refer the reader to [17] for the actual error bounds, but note that the bounds' dependence upon the values of u vary according to whether X_1 generates an analytic semigroup or merely a strongly continuous semigroup. In the former case the bounds involve only the initial value u_0 while the latter case involves u at all times.

Finally, the authors demonstrate both theoretically and numerically that the error bounds remain valid when considering spatially discretised problems as well. Continuing the treatment of the linear Schrödinger equation (27) Jahnke and Lubich discretise the problem in space by means of spectral collocation. Representing the numerical solution as a trigonometric polynomial $U(x,t) = \sum_{k=-N}^{N-1} \mathrm{e}^{\mathrm{i}kx}\, \hat{u}_k(t)$, this technique leads to the linear ODE system

$$\mathrm{i}\hat{U}' = -D^2\hat{U} + W\hat{U}, \quad t \geq 0$$

in which D^2 is the Fourier space discrete Laplacian and W is the Fourier space representation of the potential function V. In this case Jahnke and Lubich prove that for sufficiently smooth potential functions there exist constants c_1 and c_2 such that

$$\left\|[-D^2 + I, W]\, v\right\| \leq c_1 \left\|(-D^2 + I)^{1/2}\, v\right\|$$
$$\left\|[-D^2 + I, [-D^2 + I, W]]\, v\right\| \leq c_2 \left\|(-D^2 + I)\, v\right\|$$

for all $v \in \mathbf{R}^{2N}$ independently of the spectral resolution N. We thus note that even though $-D^2$ is unbounded in terms of N, the commutators remain well behaved and, moreover, that the global errors, in agreement with the general analysis presented in [17], are bounded by

$$\left\|U^n - U(\cdot, nh)\right\|_{L^2} \leq C_1 h \left\|U^0\right\|_{H^1}, \quad \left\|U^n - U(\cdot, nh)\right\|_{L^2} \leq C_2 h^2 \left\|U^0\right\|_{H^2}.$$

Note in particular that only the norms of the initial conditions enters into these expressions.

3.3 Methods based on numerical flow approximations

Numerical flow approximations have traditionally been the only viable approach to constructing splitting based numerical solutions to partial differential equations. A number of these traditional schemes are summarised in section 5.7 of [32]. The so-called Yanenko splitting scheme

$$\frac{u_{1/2} - u_0}{h} = X_1 u_{1/2}, \quad \frac{u_1 - u_{1/2}}{h} = X_2 u_1 \tag{28}$$

is unconditionally stable and first order accurate with respect to the time step h when applied to the linear problem

$$\dot{u} = X_1 u + X_2 u$$

assuming X_1 and X_2 are both negative, or at least non-positive, definite matrices. Such problems arise in the spatial discretisation of linear parabolic partial differential equations, for instance using finite element methods. Being implicit, two linear systems must be resolved at each time step when computing u_1. However, if X_1 and X_2 are discretisations of elliptic spatial operators, the systems become diagonally dominant for which efficient linear system solvers exist. Eliminating the intermediate quantity $u_{1/2}$ from (28), we observe that

$$u_1 = (\tfrac{1}{h} I - X_2)^{-1} (\tfrac{1}{h} I - X_1)^{-1} u_0$$

which is simply the LTK formula (2) when using the backward Euler scheme for approximating the flow of each constituent vector field, X_1 and X_2.

Improving the Yanenko scheme another classic splitting method, known as the Peaceman–Rachford scheme, is usually presented as a two-stage method alternately solving X_1 and X_2 implicitly as

$$\frac{u_{1/2} - u_0}{h} = X_1 u_{1/2} + X_2 u_0, \quad \frac{u_1 - u_{1/2}}{h} = X_1 u_{1/2} + X_2 u_1. \tag{29}$$

Eliminating the intermediate quantity $u_{1/2}$, the method can however be rewritten as

$$u_1 = (\tfrac{1}{h} I - X_2)^{-1} (\tfrac{1}{h} I + X_1) (\tfrac{1}{h} I - X_1)^{-1} (\tfrac{1}{h} I + X_2) u_0$$

and, accordingly, this method is the symmetric composition of the *symplectic* Euler method and its adjoint method applied to the partitioned system

$$\dot{v}_1 = X_1(v_1 + v_2), \quad \dot{v}_2 = X_2(v_1 + v_2)$$

if the function u is additively split as $u = v_1 + v_2$. The symplectic Euler method treats one part of the partitioned system by the forward Euler method and the other by the backward Euler method. Its adjoint method switches the rôle of which parts are treated explicitly and implicitly. Being a symmetric composition of two first order schemes, the Peaceman–Rachford scheme is second order accurate with respect to h.

Finally, the Strang splitting method

$$\varphi_{S,h} = \varphi_1(h/2) \circ \varphi_2(h) \circ \varphi_1(h/2) \tag{30}$$

in which $\varphi_k(h)$ denotes a numerical approximation to $\mathrm{Exp}(hX_k)$ is arguably the most well-known of the early splitting methods. The method illustrates the idea of constructing integrators by composing integrators for simpler flows. A prime advantage of this method is its attainable symmetry when composed of symmetric methods.

