SOLVING PERIODIC SEMILINEAR STIFF PDES IN 1D, 2D AND 3D WITH EXPONENTIAL INTEGRATORS

HADRIEN MONTANELLI* AND NIALL BOOTLAND†

Abstract. Dozens of exponential integration formulas have been proposed for the high-accuracy solution of stiff PDEs such as the Allen-Cahn, Korteweg-de Vries and Ginzburg-Landau equations. We report the results of extensive comparisons in MATLAB and Chebfun of such formulas in 1D, 2D and 3D, focusing on fourth and higher order methods, and periodic semilinear stiff PDEs with constant coefficients. Our conclusion is that it is hard to do much better than one of the simplest of these formulas, the ETDRK4 scheme of Cox and Matthews.

Key words. Stiff PDEs, exponential integrators, Fourier spectral methods, Chebfun

AMS subject classifications. 65L04, 65L05, 65M20, 65M70

1. Introduction. We are interested in computing smooth solutions of stiff PDEs of the form

\[ u_t = S(u) = Lu + N(u), \quad u(0, X) = u_0(X), \quad \text{periodic boundary conditions}, \quad (1.1) \]

where \( u(t, X) \) is a function of time \( t \) and space \( X \), \( L \) is a linear differential operator with constant coefficients on a domain in one, two or three space dimensions and \( N \) is a nonlinear differential (or non-differential) operator of lower order with constant coefficients and on the same domain. In applications, PDEs of this kind typically arise when two or more different physical processes are combined, and many PDEs of interest in science and engineering take this form. For example, the Korteweg-de Vries equation \( u_t = -u_{xxx} - uu_x \), the starting point of the study of nonlinear waves and solitons, couples third-order linear dispersion with first-order convection, and the Allen-Cahn equation \( u_t = \epsilon u_{xx} + u - u^3 \) couples second-order linear diffusion with a nondifferentiated cubic reaction term. Often a system of equations rather than a single scalar equation is involved, for example in the Gray-Scott and Schnakenberg equations, which involve two components coupled together. (The importance of coupling of nonequal diffusion constants in science was made famous by Alan Turing in the most highly-cited of all his papers \[60]\). Fourth-order terms also arise, for example in the Cahn-Hilliard equation, whose solutions describe structures of alloys, and in the Kuramoto-Sivashinsky equation, related to combustion problems among others, whose solutions are chaotic. Other examples of stiff PDEs include the Ginzburg-Landau, nonlinear Schrödinger and Swift-Hohenberg equations. Figure 1.1 shows six examples of solutions of such PDEs.

Solving all these PDEs by generic numerical methods can be highly challenging. This paper describes and compares specialized methods that take advantage of two special features of (1.1). The first one is the periodic boundary conditions. This allows us to discretize the spatial component of (1.1) with a Fourier spectral method on \( N \) points; equation (1.1) becomes a system of \( N \) ODEs,

\[ \dot{\hat{u}} = S(\hat{u}) = L\hat{u} + N(\hat{u}), \quad \hat{u}(0) = \hat{u}_0, \quad (1.2) \]

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\( X \) denotes a space variable in 1D, 2D or 3D. Throughout this paper, we will use the variables \( x \) in 1D, \((x, y)\) in 2D and \((x, y, z)\) in 3D. The domain will be an interval in 1D, a square in 2D and a cube in 3D.
Fig. 1.1: First row, from left to right: a metastable solution of the Allen-Cahn equation\(^{(3.1)}\), a two-soliton solution of the KdV equation\(^{(3.7)}\) and the absolute value of a breather solution of the nonlinear Schrödinger equation\(^{(3.16)}\). Second row, from left to right: the real part of a frozen state solution of the 2D Ginzburg-Landau equation\(^{(3.20)}\), a spot solution of the 2D Schnakenberg\(^{(3.23)}\) equations and convection rolls, a solution of the 2D Swift-Hohenberg equations\(^{(3.26)}\).

where \(\hat{u}(t)\) is a vector of \(N\) Fourier coefficients, and \(L\) (a \(N \times N\) matrix) and \(N\) are the discretized versions of \(L\) and \(N\). For example, in 1D on \([0, 2\pi]\) with \(Lu = u_{xx}\) and an even number \(N\) of equispaced grid points \(\{x_j = 2\pi j/N\}_{j=0}^{N-1}\), we look for a solution \(u(t, x)\) of the form\(^2\)

\[
    u(t, x) \approx \sum_{k=-N/2}^{N/2-1} \hat{u}_k(t) e^{ikx}
\]

with Fourier coefficients \(\hat{u}(t) = \{\hat{u}_k(t)\}_{k=-N/2}^{N/2-1}\) defined by\(^3\)

\[
    \hat{u}_k(t) = \frac{1}{N} \sum_{j=0}^{N-1} u(t, x_j) e^{-ikx_j}, \quad -\frac{N}{2} \leq k \leq \frac{N}{2} - 1, \quad \hat{u}_{N/2}(t) = \hat{u}_{-N/2}(t).
\]

---

\(^2\)The prime on the summation sign in\(^1\) signifies that the terms \(k = \pm N/2\) are halved.

\(^3\)Note that, in practice, the coefficient \(\hat{u}_{N/2}\) is not stored—the vector of Fourier coefficients is really \(\hat{u}(t) = \{\hat{u}_k(t)\}\), with \(-N/2 \leq k \leq N/2 - 1\).
For this PDE, $L = D^{(2)}$ is the (diagonal) second-order Fourier differentiation matrix with entries $-k^2, -N/2 \leq k \leq N/2 - 1$; see [57] for more details about Fourier spectral methods and [62] for a review of trigonometric interpolation techniques. Some basic results about Fourier spectral methods and trigonometric interpolation can be found in Appendices A (1D) and B (2D and 3D).

The main issue with solving (1.2) numerically is stiffness, characterised by the need for an explicit method to use small time-steps, much smaller than the condition required by accuracy. (Note that stiffness is related to $L$ having large eigenvalues since stability of spectral methods for time-dependent PDEs requires that the eigenvalues of $L$, scaled by the time-step, lie in the stability region of the time-stepping formula [57, Chapter 10].) When too many steps are required, this can result in an infeasibly long computation for the method.

The second special feature of (1.1) is that it is semilinear, i.e., the higher-order terms of the equation are linear. Exponential integrators are a class of numerical methods for systems of ODEs that are aimed at taking advantage of this. The linear part $L$, responsible for the stiffness, is integrated exactly using the matrix exponential while a numerical scheme is applied to $N$.

According to the 2005 review of Minchev and Wright [39], the first exponential integrators were constructed in a paper by Certaine [11], published in 1960. Subsequently, however, Hochbruck and Ostermann [24] noted, in a comprehensive theoretical review of these schemes, that Hersch [21] had previously considered exponential integrators in 1958 in an effort to find schemes that are exact for linear problems with constant coefficients. The first use of the term exponential integrator was by Hochbruck, Lubich and Selhofer [22] in a seminal paper of 1998. The extensive use of these formulas for solving stiff PDEs seems to have been initiated by the papers by Cox and Matthews [13] and Kassam and Trefethen [28]. A striking unpublished paper by Kassam [27] shows how effective such methods can be also for PDEs in 2D and 3D. A software package for such computations called EXPINT was produced by Berland, Skaflestad and Wright [4].

One of the simplest exponential integrators, first derived by Pope in 1963 [42] and commonly known as the Exponential Time Differencing (ETD) Euler method, is given by:

$$\hat{u}^{n+1} = e^{hL}\hat{u}^n + h\varphi_1(hL)N(\hat{u}^n),$$  \hspace{1cm} (1.5)

where $h = t_{n+1} - t_n$ is the time-step and

$$\varphi_1(z) = \frac{e^z - 1}{z}. \hspace{1cm} (1.6)$$

As Minchev and Wright [39] point out, this method has been rediscovered from many different viewpoints and has been known by several other names. Pope introduced it by considering the linearized version of (1.2) on $[t_n, t_{n+1}]$,

$$\hat{u}' = S(\hat{u}) + S_\hat{u}(\hat{u}')(\hat{u} - \hat{u}^n), \quad \hat{u}(t_n) = \hat{u}^n,$$ \hspace{1cm} (1.7)

with exact solution at $t_{n+1} = t_n + h$,

$$\hat{u}^{n+1} = \hat{u}^n + h\varphi_1(hS\hat{u}(\hat{u}^n))S(\hat{u}).$$ \hspace{1cm} (1.8)

Approximating $S\hat{u}(\hat{u}^n)$ by $L$ in (1.8) leads to (1.5). Note that (1.8) defines a time-stepping scheme too, known as the exponential Euler method. The problem with (1.8) is that the exact Jacobian $S\hat{u}$,
and its value under the exponential-like function \( \varphi_1 \), need to be computed at each time-step. This would involve a high computational cost, so typically one either does not compute \( \varphi_1 \) but rather an approximation, such as a Padé approximation, or else one uses an approximation to the Jacobian as opposed to the exact Jacobian. The former approach contains the Rosenbrock methods. There is a large literature on such methods, including the papers of Rosenbrock [45] andHairer [18] and the books of Hairer and Wanner [19] and van der Houwen [61]. More recent papers include Hochbruck et al. [26] andLuan and Ostermann [37]. The latter approach is what Pope did to derive (1.5) and is what we shall consider in this paper.

As we just described, exponential integrators are characterised by the use of exponential and related functions of the matrix \( L \). Standard methods for computing the matrix exponential include Krylov subspace methods and the scaling and squaring method together with a truncated Taylor series approximation to the exponential [1]. There is recent work which shows that exponential integrators together with Krylov methods are competitive, for instance see Tokman and Loffeld [35, 54]. In our case we consider periodic problems and, using Fourier spectral methods, the matrices \( L \) are diagonal, so the matrix exponential is trivial.

We compare in this paper thirty exponential integrators of fourth and higher order on eleven model problems in 1D, 2D and 3D, using MATLAB R2015b and Chebfun v5.5 [14]. Comparisons with other types of time-stepping schemes are out of the scope of the article; see, e.g., [17, 27, 29, 30, 35]. Let us emphasize that we are interested in determining if one of the high order integrators outperforms the others on a large class of problems. For a particular problem, it might be possible to design a very specific scheme, of possibly lower order than four, which performs extremely well. For example, Cano and Gonzáles-Pachón have recently shown that the low-order Lawson methods, combined with orthogonal projections onto some invariants, can be very competitive for the nonlinear Schrödinger equation [9, 10].

The paper is structured as follows. We present the thirty exponential integrators in Section 2 and the eleven model problems in Section 3. The numerical results are presented in Section 4 and show that it is hard to do much better than one of the simplest of these formulas, the ETDRK4 scheme of Cox and Matthews [13].

2. Thirty exponential integrators.

2.1. Exponential general linear methods. We consider exponential integrators, based on the approximation of the Jacobian of (1.8), that belong to the large class of exponential general linear methods, first introduced by Minchev and Wright in 2005 [39]. This class contains, in particular, the ETD Runge-Kutta (one-step), ETD Adams-Bashforth (multistep), Lawson and exponential predictor-corrector methods. For given starting values \( \hat{u}^0, \hat{u}^1, \ldots, \hat{u}^{q-1} \) at times \( t = 0, h, \ldots, (q-1)h \), the numerical approximation \( \hat{u}^{n+1} \) at time \( t_{n+1} = (n+1)h \), \( n + 1 \geq q \), is given by the formula

\[
\hat{u}^{n+1} = e^{hL}\hat{u}^n + h \sum_{i=1}^s B_i(hL)N(\hat{v}^i) + h \sum_{i=1}^{q-1} V_i(hL)N(\hat{u}^{n-i}),
\]

(2.1)

with \( q \) steps \( \hat{u}^{n-i} \) and \( s \) stages \( \hat{v}^i \), with \( \hat{v}^1 = \hat{u}^n \) and

\[
\hat{v}^i = e^{C_i hL}\hat{u}^n + h \sum_{j=1}^{i-1} A_{i,j}(hL)N(\hat{v}^j) + h \sum_{j=1}^{q-1} U_{i,j}(hL)N(\hat{u}^{n-j}), \quad 2 \leq i \leq s.
\]

(2.2)

Note that, in practice, the nonlinear evaluations \( N(\hat{v}^i) \) and \( N(\hat{u}^{n-i}) \) are carried out in value space, e.g., \( N(\hat{v}^i) \) means \( \mathcal{F}(N(\mathcal{F}^{-1}\hat{v}^i)) \), with discrete Fourier transform \( \mathcal{F} \). Methods of the form (2.1)–
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| $C_2$ | $A_{2,1}$ | $U_{2,1}$ | $U_{2,q-1}$ |
|------|-----------|-----------|-------------|
| ...  | ...       | ...       |             |
| $C_s$| $A_{s,1}$ | $A_{s,s-1}$| $U_{s,1}$   | $U_{s,q-1}$ |
|      |           |           | $B_1$       | $B_{s-1}$   |
|      |           |           | $B_s$       | $V_1$       |
|      |           |           |             | $V_{q-1}$   |

Table 2.1: Butcher tableau for the coefficients of an exponential integrator with $q$ steps and $s$ stages.

Equations (2.1)–(2.2) not only include purely one-step methods ($q = 1$, $s \geq 1$) and purely multistep methods ($q \geq 1$, $s = 1$), but also combinations of both. Each scheme is characterised by its coefficients $A$, $B$, $C$, $U$, and $V$, which can be conveniently listed in a Butcher tableau, see Table 2.1. Note that these coefficients (except $C$) depend on $L$—for instance, (1.5) uses one stage and one step, and its only non-zero coefficient is $B_1 = \varphi_1(hL)$.

The coefficients satisfy the following summation properties

\begin{align}
B_1 &= \varphi_1(hL) - \sum_{i=2}^{s} B_i(hL) - \sum_{i=1}^{q-1} V_i(hL), \\
A_{i,1} &= \psi_{1,i}(hL) - \sum_{j=2}^{i-1} A_{i,j}(hL) - \sum_{j=1}^{q-1} U_{i,j}(hL), \quad 2 \leq i \leq s,
\end{align}

where the $\varphi$- and $\psi$-functions are exponential and related functions that we shall define in the next subsection. As a consequence, it is notationally convenient to incorporate this condition by filling the corresponding entries of the Butcher tableau with a dot on the understanding that these method coefficients are given by (2.3).