3.4 Krylov subspace exponential approximations

Following the detailed exposition of [15], the main idea supporting the approximation of matrix exponentials by means of Krylov subspace techniques is the Arnoldi decomposition

$$XV_m = V_m H_m + h_{m+1,m} v_{m+1} e_m^T$$

in which X is a matrix, V_m is a matricial representation of an orthonormal basis of the Krylov subspace $K_m(X, v) = \operatorname{span}\{v, Xv, \ldots, X^{m-1}v\}$ for some initial vector v, and H_m is a Hessenberg matrix of dimension m. Furthermore, the vector e_j is the regular j'th unit vector of $\mathbf{R}^m$. Then, for a suitably chosen contour $\Gamma \subset \mathbf{C}$ encapsulating the "numerical range" of the matrix X, any function f analytic in a neighbourhood of the numerical range of X admits the relation

$$f(X)v = \frac{1}{2\pi i} \int_\Gamma f(\lambda) \, (\lambda I - X)^{-1} v \, \mathrm{d}\lambda. \tag{31}$$

The Arnoldi process is usually employed in approximating $(\lambda I - X)^{-1}v$. In particular we have $(\lambda I - X)^{-1}v \approx V_m(\lambda I - H_m)^{-1}e_1$ and inserting this into (31) we get

$$f(X)v \approx \frac{1}{2\pi i} \int_\Gamma f(\lambda) \, V_m(\lambda I - H_m)^{-1} e_1 \, \mathrm{d}\lambda = V_m f(H_m) e_1.$$

We have thus reduced the original problem to that of computing the expression $f(H_m)e_1$, a task much more tractable than $f(X)v$ whenever m is much less than the dimension of v. Diagonalising H_m may be fully feasible, thus yielding a computable expression for $f(H_m)$.

Unfortunately, in practice the Krylov subspace dimension m must still be quite large unless the matrix is e.g. Hermitian negative definite with a limited spectrum. In other words, the convergence rate of these methods though super-linear in many cases, may not be fully sufficient in the general case. The authors suggested using Lanczos type oblique projection techniques and bi-orthogonal sequences to remedy this problem, although this means abandoning the orthogonality of the basis V_m. In the recent paper [11], a method of preconditioning the Lanczos approximations has been developed, giving excellent convergence rates for matrices arising from spatial discretisation of some elliptic operators found in common partial differential equations. However, the need for preconditioning coupled to the difficulty of constructing good preconditioners shows that there is still work to do. While general-purpose black-box integrators for all problems may not be feasible, or indeed not desirable, automated procedures for finding sufficient preconditioners will benefit the Krylov subspace methodology. Other ways of computing the exponential function, at least for constant linear vector fields, are discussed Moler and van Loan in [26].

3.5 Splitting methods in incompressible fluid flow modelling

Incompressible fluid flow is usually modelled by the unsteady incompressible Navier–Stokes equations

$$\begin{gathered} \frac{\partial u}{\partial t} + (u \cdot \nabla)u + \nabla p = \tfrac{1}{Re}\Delta u + f \\ \operatorname{div} u = 0 \end{gathered} \tag{32}$$

with u denoting the fluid velocity field and p the thermodynamic pressure. External body forces are accounted for by the source term f. The Reynolds number Re is a dimensionless number measuring the effects of convection relative to diffusive forces present in the physical problem. The fluid's interaction with the outside world is incorporated in additional

boundary condtions. Such conditions typically specify the fluid's velocity or contact shear forces at the boundary of the physical domain. Additionally, an initial condition must be specified. Discretising this system in space by some method, e.g. finite elements or spectral elements, we arrive at a system of non-linear ordinary differential equations

$$\begin{aligned} M\frac{\mathrm{d}u}{\mathrm{d}t} + C(u)u + D^T p &= -Au + F(t) \\ Du &= 0 \end{aligned} \tag{33}$$

in which M is known as the *mass matrix*, $C(u)$ is the non-linear discrete convection operator, and $-A$ is the discrete diffusion operator. Furthermore, D is the discrete divergence operator, D^T is the discrete pressure gradient, and $F(t)$ is a spatially discretised source term associated with the body forces f of (32).

A challenging aspect of both problems (32) and (33) is that the pressure variable p is not dynamically determined by the equations themselves. This is in contrast to *compressible* fluid flow in which equations of state uniquely determine the pressure in terms of the velocity field and, possibly, the temperature distribution throughout the domain. This fact is reflected in the construction of numerical methods for simulating fluid flows, and the usual approach is to view p as a Lagrange variable associated with the incompressibility constraint $\operatorname{div} u = 0$. As such, the pressure is determined so as to enforce divergence free velocity fields at all time steps.

Splitting methods for (32) orignated with Chorin's projection method in 1967. A single step of this method is divided into two substeps. The first substep splits the convection and diffusion operators into one-dimensional single coordinate components and, by treating the convection operator explicitly, resolves the resulting linear systems one coordinate component at a time. This produces a velocity field which only weakly satisfies the Navier–Stokes equations. The second substep recovers the final velocity field by projecting this velocity field onto divergence free vector fields as a post-processing step. This method implicitly assumes that the velocity field is divergence free at all times, thus eliminating the pressure variable from the equation. Consequently, the pressure values cannot be recovered directly from the method.

In particular, for two-dimensional fluid flows, Chorin's method uses the splitting

$$Au + C(u)u = (A_1 + A_2)u + (C_1(u) + C_2(u))u$$

with A_i and C_i representing, respectively, diffusive and convective contributions in direction $i = 1, 2$. The resulting algorithm is

1a. Solve
$$M\frac{u_{1/3} - u_0}{h} + \tfrac{1}{Re}A_1 u_{1/3} + C_1(u_0)u_{1/3} = F_1$$
with respect to $u_{1/3}$.

1b. Solve
$$M\frac{u_{2/3} - u_{1/3}}{h} + \tfrac{1}{Re}A_2 u_{2/3} + C_2(u_{1/3})u_{2/3} = F_2$$
with respect to $u_{2/3}$.