2.2. Evaluating the $\varphi$-functions. The coefficients $A$, $B$, $C$, $U$, and $V$ involve the $\varphi$ and $\psi$-functions applied to $L$. Because $L$ is diagonal, $\varphi(L)$ and $\psi(L)$ reduce to $\varphi$ and $\psi$ applied to the diagonal elements $\lambda$ of $L$, so all we have to be able to is to compute $\varphi(\lambda)$ and $\psi(\lambda)$ for $\lambda \in \mathbb{C}$. The $\varphi$-functions are defined by the recurrence relation

\[ \varphi_{l+1}(z) = \frac{\varphi_l(z) - 1/l!}{z}, \quad l \geq 1, \]

where the $\varphi$- and $\psi$-functions are exponential and related functions that we shall define in the next subsection. As a consequence, it is notationally convenient to incorporate this condition by filling the corresponding entries of the Butcher tableau with a dot on the understanding that these method coefficients are given by (2.3). Note that the exponential integrators of the form (2.1)–(2.2) do not include the Exponential Propagation Iterative methods of Runge-Kutta type (EPIRK) \[43, 44, 52, 53, 55\] and the EMAM4 scheme of Calvo and Palencia \[8\]. The second author showed in \[6\] that the former—derived with the use of Krylov methods in mind where they perform well—are less competitive in this context, and that the latter often suffers from stability problems.

Let us finish this section with a few words about the computational cost per time-step. Since the matrices in (2.1)–(2.2) are diagonal, the matrix-vector products cost only $O(N)$ operations, where $N$ is the number of grid points. The dominant cost per time-step is then of the order of the cost of an FFT \[12\], i.e., $O(N \log N)$ operations. For exponential integrators of the form (2.1)–(2.2), it is therefore $O(2sN \log N)$. As a consequence, purely multistep methods have a low computational cost per time-step.

There are two exceptions: the coefficients of the Lawson4 and ABLawson4 schemes do not satisfy (2.3).
with \( \varphi_0(z) = e^z \). After \( \varphi_0 \), the first few \( \varphi \)-functions are (1.6) and

\[
\varphi_2(z) = \frac{e^z - z - 1}{z^2}, \quad \varphi_3(z) = \frac{e^z - z^2 - z - 1}{z^4},
\]

(2.5)

while the \( \psi \)-functions are defined via the \( \varphi \)-functions and the coefficients \( C \),

\[
\psi_{l,m}(z) = C_{l}^{m} \varphi_{l}(C_{m}z), \quad l \geq 0, \quad 1 \leq m \leq s.
\]

(2.6)

Equations (2.4) and (2.6) can be implemented recursively, but the accurate evaluation of \( \varphi \) and \( \psi \) is not straightforward because it can suffer from cancellation error. Following the idea of Kassam and Trefethen in [28], to compute the functions at some \( \lambda \in \mathbb{C} \), we use Cauchy’s integral formula

\[
\varphi(\lambda) = \frac{1}{2\pi i} \oint_{\Gamma} \frac{\varphi(z)}{z - \lambda} dz,
\]

(2.7)

which can be approximated with exponential accuracy by the trapezoidal rule [58],

\[
\varphi(\lambda) \approx \frac{1}{M} \sum_{k=1}^{M} \varphi(\lambda + e^{2\pi i(k-0.5)/M}),
\]

(2.8)

taking \( \Gamma \) to be the circle of radius 1 centred at \( \lambda \), oriented counter-clockwise, discretized with \( M \) equally spaced points. Note that the \( \varphi \)-functions satisfy \( \varphi(\bar{z}) = \bar{\varphi}(z) \) for all \( z \in \mathbb{C} \). As a consequence, when \( \lambda \) is on the real axis, we can take \( \Gamma \) to be the upper half of the circle of radius 1 centred at \( \lambda \) and take the real part of the result, i.e.,

\[
\varphi(\lambda) = \frac{1}{\pi} R \left( \int_{0}^{\pi} \varphi(\lambda + e^{i\theta}) d\theta \right),
\]

(2.9)

which can be discretized by

\[
\varphi(\lambda) \approx \frac{1}{M} R \left( \sum_{k=1}^{M} \varphi(\lambda + e^{\pi i(k-0.5)/M}) \right).
\]

(2.10)

If this symmetry is not explicitly used in the computation of the \( \varphi \)-functions when \( \lambda \) is real, rounding errors appear that lead to numerical instability. Note that the evaluation of the \( \varphi \)-functions using (2.8) or (2.10) requires \( O(M) \) operations per \( \lambda \).

Let us emphasize that we can use circles or radius 1 around each eigenvalue \( \lambda \) of \( L \) because \( L \) is diagonal. When the matrix is not diagonal, one has to use a single contour that encloses all the eigenvalues, and the best possible contour depends on the problem. For example, for parabolic problems (also called diffusive problems), all the eigenvalues are on the real negative axis and the best contour is a Hankel contour [46, 59].

Using contour integrals is not the only possible remedy for cancellation error. When Pope introduced (1.5), he suggested the use of Taylor series for small \( \lambda \) and the direct formula for large \( \lambda \). The problem with this approach is that, for some intermediate values, neither method gives full precision, as noted by Cox and Matthews [13] and Kassam and Trefethen [28]. Another approach is to use Padé approximations, combined with a scaling and squaring technique [6]. This method is also effective, but the contour integral method is particularly appealing because of its greater generality for dealing with arbitrary functions.
2.3. Introducing the thirty exponential integrators. Table 2.2 lists the exponential integrators considered in this paper. Their Butcher tableaux can be found in the supplementary material.

Table 2.2: A reference table for the exponential integrators considered in this article. Note that some methods do not appear explicitly in the references listed but can be derived using order conditions or recurrence formulas found there; these cases are marked by asterisks. The Butcher tableaux for all of these formulas can be found in the supplementary material.

The first category of exponential integrators is the ETD Adams-Bashforth schemes of orders four to six. These are ETD (purely) multistep methods, which reduce to Adams-Bashforth schemes when $L = 0$, and go back to Nørsett in 1969 [40]. Since $s = 1$, (2.1)–(2.2) reduces to

$$
\hat{u}^{n+1} = e^{hL} \hat{u}^n + hB_1 (hL) N(\hat{u}^n) + h \sum_{i=1}^{q-1} V_i (hL) N(\hat{u}^{n-i}),
$$

(2.11)
i.e., the only non-zero coefficients are $B_1$ and those in $V$. Note that since these schemes are purely
often known as integrating factor (IF) methods, the motivation behind Lawson methods is to

\[
\begin{align*}
C_2 &= \frac{1}{2} \\
C_3 &= \frac{1}{2} \\
C_4 &= 1
\end{align*}
\]

\[
\begin{align*}
A_{3,2} &= \psi_{1,2} \\
A_{4,2} &= 0 \\
A_{4,3} &= 2\psi_{1,2}
\end{align*}
\]

\[
\begin{align*}
B_2 &= 2\varphi_2 - 4\varphi_3 \\
B_3 &= 2\varphi_2 - 4\varphi_3 \\
B_4 &= -\varphi_2 + 4\varphi_3
\end{align*}
\]

Table 2.3: Butcher tableau for ETDRK4. Note the dots in the first column, which indicate that
these coefficients are computed using (2.23). These coefficients are (from top to bottom): \(A_{2,1} = \psi_{1,2}\), \(A_{3,1} = 0\), \(A_{4,1} = \varphi_1 - 2\psi_{1,2}\) and \(B_4 = 2\varphi_1 - 3\varphi_2 + 4\varphi_3\).

We label these methods as ABNørsett\(q\), where \(4 \leq q \leq 6\) is the order and also the number of steps. For more details on the derivation of ABNørsett methods see Minchev and Wright [39], who also show a connection between these schemes and the IMEX schemes of Ascher, Ruuth and Wetton [3]. One can also derive methods based on Adams-Moulton methods, known as AMNørsett methods. These are implicit but can be used within predictor-corrector pairs, as we will see when introducing exponential predictor-corrector schemes (the last category in the table). A comprehensive look at both the Adams-Bashforth and Adams-Moulton exponential integrators can be found in the paper by Hochbruck and Ostermann [25].

The second category is the ETD Runge-Kutta schemes of order four to five. These are (purely) one-step methods and go back to Friedli in 1978 [10] and Strehmel-Weiner in 1982 [50]. More recently, inspired by Cox and Matthews’ ETDRK4 scheme [13], Minchev [38] in 2004 and Krogstad [32] and Hochbruck and Ostermann [23] in 2005 derived ETD Runge-Kutta schemes of order four. Luan and Ostermann proposed a scheme of order five (EXPRK5S8) in 2014 [36]. Overviews of ETD Runge-Kutta methods and some of their history can be found in the reviews of Hochbruck and Ostermann [24] and Minchev and Wright [39], where connections are described between ETD Runge-Kutta, generalised Runge-Kutta and semi-implicit methods. Since \(q = 1\), (2.11)–(2.22) reduces to

\[
\hat{u}^{n+1} = e^{hL}\hat{u}^n + h \sum_{i=1}^{s} B_i(hL)N(\hat{v}^i),
\]

\[
\hat{v}^1 = \hat{u}^n, \quad \hat{v}^i = e^{hL}\hat{u}^n + h \sum_{j=1}^{i-1} A_{i,j}(hL)N(\hat{v}^j), \quad 2 \leq i \leq s.
\]

The only non-zero coefficients are those in \(A\), \(B\) and \(C\). The coefficients for the ETDRK4 scheme can be found in Table 2.3 and correspond to the following formula:

\[
\begin{align*}
\hat{v}^1 &= \hat{u}^n, \\
\hat{v}^2 &= e^{Lh/2}\hat{u}^n + (h/2)\varphi_1(Lh/2)N(\hat{v}^1), \\
\hat{v}^3 &= e^{Lh/2}\hat{u}^n + (h/2)\varphi_1(Lh/2)N(\hat{v}^2), \\
\hat{v}^4 &= e^{Lh/2}\hat{v}^2 + (h/2)\varphi_1(Lh/2)[2N(\hat{v}^1) - N(\hat{v}^1)], \\
\hat{u}^{n+1} &= e^{Lh}\hat{u}^n + hB_1(hL)N(\hat{v}^1) + hB_2(hL)[N(\hat{v}^2) + N(\hat{v}^3)] + hB_4(hL)N(\hat{v}^4).
\end{align*}
\]

The third category is the Lawson methods. First developed by Lawson in 1967 [34], and often known as integrating factor (IF) methods, the motivation behind Lawson methods is to
use a change of variable in \((1.2)\) to get rid of the stiff linear part, and then apply a numerical
solver to the transformed equation. The Lawson transformation consists of the change of variables
\(\hat{v}(t) = e^{-Lt} \hat{u}(t)\). If we differentiate this and substitute into \((1.2)\), the transformed equation is
\[
\hat{v}' = e^{-Lt} N(e^{Lt} \hat{v}), \quad \hat{v}(0) = \hat{u}_0. \tag{2.13}
\]
The linear term is gone, and the transformed equation \((2.13)\), while no longer stiff, now has rapidly
varying coefficients. Once we have decided on a scheme to solve \((2.13)\), we can transform back to \(\hat{u}\).
Lawson, in his 1967 paper, used the classical fourth order Runge-Kutta scheme on the transformed
equation \((2.13)\); we call this method Lawson4. Using the classical fourth order Adams-Bashforth
scheme gives the ABLawson4 method. Ehle and Lawson observed in [15] that Runge-Kutta based
Lawson methods only work well when the problem is moderately stiff. Another problem with Lawson
methods, as indicated by Krogstad [32], is that they do not preserve fixed points of the differential
equation. Krogstad worked around these problems to derive generalised Lawson methods, also
called generalised integrating factor (GIF) methods, the fourth category in the table.

**Generalised Lawson** methods are based on the transform
\[
\hat{v}(t) = e^{-Lt} \hat{u}(t) - e^{-Lt} \sum_{l=1}^{q} t^l \varphi_l(tL)p_{l-1}, \tag{2.14}
\]
where the \(p_l\) are the coefficients, in a (scaled) monomial basis, of the polynomial \(P(t)\) of degree
\(q - 1\) that interpolates the values \(\{N(\hat{u}^{n-1})\}_{l=1}^{q}\) at the points \(\{t_{n-1}\}_{l=1}^{q}\); see [24, 39] for details.
Differentiating this and substituting into \((1.2)\) leads to the transformed equation
\[
\hat{v}' = e^{-Lt} \left( N(e^{Lt} \hat{v} + \sum_{l=1}^{q} t^l \varphi_l(tL)p_{l-1}) - P(t) \right), \quad \hat{v}(0) = \hat{u}_0. \tag{2.15}
\]
Note that \((2.13)\) is the special case of \((2.15)\) with \(P(t) = 0\). The idea of Krogstad is to apply, for
various values of \(q\), the classical fourth order Runge-Kutta scheme on \((2.15)\), and then transform
back to \(\hat{u}\). It leads to methods with four stages and \(q\) steps, called the GenLawson4q methods.

As we increase \(q\) in the generalised Lawson methods we incorporate more of the nonlinearity
and the methods have improved accuracy. However, this in part comes at the cost of stability,
especially for dispersive problems, as was demonstrated by Krogstad [32]. A modification, based
on satisfying order conditions, given by Ostermann, Thalhammer and Wright [41], significantly
improves stability. The modification is given by the requirement that
\[
\sum_{i=1}^{4} B_i(hL)^j \frac{j!}{j^j} + \sum_{i=1}^{q-1} V_i(hL) \frac{(-1)^j}{j!} = \varphi_{j+1}(hL), \quad 0 \leq j \leq q - 1, \tag{2.16}
\]
where, as before, \(q - 1\) is the degree of the polynomial approximation. These are the **modified
generalised Lawson** methods, labelled as ModGenLawson4q.