2. Project $u_{2/3}$ onto divergence free vector fields to recover u_1.

The source terms F_1 and F_2 are temporally averaged parts of the body force $F(t)$. We note that the exact representations of A_i and C_i depend upon the chosen spatial discretisation

and formulation of the original problem (33). In particular, it is common to choose the convective contributions C_i to be single coordinate components of a *symmetrised* convection operator as this leads to symmetric linear systems when computing the intermediate velocities $u_{1/3}$ and $u_{2/3}$. Another numerical method for modelling incompressible fluid flow, based on dimensional splitting of the diffusive operator to simplify the linear algebra problems and explicit treatment of the convection operator, was analysed by Kim and Moin in [19].

Subsequent development has produced a splitting method for the Navier–Stokes equations which has been much used and which guarantees divergence free velocity fields. This method decomposes the physical operators into convective and diffusive sub-problems. A basic step of this method consists of a convective sub-step followed by a pressure projection step to enforce the incompressibility contstraint. Finally a linear system is resolved to balance the viscous forces. Symbolically, the algorithm is described by the following sequence

$$\begin{aligned} u_{1/3} &= \varphi_{M^{-1}C(u)}(h)u_0 \\ (DMD^T)\,p_1 &= \tfrac{1}{h}DMu_{1/3} \\ u_{2/3} &= u_{1/3} - hMD^Tp_1 \\ u_1 &= \varphi_{(\frac{1}{h}M+\frac{1}{Re}A)^{-1}}(h)\big(Mu_{2/3} + b_1(t)\big) \end{aligned}$$

in which $b_1(t)$ is the source term $F(t)$ and, possibly, additional terms arising from using linear multistep methods for evaluating the flow of $(\frac{1}{h}M+\frac{1}{Re}A)^{-1}$. Linear multistep methods have traditionally been the common choice for computing $u_{1/3}$ and u_1 due to only a single linear diffusive system at each basic step of the global algorithm. Originally developed from the point of view of temporal discretisation prior to spatial discretisation, the pressure evaluation step amounts to solving a spatial Poisson problem for which efficient solvers exist. However, this approach is adversely affeceted by a need to supply boundary conditions for the pressure field. Such boundary conditions are artificial and have been the subject of much study. Early implementations used non-homogeneous Neumann type boundary conditions derived from the normal component of $u_{1/3} - u_0$, but this approach in some cases introduces large splitting errors which degrade the performance of the method. Karniadakis and co-workers in [18] derived more general boundary conditions for the Poisson pressure problem and through several numerical tests showed that the resulting numerical scheme was second order accurate with respect to h.

Advantages of physical decomposition of the Navier–Stokes equations into their convective and diffusive constituents led Maday and co-workers [22] to using integrating factors for the convective forces. Focusing on the action of the integrating factors rather than explicit formation of the exponential matrix, this framework is a general procedure for generating splitting methods for problems of the form (1). The underlying idea of the "operator integrating-factor splitting (OIFS) methods", is the introduction of the integrating factor $\mathrm{Exp}((t^*-t)X_1)$ with X_1 defined in (1) and $t^* \geq t$ a fixed parameter. Then

$$\frac{\mathrm{d}}{\mathrm{d}t}\big(\mathrm{Exp}((t^*-t)X_1)u\big) = \mathrm{Exp}((t^*-t)X_1)X_2(u) \tag{34}$$

Splitting schemes for (1) are generated through various discretisations of (34). Generating the flow $\mathrm{Exp}((t^*-t)X_1)u$ is typically accomplished by solving

$$\frac{\mathrm{d}v}{\mathrm{d}s} = X_1(v), \quad 0 < s < t^* - t \tag{35}$$

using $v(0) = u(t)$ as an initial value. Discretising problems (34) and (35) using numerical schemes $\varphi_2(h)$ and $\varphi_1(h)$ respectively, the complete scheme for (1) is denoted by

$\varphi_2(h)/\varphi_1(h)$. In the context of the incompressible Navier–Stokes equations, $\varphi_2(h)$ is commonly chosen as a BDF scheme of order $k \geq 1$ while φ_1 is some one-step Runge–Kutta method, usually explicit. Choosing BDF schemes for φ_2 makes the choice of t^* simpler. Using $t^* = t + h$ reduces $\mathrm{Exp}((t^* - t)X_1)$ to the identity in this case. Consequently, the right hand side of (34) becomes $X_2(u)$. The original paper [22] specifically studied the "BDF3/RK4" scheme in this context.

An immediate consequence of splitting the vector field is that φ_1 and φ_2 need not use the same step sizes. This can be used to good effect when solving incompressible fluid flow problems, as numerical schemes and step sizes can be tuned to a specific sub-problem while temporarily disregarding the coupling effects. Schemes derived from the OIFS framework enable treating the diffusive contributions implicitly leading to less frequent inversions of the indefinite Stokes operator, whilst the convection forces can be treated explicitly to remove the need for solving non-linear systems of algebraic equations. Furthermore, the incompressibility constraint can be naturally incorporated into the overall scheme to ensure that the output velocity field is divergence free. A drawback to the OIFS approach, however, is that using step sizes for the convective sub-problems and diffusive outer problems that are too disparate may lead to unstable computations due to steepening boundary layers in the solution. This steepening effect may occur because the splitting does not necessarily balance the convective and diffusive forces at all times, and is observed in actual simulations of flows exhibiting narrow boundary layers.