Just as with the standard Adams-Bashforth and Adams-Moulton multistep methods, the exponential
versions can be used in predictor-corrector pairs. These are the **exponential predictor-corrector**
methods, the last category in the table. For instance, using ABNørsett3 for a predictor
step and AMNørsett4 for the corrector step yields the fourth order method called PEC433 in the
MATLAB package EXPINT [4]. (PEC stands for predict-evaluate-correct, four is the order, two is
the number of stages and three is the number of steps.) One can evaluate and correct again, that
is, use the corrector twice. The name PEC433 is given in EXPINT for the fourth order method
that uses ABNørsett3 for a predictor step and AMNørsett4 for two corrector steps.
Table 3.1: The model problems we consider in this paper. The linear operator of a diffusive PDE has real eigenvalues while it has purely imaginary eigenvalues for dispersive PDEs. Note that we take $A = 0$ for the Ginzburg-Landau equation (3.20). For $A \neq 0$, the linear part would have complex eigenvalues.

3. Eleven model problems. In this section we describe the PDEs used in the numerical comparisons of Section 4, including the initial conditions, the domains and the time intervals. There are five PDEs in 1D and three PDEs considered in both 2D and 3D, see Table 3.1.

3.1. Model problems in 1D. The Allen-Cahn equation, derived by Allen and Cahn in the 1970s, is a reaction-diffusion equation which describes the process of phase separation in iron alloys (see, e.g., [2]). It is given in one dimension as

$$u_t = \epsilon u_{xx} + u - u^3,$$

with linear diffusion $\epsilon u_{xx}$ and a cubic reaction term $u - u^3$. The function $u$ is the order parameter, a correlation function related to the positions of the different components of the alloy. The Allen-Cahn equation exhibits stable equilibria at $u = \pm 1$ while $u = 0$ is an unstable equilibrium. Solutions often display metastability where wells $u \approx -1$ compete with peaks $u \approx 1$, and structures remain almost unchanged for long periods of time before changing suddenly. This can be quantified: features with width $L$ persist for time scales on the order of $e^{L/\epsilon}$. In Fourier space, (3.1) becomes

$$\hat{u}' = -\epsilon k^2 \hat{u} + \hat{u} - \mathcal{F}\left((\mathcal{F}^{-1}\hat{u})^3\right).$$

Note that $-k^2 \hat{u}$ is an abuse of notation and means $D^{(2)} \hat{u}$. We take $\epsilon = 5 \times 10^{-2}$,

$$u(0, x) = \frac{1}{3} \tanh(2 \sin(x)) - e^{-23.5(x-\pi/2)^2} + e^{-27(x-4.2)^2} + e^{-38(x-5.4)^2}, \quad x \in [0, 2\pi],$$

and solve up to $t = 60$. This initial condition quickly converges to a set of wells $u \approx -1$ and peaks $u \approx 1$ (at around $t = 4$) and eventually to a two-plateau solution (at around $t = 500$). Figure 1.1 shows the solution at time $t = 113$, when the peak on the far right is switching to $u \approx -1$.

The Cahn-Hilliard equation,

$$u_t = D(-u_{xx} - \gamma u_{xxxx} + (u^3)_{xx}),$$

is a fourth order reaction-diffusion problem which Cahn and Hilliard suggested in 1958 as a model for the process of phase separation in binary alloys [7]. It couples second-order destabilizing diffusion
−u_{xx} with fourth-order stabilizing diffusion −u_{xxxx} and a differentiated cubic reaction term \((u^3)_{xx}\). The function \(u\) is defined as \(u = 1 - 2c_A\) where \(0 \leq c_A \leq 1\) and \(c_B = 1 - c_A\) denote the concentrations of the two components \(A\) and \(B\) of the alloy, that is, \(u = -1\) means pure \(A\) while \(u = 1\) means pure \(B\). The Cahn-Hilliard equation also exhibits metastable solutions. When quenched below a critical temperature, alloys described by (3.4) become unstable in the sense that small metastable pockets of relatively pure \(A\) and \(B\) may soon appear, corresponding to wells \(u = -1\) and peaks \(u = 1\). These pockets may coarsen into larger pockets at progressively larger times. In Fourier space, (3.4) becomes

\[
\hat{u}' = D(k^2 - \gamma k^4)\hat{u} - Dk^2\mathcal{F}\left((\mathcal{F}^{-1}\hat{u})^3\right).
\]  

We take \(D = 10^{-2}, \gamma = 10^{-3}\),

\[
u(0, x) = \frac{1}{5} \sin(4\pi x)^5 - \frac{4}{5} \sin(\pi x), \quad x \in [-1, 1],
\]

and solve up to \(t = 12\). This initial condition evolves to a four-plateau solution (two wells \(u \approx -1\), two peaks \(u \approx 1\)) at around \(t = 12\) before switching to a two-plateau solution (one well, one peak) at around \(t = 70\).

The Korteweg-de Vries (KdV) equation,

\[
u_t = -u_{xxx} - uu_x,
\]

was derived by Korteweg and de Vries in 1895 to model the propagation of waves in shallow water [31]. It couples dispersion \(−u_{xxx}\) with nonlinear convection \(−uu_x\). Among the solutions of (3.7) are solitary waves or solitons. These are waves that maintain their shapes as they travel and are given by

\[
u(t, x) = 3c \text{sech}^2\left(\frac{\sqrt{c}}{2}(x - x_0 - ct)\right), \quad c > 0.
\]  

Waves of the form (3.8) have amplitude \(3c\) and travel at constant speed \(c\). This is contrast to solutions of linear wave equations \(\nu_t = -cu_x\), which all travel at velocity \(c\), regardless of their amplitudes. In Fourier space, (3.7) becomes

\[
\hat{u}' = ik^3\hat{u} - \frac{ik}{2}\mathcal{F}\left((\mathcal{F}^{-1}\hat{u})^2\right).
\]  

We take

\[
u(0, x) = 3A^2\text{sech}^2\left(\frac{A}{2}(x + 2)\right) + 3B^2\text{sech}^2\left(\frac{B}{2}(x + 1)\right), \quad x \in [-\pi, \pi],
\]

with \(A = 25\) and \(B = 16\), and solve up to \(t = 10^{-2}\). This is a superposition of two solitons with speed \(A^2\) and \(B^2\) initially centred at \(x = -2\) and \(x = -1\), respectively. The stronger wave \((A = 25)\) catches up with the weaker one \((B = 16)\) at around \(t = 10^{-3}\). Both waves remain unchanged after the interaction, the only nonlinear effect being a forward shift

\[
\frac{1}{A^2} \log \left(\frac{A^2 + B^2}{A^2 - B^2}\right)^2
\]  

(3.11)
for the stronger wave and a backward shift
\[- \frac{1}{B^2} \log \left( \frac{A^2 + B^2}{A^2 - B^2} \right)^2 \] (3.12)
for the weaker one. The interaction ends at around \( t = 3.5 \times 10^{-3} \). Figure 1.1 shows the initial condition.