Applied to the spatially discretised Navier–Stokes equations (33), the OIFS methods become

$$\begin{bmatrix} \frac{\alpha_0}{h}M + A & D^T \\ D & 0 \end{bmatrix} \begin{bmatrix} u^{n+1} \\ p^{n+1} \end{bmatrix} = \begin{bmatrix} M(f^{n+1} - \frac{1}{h}\sum_{s=1}^{k} \alpha_s \tilde{u}^{n+1-s}) \\ 0 \end{bmatrix} \tag{36}$$

if the outer, diffusive Stokes problem is discretised using a BDF scheme of order k. In the right hand side of (36), we denote by $\tilde{u}^{n+1-s}$ the quantities $\mathrm{Exp}((t+h-sh)(-C))u^{n+1-s}$.

Equation (36) is an algebraic saddle-point problem which must be resolved at each time step. A Uzawa type decoupling of the global discrete operator using the pressure variable for enforcing divergence free velocity fields is possible, but the resulting algorithm is normally too expensive in terms of computer resources. However, accepting an additional algebraic splitting error, equation (36) may be resolved at the expense of one scalar and strongly diagonally dominant Helmholtz problem for each velocity component and one system solve involving the consistent Poisson (DMD^T) operator at each time step.

This algorithm involves the following three stages at each time step

1. Solve
$$(\frac{\alpha_0}{h}M + A)u_i^* = (F^{n+1} - \tfrac{1}{h}M\sum_{s=1}^{k} \alpha_s \tilde{u}^{n+1-s})_i - D_i^T p^*$$
for each velocity component $i = 1, \ldots, d$. The pressure p^* is an extrapolated estimate of the pressure at the next time step. This demands caution in the case of high-order outer stepping schemes.

2. Solve
$$(DMD^T)\,\delta p^n = \tfrac{\alpha_0}{h}\,Du^*$$
obtaining the pressure update $\delta p^n = p^{n+1} - p^*$.

3. Update the velocity and pressure variables
$$\begin{aligned} p^{n+1} &= p^* + \delta p^n \\ u^{n+1} &= u^* - \tfrac{h}{\alpha_0}M^{-1}\,D^T\delta p^*, \end{aligned}$$

the latter system being trivial as the mass matrix is diagonal.

The non-vanishing algebraic splitting error present in this algorithm is explicitly given by $A(u^{n+1} - u^*)$ at each time step.

4 Exponential integrators

4.1 Order conditions for exponential integrators

Connecting splitting methods based on exact flows for each vector field component X_k and methods based on numerical flow approximations for all vector field components, are methods which employ exact flows for some components and flow map approximations for the remaining vector field components. A particular class of such methods is useful if the additional structure of a linear and a non-linear term can be imposed on the prototypical vector field splitting (1). We will in the following assume that X_1 is a constant, linear vector field. This vector field may either be a matrix in the case of ordinary differential equations, or a constant linear differential operator in the case of partial differential equation. Moreover, as previously indicated in equation (5), we will consider explicit schemes of the form

$$k_r = X_2(\mathrm{Exp}(c_r h X_1)u_0 + \sum_{j=1}^{r-1} a_r^j(hX_1)\, hk_j), \quad r = 1, \ldots, s$$

$$u_1 = \mathrm{Exp}(hX_1)u_0 + \sum_{r=1}^{s} b^r(hX_1)\, hk_r.$$

This format is not fully general, but nevertheless covers all of the classic exponential integrators. We note, however, that generalisations to schemes based on underlying general linear methods have recently been derived in [30]. Implementation of such schemes are available in EXPINT MATLAB package described in the technical report [4].

Early exponential integrators were used by Certaine [9] for solving ODEs with large time constants. These integrators were all from the class now known as exponential time differencing (ETD) schemes. This class may be derived by rewriting the original problem using the "variation of constants formula"

$$u(t_0 + h) = \mathrm{Exp}(hX_1)u(t_0) + \mathrm{Exp}(hX_1)\int_0^h \mathrm{Exp}(-\tau X_1)X_2(u(\tau))\,\mathrm{d}\tau \tag{37}$$

and subsequently approximating the integral term in some way. Integrating an interpolating polynomial representation of X_2 produces multistep ETD schemes. This class was also analysed by Nørsett in [28] as a means of producing high order A-stable explicit linear multistep methods.

The Nørsett methods may be summarised as

$$u_{n+1} = \mathrm{Exp}(hX_1)u_n + h\sum_{j=0}^{k-1} b_j(hX_1)\, X_2(u_{n-j}) \tag{38}$$

in which n denotes the time level, $t_n = t_0 + nh$, and the coefficient functions are given by

$$b_j(z) = (-1)^j \sum_{i=j}^{k} \binom{k}{i} S_i(z), \quad S_i(z) = -\frac{1}{z}\sum_{m=1}^{i} \left(\tfrac{1}{k} S_{i-m}(z)\right).$$

We note that $S_0(z) = -(\mathrm{Exp}(z) - 1)/z$. The explicit coefficient function formulae arise from the well known representation of the interpolating polynomial in terms of backwards differences. In his seminal paper [28] Nørsett proved that (38) are, in fact, A-stable and, moreover, that the methods' truncation error behaves as $\mathcal{O}(h^k)$. Finally, as $X_1 \to 0$, we recover the underlying explicit linear multistep scheme. We remark that the Nørsett methods employ the variation of constants formula over a single time step of size h.

In contrast, another class of multistep based exponential integrators recently investigated by Calvo and Palencia in [8], uses (37) across a k-step time interval $[t_n, t_n + kh]$ and are thus derived by representing the exact solution as

$$u(t_n + kh) = \mathrm{Exp}(khX_1)\, u(t_n) + h \int_0^k \mathrm{Exp}\big((k-\tau)hX_1\big) X_2(u(t_n + \tau h))\, \mathrm{d}\sigma$$

for all $n \geq 0$. Using the data $\{(t_j, X_2(u_j))\}_{j=n}^{n+k-1}$ to define an interpolating polynomial $I_{n,k}(t)$ and substituting this into the integral, these schemes may be written in an "unevaluated" form as

$$u_{n+k} = \mathrm{Exp}(khX_1)\, u_n + h \int_0^k \mathrm{Exp}\big((k-\tau)hX_1\big)\, I_{n,k-1}(\tau h)\, \mathrm{d}\tau. \tag{39}$$

Then, choosing an explicit representation of the interpolating polynomial in terms of ordinates and evaluating the required integrals, the schemes may also be written as

$$u_{n+k} = \mathrm{Exp}(khX_1)\, u_n + h \sum_{j=0}^{k-1} b_j(hX_1)\, X_2(u_{n+j})$$

in which the coefficient functions $b_j(hX_1)$, given by

$$b_j(z) = \int_0^k \mathrm{Exp}((k-\tau)z) \prod_{\substack{\ell=0 \\ \ell \neq j}}^{k-1} \frac{\tau - t_\ell}{t_j - t_\ell}\, \mathrm{d}\tau,$$

need be evaluated only once unless the step size h is changed. We note, however, that Calvo and Palencia cite implementational and analytical reasons for preferring the forward difference representation of the interpolating polynomial $I_{n,k-1}(t)$. In this case, the schemes are given by

$$u_{n+k} = \mathrm{Exp}(khX_1)\, u_n + h \sum_{j=0}^{k-1} \gamma_j(hX_1)\, \Delta^j X_2(u_n), \quad \gamma_j(z) = \int_0^k \mathrm{Exp}((k-\tau)z) \binom{\tau}{j} \mathrm{d}\tau.$$

Irrespective of the actual representation of the interpolating polynomial, the main distinguishing feature of the Calvo–Palencia schemes compared to the Nørsett modified Adams–Bashforth schemes is the fact that u_n is exponentially pushed k steps forward in the former and only a single step in the latter. When implementing the Calvo–Palencia schemes, this increased delay either doubles the scheme's memory requirements or forces additional evaluations of X_2.

Asserting a number of technical conditions on the regularity of X_2 and the domain of X_1, mainly to guarantee existence and uniqueness of the solution, Calvo and Palencia study the behaviour of (39) with respect to order of convergence for parabolic problems. Their main result is that when solving the problem to final time T,

$$\|u(t_n) - u_n\|_\alpha \leq K \cdot h^k \cdot \|g^{(k)}\|_\infty, \quad 0 \leq n \leq T/h. \tag{40}$$

Here, $g(t) = X_2(u(t))$, and $\|\cdot\|_\alpha$ is a problem dependent norm involving fractional powers of $X_1 + \nu I$ for some ν guaranteeing positivty of $X_1 + \nu I$. In other words, the Calvo–Palencia schemes attain correct order even in the case of unbounded linear operators X_1. The constant K in (40) is independent of h and g but may otherwise depend on the characteristics of the problem itself.

Defining the quantities $U_n = (u_n, \ldots, u_{n+k-1})^T$, and $U(t_n) = (u(t_n), \ldots, u(t_{n+k-1})^T$, the multistep method (39) is rewritten as a one step method in the proof of (40). The resulting one step method is

$$U_{n+1} = A(hX_1)U_n + B(hX_1)\, X_2(U_n)$$

in which

$$A(z) = \begin{pmatrix} 0 & I & 0 & \cdots & 0 \\ 0 & 0 & I & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & 0 \\ 0 & \ddots & \ddots & \ddots & I \\ \mathrm{Exp}(kz) & 0 & \cdots & 0 & 0 \end{pmatrix}, \quad B(z) = \begin{pmatrix} 0 & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & 0 \\ b_0(z) & \cdots & b_{k-1}(z) \end{pmatrix}.$$

The circulant structure of $A(z)$ provides bounds on its operator norm when applied repeatedly and when combined with $B(z)$. These bounds are then subsequently used in a somewhat technical analysis to establish upper bounds on the defects $U(t_n) - U_n$, and, ultimately on $\|u(t_n) - u_n\|_\alpha$. Moreover, the authors note that the proof may be modified to give similar results for the Nørsett schemes (38). However, recent research by Ostermann and co-workers [30] has revealed that the Calvo–Palencia schemes are less desirable than the Adams–Bashforth schemes from a stability point of view.

We finally mention one of the technical assumptions used by Calvo and Palencia. The "starting values" $u_0, u_1, \ldots, u_{k-1}$ are all assumed to be in a suitable subspace of a Banach space. The initial value satisfies this condition by default but the remaining values may not. The authors describe a procedure by which suitable starting values may be constructed and give practical details on how this procedure may be realised. This procedure employs a one step scheme, such as the Nørsett–Euler, to construct initial approximations to the starting values and subsequently uses fixed point iteration to solve a nonlinear system of equations for the starting values. The fixed point iteration is continued until the starting values are suitably accurate.