The Kuramoto-Sivashinsky equation,
\[ u_t = -u_{xx} - u_{xxxx} - uu_x, \] (3.13)
dates to the mid-1970s with the work of Kuramoto [33] and Sivashinsky [48]. It couples destabilizing \(-u_{xx}\) and stabilizing \(-u_{xxxx}\) diffusions with nonlinear convection \(-uu_x\). The nonlinear term shifts energy created at low wavenumbers by the second-order term to high wavenumbers where the fourth-order term stabilises. The Kuramoto-Sivashinsky equation models various physical phenomena, from unstable drift waves in plasmas to thermal instabilities in laminar flame fronts. In the latter, the function \( u \) represents the perturbation of the flame front surface. The solutions of (3.13) can demonstrate a wide range of spatio-temporal dynamics, including chaos. In Fourier space, (3.13) becomes
\[ \hat{u}' = (k^2 - k^4)\hat{u} - \frac{ik}{2} F \left( \left| F^{-1} \hat{u} \right|^2 F^{-1} \hat{u} \right). \] (3.14)

We take
\[ u(0, x) = \cos \left( \frac{x}{16} \right) \left( 1 + \sin \left( \frac{x}{16} \right) \right), \quad x \in [0, 32\pi], \] (3.15)
and solve up to \( t = 100 \). This simple initial data progressively evolves into a much more complicated superposition of wavenumbers and, even though the solution looks quite complicated, a characteristic pattern emerges from \( t \approx 50 \).

The (focusing) nonlinear Schrödinger equation,
\[ u_t = iu_{xx} + i|u|^2u, \] (3.16)
models several physical phenomena, including the nonlinear propagation of light in optical fibres. A nonlinear variant of the Schrödinger equation, it couples dispersion \( iu_{xx} \) with a nonlinear potential \( i|u|^2u \). Note that the wave function \( u \) is complex-valued. Among the solutions of (3.16) are breathers, given by
\[ u(t, x) = A \left( \frac{2B^2 \cosh(\theta) + 2iB\sqrt{2 - B^2} \sinh(\theta)}{2\cosh(\theta) - \sqrt{2}\sqrt{2 - B^2} \cos(ABx)} - 1 \right) e^{i\lambda^2 t}, \quad \theta = A^2 B \sqrt{2 - B^2} t, \ B \leq \sqrt{2}. \] (3.17)
These are nonlinear waves in which energy concentrates in a localized and oscillatory fashion. In Fourier space, (3.16) becomes
\[ \hat{u}' = -ik^2 \hat{u} + iF \left( \left| F^{-1} \hat{u} \right|^2 F^{-1} \hat{u} \right). \] (3.18)

We take
\[ u(0, x) = \frac{2AB^2}{2 - \sqrt{2}\sqrt{2 - B^2} \cos(ABx)} - A, \quad x \in [-\pi, \pi], \] (3.19)
with \( A = 2 \) and \( B = 1 \), and solve up to \( t = 2 \). This is a breather whose amplitude oscillates in time around the value \( A \). Figure 1.1 shows the initial condition.
3.2. Model problems in 2D and 3D. The (complex) Ginzburg-Landau equation,

\[ u_t = (1 + iA)\Delta u + u - (1 + iB)u|u|^2, \]  

(3.20)

was first derived in 2D by Stewartson and Stuart in 1971 to study non-linear instabilities in plane Poiseuille flow [49], using concepts from Ginzburg-Landau theory for superconductivity. The function \( u \) is the amplitude of a non-linear perturbation wave for values of the Reynolds number close to the critical value, above which perturbations may grow. Equation (3.20) admits solutions known as frozen states which correspond to quasi-frozen spiral defects surrounded by shock lines. In this regime, \(|u|\) is stationary in time. We take \( A = 0 \) and \( B = 1.5 \),

\[ u(0, x, y) = e^{-0.1((x-50)^2+(y-50)^2)}, \quad (x, y) \in [0, 100]^2, \]  

(3.21) and

\[ u(0, x, y, z) = e^{-0.1((x-50)^2+(y-50)^2+(z-50)^2)}, \quad (x, y, z) \in [0, 100]^3, \]  

(3.22)

and solve up to \( t = 10 \) in both 2D and 3D. These two initial conditions generate spiral waves. Figure 1.1 shows an example of a 2D frozen state solution at \( t = 30 \), obtained with an initial condition of amplitude 0.1 involving random noise on the grid.

The Schnakenberg equations,

\[
\begin{aligned}
    u_t &= \epsilon_u \Delta u + \gamma (a - u + u^2 v), \\
    v_t &= \epsilon_v \Delta v + \gamma (b - u^2 v),
\end{aligned}
\]

(3.23)

are reaction-diffusion equations derived by Schnakenberg in 1979 to study limit cycle behaviours of two-component chemical reactions [17]. The system (3.23) models the chemical reaction \( 2U + V \rightarrow 3U \); \( U \rightarrow A \); \( B \rightarrow V \); \( u \) and \( v \) are the concentrations of \( U \) and \( V \), and \( A \) and \( B \) are another two chemical species, assumed to be maintained at constant concentrations \( a \) and \( b \). We take \( \epsilon_u = 1 \), \( \epsilon_v = 0.1 \), \( \gamma = 1 \), \( a = 0.1 \) and \( b = 0.9 \). The initial conditions are

\[
\begin{aligned}
    u(0, x, y) &= 1 - e^{-2((x-G/2.15)^2+(y-G/2.15)^2)}, \\
    v(0, x, y) &= 0.9 \left( 1.1^2 + .9^2 \right) + e^{-2((x-G/2)^2+2(y-G/2)^2)},
\end{aligned}
\]

(3.24)

with \( (x, y) \in [0, G]^2 \) and \( G = 30 \) in 2D, and

\[
\begin{aligned}
    u(0, x, y, z) &= 1 - e^{-2((x-G/2.15)^2+(y-G/2.15)^2+(z-G/2.15)^2)}, \\
    v(0, x, y, z) &= 0.9 \left( 1.1^2 + .9^2 \right) + e^{-2((x-G/2)^2+2(y-G/2)^2+2(z-G/2)^2)},
\end{aligned}
\]

(3.25)

with \( (x, y, z) \in [0, G]^3 \) and \( G = 30 \) in 3D. We solve up to \( t = 20 \) in both 2D and 3D. Note that these initial conditions are small perturbations from the constant solution \((u, v) = (a + b, b/(a + b)^2)\). They lead to a set of spots at around \( t = 500 \) in 2D and \( t = 300 \) in 3D. Figure 1.1 shows the 2D solution at \( t = 500 \).

The Swift-Hohenberg equation,

\[ u_t = ru - (1 + \Delta)^2 u + gu^2 - u^3, \]

(3.26)

was first derived in 2D by Swift and Hohenberg in 1977 to study thermal fluctuations on a fluid near the Rayleigh-Bénard convective instability [51]. In 2D, the function \( u \) is the temperature field.
Fig. 4.1: Fourier coefficients of the initial condition \((3.3)\) of the Allen-Cahn equation (left) and of the solution at \(t = 60\) computed with time-step \(h = 10^{-2}\) (right). With \(N = 512\) grid points, the Fourier coefficients decay to about \(10^{-17}\). In our computations for the Allen-Cahn equation, the smallest error due to the time discretization is equal to about \(10^{-12} \gg 10^{-17}\).

in a plane horizontal layer of fluid heated from below. Equation (3.26) is another example of a PDE that exhibits pattern formation, including stripes, spots and spirals. We take \(r = 0.1, g = 1\),

\[
    u(0, x, y) = \frac{1}{4} \left( \sin(\pi x/10) + \sin(\pi y/10) \right) + \sin(\pi x/2) \sin(\pi y/2), \quad (x, y) \in [0, 20]^2,
\]

and

\[
    u(0, x, y, z) = \frac{1}{4} \left( \sin(\pi x/10) + \sin(\pi y/10) + \sin(\pi z/10) + \sin(\pi x/2) \sin(\pi y/2) + \sin(\pi x/2) \sin(\pi z/2) + \sin(\pi y/2) \sin(\pi z/2) \right), \quad (x, y, z) \in [0, 20]^3,
\]

and solve up to \(t = 20\). Both of these two initial conditions lead to a set of spots. Figure 1.1 shows the 2D solution at \(t = 1000\) obtained with \(r = 0.1, g = 0\) and an initial condition of amplitude 0.1 involving random noise on the grid. This solution corresponds to the so-called convection rolls.