Exponential integrator methods based on Runge–Kutta processes were introduced by Lawson [21] as a means of constructing explicit one-step methods for stiff, semilinear problems. The integrating factor methods

$$\begin{aligned} k_r &= X_2(\mathrm{Exp}(c_r hX_1)u_0 + \sum_{j=1}^{r-1} a_r^j\ \mathrm{Exp}((c_r - c_j)\, hX_1)\, hk_j) \quad r = 1, \ldots, s \\ u_1 &= \mathrm{Exp}(hX_1)u_0 + \sum_{r=1}^{s} b^r\ \mathrm{Exp}((1 - c_r)\, hX_1)\, hk_r \end{aligned} \tag{41}$$

may thus be viewed as the initial work on exponential integrators. The method parameters a_r^j, b^r and c_r are usually chosen from an *underlying* Runge–Kutta scheme on which we impose the coefficient "summability condition" $c_r = \sum_{j=1}^{r-1} a_r^j$.

Friedli [12] extended the integrating factor methods to the general format shown above and also derived order conditions for methods up to order four. Recent analysis by Berland

et al [3] provides non-stiff order conditions of any order for exponential integrators in this format. These non-stiff order conditions are valid whenever $\|hX_1\| \leq \mathcal{O}(1)$. However, additional requirements must be asserted in the stiff regime of $\|hX_1\| \gg \mathcal{O}(1)$. Stiff order conditions are derived and analysed by Hochbruck and Ostermann [16] in the context of explicit exponential integrators for semilinear parabolic problems.

4.2 Stiff order conditions

Hochbruck and Ostermann consider non-autonomous semilinear parabolic systems of the form

$$\frac{\mathrm{d}u}{\mathrm{d}t} = X_1 u + X_2(t,u), \quad u(t_0) = u_0$$

viewed as an evolution equation in a Banach space $(V, \|\cdot\|)$. The linear operator $-X_1$, defined on the domain $\mathcal{D}(-X_1) = \mathcal{D}(X_1) \subset V$, is assumed to be sectorial. That is, a densly defined and closed linear operator on V satisfying the resolvent condition

$$\|(\lambda I - (-X_1))^{-1}\| \leq \frac{M}{|\lambda - a|} \tag{42}$$

on the sector $\{\lambda \in \mathbf{C} : \theta \leq |\arg(a-\lambda)| \leq \pi, \lambda \neq a\}$ for some $M \geq 1$, $a \in \mathbf{R}$, and $\theta \in [0, \pi/2]$. This assumption guarantees the existence of fractional powers of the shifted linear operator $\tilde{X}_1 = (-X_1) + \omega I$ whenever $\omega > -a$, and moreover, that X_1 is the infinitesimal generator of an analytic semigroup $\{\mathrm{Exp}(tX_1)\}_{t \geq 0}$.

The authors additionally assume that X_2 is locally Lipschitz continuous in a strip around the exact solution u. Moreover, in order to obtain high order convergence results, it is assumed that the exact solution $u : [0,T] \to \mathcal{D}(\tilde{X}_1^\alpha)$, with derivatives in $\mathcal{D}(\tilde{X}_1^\alpha)$ is sufficiently smooth and that X_2 is sufficiently Frechét differentiable in a strip around u. These assumptions ensures that the composition

$$f : [0,T] \to V : t \mapsto f(t) = X_2(t, u(t))$$

is a smooth mapping. Finally, the coefficient functions a_r^j and b^r are assumed to satisfy a stability condition of the form

$$\|c(tX_1)\| + \|t^\gamma \tilde{X}_1^\gamma c(tX_1)\| \leq C, \quad 0 \leq \gamma \leq 1 \tag{43}$$

for some constant C and coefficient function $c(z)$.

As X_1 may be unbounded and is not generally a closed operator on $\mathcal{D}(X_1)$, defining integral powers of X_1 is not generally meaningful in this setting. Thus, power series expansion in terms of X_1 is not generally meaningful either, though analytic functions of X_1 may still be defined by means of the Cauchy integral formula. However, the function f is not directly affected by these characteristics of X_1 and may thus still be represented by Taylor polynomial with a remainder term in the form of an integral. This representation yields, through a somewhat technical derivation, explict expressions of the local numerical defects Δ_{nr} and δ_{n+1} defined by inserting the exact solution into the stages and updates of the numerical method respectively. These defect expressions involve the functions

$$\psi_{\ell,r}(z) = \varphi_\ell(c_r z) c_r^\ell - \sum_{j=1}^{r-1} a_r^j(z) \tfrac{c_j^{\ell-1}}{(\ell-1)!}, \quad \psi_\ell(z) = \varphi_\ell(z) - \sum_{r=1}^{s} b^r(z) \tfrac{c_r^{\ell-1}}{(\ell-1)!} \tag{44}$$

of fundamental importance in deriving and expressing the stiff order conditions. Given $0 < \gamma \leq 1$ and $\tilde{X}_1^{\nu-1} f^{(m)} \in L^\infty\big(0,T; \mathcal{D}(\tilde{X}_1^\alpha)\big)$, the explicit defect expressions yield the

bounds

$$h^{1-\nu}\left\|\Delta_{nr}^{(m)}\right\|_{\mathcal{D}(\tilde{X}_1^\alpha)} + \left\|\tilde{X}_1^{\nu-1}\right\|_{\mathcal{D}(\tilde{X}_1^\alpha)} \leq Ch^{m+1} \sup_{0\leq\tau\leq 1} \left\|\tilde{X}_1^{\nu-1} f^{(m)}(t_n+\tau h)\right\|_{\mathcal{D}(\tilde{X}_1^\alpha)}$$

$$\left\|\sum_{j=0}^{n-1} \mathrm{Exp}(jhX_1)\,\delta_{n-j}^{(m)}\right\|_{\mathcal{D}(\tilde{X}_1^\alpha)} \leq Ch^m \sup_{0\leq t\leq t_n} \left\|\tilde{X}_1^{\nu-1} f^{(m)}(t)\right\|_{\mathcal{D}(\tilde{X}_1^\alpha)},$$

which subsequently relate attainable scheme order to the differentiability of f.

Assuming sufficient differentiability of f and repeatedly applying the explicit defect recursion formulae, Hochbruck and Ostermann's main result is the existence of a family of bounded operators $\mathcal{N}_n(v)$ on V such that the global errors $e_n = u_n - u(t_n)$ satify the recursion relation

$$\begin{aligned} e_{n+1} = \mathrm{Exp}(hX_1)\,e_n + h\mathcal{N}_n(e_n)\,e_n - h^2\psi_2(hX_1)f'(t_n) \\ - h^3\psi_3(hX_1)f''(t_n) - h^3\sum_{r=1}^{s} b^r(hX_1)J_n\psi_{2,r}(hX_1)f'(t_n) \\ - h^4\psi_4(hX_1)f'''(t_n) - h^4\sum_{r=1}^{s} b^r(hX_1)J_n\psi_{3,r}(hX_1)f''(t_n) \\ - h^4\sum_{r=1}^{s} b^r(hX_1)J_n\sum_{j=1}^{r-1} a_r^j(hX_1)J_n\psi_{2,j}(h_X 1)f'(t_n) \\ - h^4\sum_{r=1}^{s} b^r(hX_1)c_r K_n\psi_{2,r}(hX_1)f'(t_n) + h^5\mathcal{R}_n, \end{aligned} \tag{45}$$

with uniformly bounded remainders $\|\mathcal{R}_n\| \leq C$. The paper gives explicit expressions for operators J_n and K_n, though the actual expressions are suppressed in the list of algebraic order conditions.

Those algebraic order conditions may be directly extracted from equation (45) as a numerical scheme of order p must eliminate all terms of orders less than and including p from the recursion (45). Table 1 lists the algebraic order conditions which must be satisfied in order to construct numerical schemes of orders up to and including $p = 4$. This table is replicated from [16] and the operators J and K denote here general bounded operators on V. As a further refinement, we note that the complexity of constructing numerical schemes of high order which satisfy these conditions is somewhat ameliorated through theorem 4.7 of [16]. This theorem states that in order to achieve order p, $2 \leq p \leq 4$, one need only satisfy the conditions for schemes of order $p-1$ for all z. The conditions associated with p may be replaced by the weaker conditions $\psi_p(0) = 0$ and by subsituting $b^r(0)$ for $b^r(z)$ in the other relations. Nevertheless, the task of constructing such high order schemes remains considerable.

There are some practical consequences of these conditions. Hochbruck and Ostermann demonstrate the impossibility of constructing explicit fourth order schemes using only four stages. At least five stages must be employed to achieve guaranteed fourth order schemes for semilinear parabolic problems. The authors explicitly construct an example of such a scheme. Moreover, the coefficient functions $a_r^j(z)$ and $b^r(z)$ are restricted to linear combinations of φ functions to even satisfy $\psi_1(z) = 0$. Consequently, Lawson's integrating factor schemes (41) will, in general, exhibit order reduction down to order 1 when applied to this class of problems.

Order reduction phenomena occur for other classes of schemes as well, even schemes using φ-based coefficient functions, although not generally as severe as in the case of no

Table 1: Stiff algebraic order conditions

Order	Order condition, $z = hX_1$
1	$\psi_1(z) = 0$
2	$\psi_2(z) = 0$
2	$\psi_{1,r}(z) = 0, \quad r = 1, \ldots, s$
3	$\psi_3(z) = 0$
3	$\sum_{r=1}^{s} b^r(z) J \psi_{2,r}(z) = 0$
4	$\psi_4(z) = 0$
4	$\sum_{r=1}^{s} b^r(z) J \psi_{3,r}(z) = 0$
4	$\sum_{r=1}^{s} b^r(z) J \sum_{j=1}^{r-1} a_r^j(z) J \psi_{2,j}(z) = 0$
4	$\sum_{r=1}^{s} b^r(z) c_r K \psi_{2,r}(z) = 0$

φ functions. The so-called ETD4RK scheme of Cox and Matthews constructed in [10] exhibits order reduction when applied to both test problems in [16], a fact explained by the scheme's failure to fully satisfy all the stiff order conditions even though the conditions are satisfied in a very weak sense.

On the other hand, numerical and empirical evidence suggest [2] that satisfying the stiff order conditions may not be crucial whenever the problem is not parabolic. The complete characterisation of conditions under which exponential integrators perform well thus remains, at present, unresolved.

5 Conclusion

We have presented a brief review of some of the error analysis available in the literature for splitting methods in various forms. A significant body of work is devoted to the topic, yet important issues remain unresolved—particularly for the exponential integrators. Extending the order theory for exponential integrators to non-parabolic problems and constructing good methods, possibly using variable step sizes, are directions for future research.

References

[1] H. Baker, *Alternants and Continuous Groups*, Proc. London Math. Soc., 3 (1905), pp. 24–47.

[2] H. Berland and B. Skaflestad, *Solving the nonlinear Schrödinger equation using exponential integrators*, in Proceedings of SIMS conference 2005, 2005. To appear.

[3] H. Berland, B. Skaflestad, and B. Owren, *B-series and order conditions for exponential integrators*, SIAM J. Numer. Anal., (2005). To appear.