4. Numerical comparisons.

4.1. Methodology. To compare exponential integrators, we follow the methodology of [28], though the experiments described here are far more extensive. We solve a given PDE up to \(t = T\) for various time-steps \(h\) and a fixed number of grid points. We estimate the “exact” solution \(u_{ex}(T, X)\) at \(t = T\) by using a “very small” time-step (half the smallest time-step \(h\)) and the PECEC736 scheme (one of the two seventh-order accurate schemes in Table 2.2). The relative error between the computed solution \(u_{comp}(T, X)\) and \(u_{ex}(T, X)\) is then defined as

\[
    err = \frac{\|u_{comp}(T, X) - u_{ex}(T, X)\|_{\infty}}{\|u_{ex}(T, X)\|_{\infty}}.
\]

For both \(u_{ex}\) and \(u_{comp}\) we use \(N = 512\) grid points in 1D, \(N_x N_y = 128^2\) grid points in 2D and \(N_x N_y N_z = 128^3\) grid points in 3D. (With these grid sizes, the error due to the spatial discretization
is small compared to the error due to the time discretization, see Figure 4.1.) For the contours integrals, we use $M = 64$ points in 1D and $M = 32$ points in 2D and 3D. We plot (4.1) against relative time-steps $h/T$ and computer time on a pair of graphs. The former gives a measure of the accuracy of the exponential integrator for various time-steps or, equivalently, for various number of integration steps. (If the relative time-step is $10^{-3}$, it means that the integrator performed $10^3$ steps to reach $t = T$.) However, it is possible that each step is more costly, so it is the latter which ultimately matters. We compare different families on different pairs of graphs with curves for ETDRK4 included on all plots as a baseline. We have tested every integrator on every PDE, but we shall only show graphs that correspond to the characteristic behaviour of a family of integrators, or highlight notable features such as instability or particularly good/bad performances. The rest of the graphs can be found in the supplementary material.

4.2. Starting multistep schemes. To start a multistep scheme with $q$ steps, one needs $q$ values: the initial condition $\hat{u}^0$ and $q - 1$ extra values $\hat{u}^1, \ldots, \hat{u}^{q-1}$. It is suggested in [8] to use the following strategy: first, compute an approximation of $\hat{U} = (\hat{u}^1, \ldots, \hat{u}^{q-1})^T$ using a low-order exponential integrator (e.g., ETDRK2, the second-order version of ETDRK4, also introduced by Cox and Matthews in [13]), and then, use a fixed point iteration to refine this approximation. The fixed point iteration is applied to the following system of nonlinear equations,

$$\hat{u}^j = e^{jhL} \hat{u}^0 + h \sum_{i=0}^{q-1} \gamma_i(j, hL) \Delta^i N(\hat{u}^0), \quad 1 \leq j \leq q - 1,$$

(4.2)

where $\Delta^j$ is the forward difference operator,

$$\Delta^0 N(\hat{u}^0) = \hat{u}^0, \quad \Delta^i N(\hat{u}^0) = \sum_{i=0}^{l} (-1)^i \binom{l}{i} N(\hat{u}^{l-i}), \quad l \geq 1,$$

(4.3)

and the $\gamma$-functions are defined by the recurrence relation,

$$\gamma_0(k, z) = \frac{e^{kz} - 1}{z},
$$

$$\gamma_j(k, z) = \left( \sum_{m=1}^{j} \frac{(-1)^{m-1}}{m} \gamma_{j-m}(k, z) \right) - \frac{k}{j}, \quad 1 \leq j \leq k,$$

(4.4)

$$\gamma_j(k, z) = \left( \sum_{m=1}^{j} \frac{(-1)^{m-1}}{m} \gamma_{j-m}(k, z) \right) \frac{1}{z}, \quad j > k.$$

Note that, like the $\varphi$-functions, the $\gamma$-functions can be evaluated by contour integrals and satisfy the symmetry property $\gamma(\bar{z}) = \bar{\gamma}(z)$ for all $z \in \mathbb{C}$. Let us write (4.2) as $\hat{U} = F(\hat{U})$. The fixed point iteration is then given by

$$\hat{U}_{[n+1]} = F(\hat{U}_{[n]}),$$

(4.5)

6The precomputation of the coefficients of the exponential integrators and the starting phase of multistep methods are not included in the computing time. Timings were done on a 2.8 GHz Intel i7 machine with 16 GB of RAM.
where $\hat{U}_{[n]} = (\hat{u}_1^{[n]}, \ldots, \hat{u}_q^{[n]-1})^T$ denotes the approximation obtained after $n$ iterations ($\hat{U}_{[0]}$ corresponding to the approximation given by ETDRK2). The fixed point iteration (4.5) is carried out until the norm of the difference between two successive iterations is of the order of $h^q$.

4.3. Results. We now report on the results of our numerical testing and present plots showing the typical behaviours and notable features we see from each set of methods.

Figure 4.2 shows results for ETD Adams-Bashforth methods. These formulas are often unstable for large time-steps but can be competitive at high accuracies. For the Cahn-Hilliard and KdV equations, we could not get them to work at all with the spatial discretization that we used.

Figure 4.3 shows results for ETD Runge-Kutta methods. These formulas have good stability properties. The fourth-order methods have similar performance to ETDRK4. The fifth-order EX-PRK5S8 integrator is impressively efficient in 1D, but it exhibits instability for the Cahn-Hilliard and KdV equations. In 2D and 3D, it is more accurate than the fourth-order methods for the six PDEs we have considered, and more efficient for the Ginzburg-Landau equation. For the Schnakenberg and Swift-Hohenberg equations, it is not accurate enough to counterbalance its high cost per time-step.

Figure 4.4 shows results for Lawson methods. These formulas are not accurate enough to be competitive. For the ABLawson4 formula, this lack of accuracy is partly compensated by its low computational cost per time-step (it is a purely multistep method).

Figure 4.5 shows results for generalised Lawson methods. In 1D, these formulas suffer from instabilities for most PDEs, especially for the Cahn-Hilliard and KdV equations. In 2D and 3D, the GenLawson41 formula has virtually identical performance to ETDRK4, the GenLawson42 formula is always less efficient than ETDRK4, while the other variants with three to five steps perform well for the Ginzburg-Landau equation but are less efficient for the Schnakenberg and Swift-Hohenberg equations.