[4] H. Berland, B. Skaflestad, and W. Wright, *Expint — A Matlab package for exponential integrators*, Tech. Rep. 4/05, Department of Mathematical Sciences, NTNU, Norway, 2005. http://www.math.ntnu.no/preprint/.

[5] S. Blanes and F. Casas, *On the necessity of negative coefficients for operator splitting schemes of order higher than two.* To appear in Appl. Numer. Math.

[6] S. Blanes, F. Casas, and A. Murua, *Composition methods for differential equations with processing.* To appear in SIAM J. Sci. Comp.

[7] ——, *On the numerical integration of ordinary differential equations by processed methods*, SIAM J. Numer. Anal., 42 (2004), pp. 531–552.

[8] M. Calvo and C. Palencia, *A class of explicit multistep exponential integrators for semilinear problems.* Preprint, 2004.

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

[10] S. Cox and P. Matthews, *Exponential time differencing for stiff systems*, J. Comput. Phys., 176 (2002), pp. 430–455.

[11] J. Eshof and M. Hochbruck, *Preconditioning Lanczos Approximations to the Matrix Exponential.* To appear in SIAM J. Sci. Comp.

[12] A. Friedli, *Verallgemeinerte Runge–Kutta Verfahren zur Lösung steifer Differentialgleichungssysteme*, in Numerical treatment of differential equations, vol. 631 of Lecture Notes in Math., Springer, 1978, pp. 35–50. In German.

[13] E. Hairer, C. Lubich, and G. Wanner, *Geometric Numerical Integration, Structure-Preserving Algorithms for Ordinary Differential Equations*, vol. 31 of Springer Series in Computational Mathematics, Springer-Verlag, 2002.

[14] E. Hairer, S. Nørsett, and G. Wanner, *Solving Ordinary Differential Equations I, Nonstiff Problems*, vol. 8 of Springer Series in Computational Mathematics, Springer-Verlag, second revised ed., 1993.

[15] M. Hochbruck and C. Lubich, *On Krylov Subspace Approximation to the Matrix Exponential*, SIAM J. Numer. Anal., 34 (1997), pp. 1911–1925.

[16] M. Hochbruck and A. Ostermann, *Explicit Exponential Runge–Kutta Methods for Semilinear Problems.* Manuscript, 2004. To appear in SIAM J. Numer. Anal.

[17] T. Jahnke and C. Lubich, *Error bounds for exponential operator splittings*, BIT, 40 (2000), pp. 735–744.

[18] G. Karniadakis, M. Israeli, and S. Orszag, *High-Order Splitting Methods for the Incompressible Navier–Stokes Equations*, J. Comp. Phys, 97 (1991), pp. 414–443.

[19] J. Kim and P. Moin, *Application of a Fractional-Step Method to Incompressible Navier–Stokes Equations*, J. Comp. Phys, 59 (1985), pp. 308–323.

[20] R. Kozlov, A. Kværnø, and B. Owren, *The behaviour of the local error in splitting methods applied to stiff problems*, J. Comp. Phys, 195 (2004), pp. 576–593.

[21] D. Lawson, *Generalized Runge–Kutta processes for stable systems with large Lipschitz constants*, SIAM J. Numer. Anal., 4 (1967), pp. 372–380.

[22] Y. Maday, A. Patera, and E. Rønquist, *An Operator-Integration-Factor Splitting Method for Time-Dependent Problems: Application to Incompressible Fluid Flow*, J. Sci. Comp., 5 (1990), pp. 263–292.

[23] G. Marchuk, *On the Theory of the Splitting-Up Method*, in Numerical Solution fo Partial Differential Equations II, B. Hubbard, ed., Academic Press, New York, 1971, pp. 469–500.

[24] R. McLachlan, *On the Numerical Integration of Ordinary Differential Equations by Symmetric Composition Methods*, SIAM J. Sci. Comp., 16 (1995), pp. 151–168.

[25] R. McLachlan and G. Quispel, *Splitting Methods*, Acta Numerica, (2002), pp. 341–434.

[26] C. Moler and C. Van Loan, *Nineteen Dubious Ways to Compute the Exponential of a Matrix, Twenty-Five Years Later*, SIAM Review, 45 (2003), pp. 3–49.

[27] A. Murua and J. Sanz-Serna, *Order Conditions for Numerical Integrators Obtained by Composing Simpler Integrators*, Philos. Trans. Royal Soc. London, Ser. A, 357 (1999), pp. 1079–1100.

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

[29] P. Olver, *Application of Lie Groups to Differential Equations*, GTM 107, Springer–Verlag, second ed., 1993.

[30] A. Ostermann, M. Thalhammer, and W. M. Wright, *A class of explicit exponential general linear methods.* In preparation, 2005.

[31] A. Pazy, *Semigroups of linear operators and applications to partial differential equations*, vol. 44 of Applied Mathematical Sciences, Springer-Verlag, New York, 1983.

[32] A. Quarteroni and A. Valli, *Numerical Approximation of Partial Differential Equations*, vol. 23 of Springer Series in Computational Mathematics, Sprinver-Verlag, second ed., 1997.

[33] G. Strang, *On the Construction and Comparison of Difference Schemes*, SIAM J. Numer. Anal., 5 (1968), pp. 506–517.

[34] V. Varadarajan, *Lie Groups, Lie Algebras, and Their Representations*, vol. 102 of GTM, Springer–Verlag, 1984.

[35] H. Yoshida, *Construction of Higher Order Symplectic Integrators*, Phys. Lett. A, 150 (1990), pp. 262–268.