Figure 4.6 shows results for modified generalised Lawson methods. In 1D, these formulas are much more stable than the generalized Lawson schemes and are quite efficient, but still suffer from
Fig. 4.3: Accuracy versus time-step and computer time for the ETD Runge-Kutta methods for the 1D Cahn-Hilliard (top), 1D KdV (centre) and 3D Schnakenberg (bottom) equations. The EXPRK5S8 scheme is impressively efficient in 1D but is unstable at low accuracies for the Cahn-Hilliard and KdV equations. In 2D and 3D, it does not beat the fourth-order methods for the Schnakenberg and Swift-Hohenberg equations.

instabilities for the 1D KdV equation. In 2D and 3D, we reach the same conclusions as for the generalized Lawson methods: the ModGenLawson41 formula has virtually identical performance to ETDRK4, the ModGenLawson42 formula is always the least efficient and the other variants perform well for some problems but are less efficient for others.
Fig. 4.4: Accuracy versus time-step and computer time for the Lawson methods for the 1D nonlinear Schrödinger equation. These formulas are too inaccurate to be competitive. The constants involved in the convergence bounds are too great.

Figure 4.7 shows results for exponential predictor-corrector methods. These formulas are particularly efficient in 1D, especially for the Kuramoto-Sivashinsky and nonlinear Schrödinger equations, but do not clearly outperform ETDRK4 for the Allen-Cahn equation. Most of them are unstable at low accuracies for the Cahn-Hilliard equation, especially the higher-order ones, and some of them are also unstable at low accuracies for the KdV equation. In 2D and 3D, they are more efficient than ETDRK4 for the Ginzburg-Landau equation and have similar performance to it for the Schnakenberg equations. The higher-order ones with two steps (PEC625 and PEC726) also beat ETDRK4 for the Swift-Hohenberg equations. Note that these methods are particularly unstable for the Cahn-Hilliard and KdV equations.

5. Discussion. We have tested thirty exponential integrators on eleven model problems in 1D, 2D and 3D, and have observed considerable differences in stability and efficiency. The main conclusion is that it is difficult to find a method that outperforms ETDRK4 for all the PDEs we have considered.

Our experiments show that the ETD Adams-Bashforth and the generalised Lawson methods are highly unstable while the Lawson methods are not accurate enough. Within the ETD Runge-Kutta methods, it is hard to do much better than ETDRK4. The fourth-order schemes are quite similar in terms of efficiency and stability. The fifth-order EXPRK5S8 integrator is more efficient than ETDRK4 for most PDEs in 1D, but is unstable at low accuracies for the KdV and Cahn-Hilliard equations. In 2D and 3D, it outperforms ETDRK4 only for the Ginzburg-Landau equation. Since it requires the precomputation of more than twice as many coefficients as ETDRK4, it makes it much more complicated to implement and probably less appealing to general users. The high-order modified generalised Lawson and exponential predictor-corrector methods are competitive stiff solvers for some PDEs, but for others do not beat ETDRK4 or else suffer from instabilities.

Our numerical experiments were performed using Chebfun, a MATLAB-based package for computing with functions to about 15 digits of accuracy. Its extensions to periodic problems [62], 2D [56] and 3D [20] provide a very convenient framework for solving semilinear stiff PDEs in 1D/2D/3D periodic domains. More specifically, the spin, spin2 and spin3 codes implement a Fourier spectral
Fig. 4.5: Accuracy versus time-step and computer time for the generalised Lawson methods for the 1D Kuramoto-Sivashinsky (top) and 2D Ginzburg-Landau (bottom) equations. These methods are highly unstable for most PDEs in 1D. In 2D and 3D, the GenLawson41 formula has virtually identical performance to ETDRK4 while the other variants with three to five steps perform well for some problems (e.g., 2D Ginzburg-Landau equation) but are less efficient for others.

method in space with an exponential integrator in time. The simplest way to see spin in action is to type simply \texttt{spin(‘ks’)} (for the Kuramoto-Sivashinsky equation) or \texttt{spin2(‘g12’)} (for the 2D Ginzburg-Landau equation) to invoke an example computation. It is also possible to define your own PDE using the \texttt{spinop} class. To produce the graphs of Section 4, we have used the \texttt{spincomp} code—check out \url{www.chebfun.org} to learn more about \texttt{spin}, \texttt{spinop} and \texttt{spincomp}.

Acknowledgements. This paper is dedicated to Nick Trefethen on his 60th birthday and his inspirational contributions to the field of numerical analysis.

Appendix A: Trigonometric interpolation and Fourier spectral methods in 1D. Let $u(x)$ be a periodic function on $[0, 2\pi]$, possibly complex-valued. Let \{\(x_j = 2\pi j/N\), $0 \leq j \leq N - 1$\}, denote $N$ equispaced points in $[0, 2\pi)$ and \{\(u_j = u(x_j)\), $0 \leq j \leq N - 1$\}, the values of $u$ at the points $x_j$. For an even number $N$, the trigonometric interpolant $p_N(x)$ of $u(x)$ at these points is
Fig. 4.6: Accuracy versus time-step and computer time for the modified generalised Lawson methods for the 1D Kuramoto-Sivashinsky (top), 1D KdV (centre) and 3D Swift-Hohenberg (bottom) equations. In 1D, these methods are much more stable than the generalised Lawson methods (e.g., 1D Kuramoto-Sivashinsky equation) but are still highly unstable for the KdV equation. In 2D and 3D, they are very similar to the generalised Lawson methods.

defined by

\[ p_N(x) = \sum_{k=-N/2}^{N/2} \hat{u}_k e^{ikx}, \quad \hat{u}_k = \frac{1}{N} \sum_{j=0}^{N-1} u(x_j) e^{-ikx_j}, \quad -\frac{N}{2} \leq k \leq \frac{N}{2} - 1, \quad \hat{u}_{N/2} = \hat{u}_{-N/2}, \quad (5.1) \]
Fig. 4.7: Accuracy versus time-step and computer time for the predictor-corrector methods for the 1D Allen-Cahn (top), 1D Cahn-Hilliard (centre) and 2D Schnakenberg equations (bottom). In 1D, these schemes are efficient, but do not clearly outperform ETDRK4 for the Allen-Cahn equation and are unstable at low accuracies for the Cahn-Hilliard equation. In 2D and 3D, they beat ETDRK4 for some problems but have similar performance for others (e.g., 2D Schnakenberg equations).

while, for an odd number $N$, it is defined by

$$p_N(x) = \sum_{k=-\frac{N-1}{2}}^{\frac{N-1}{2}} \hat{u}_k e^{ikx}, \quad \hat{u}_k = \frac{1}{N} \sum_{j=0}^{N-1} u(x_j) e^{-ikx_j}, \quad -\frac{N-1}{2} \leq k \leq \frac{N-1}{2}. \quad (5.2)$$
The prime on the summation sign in (5.1) signifies that the terms \( k = \pm N/2 \) are halved.

The philosophy of Fourier spectral methods (in coefficient space) is the following: interpolate \( u(x) \) by \( p_N(x) \) with Fourier coefficients \( \hat{u}_k \), and, to compute derivatives, multiply \( \hat{u}_k \) by the appropriate power of \( ik \). Since differentiation is a linear operation, it can be represented by matrices. The (diagonal) first-order Fourier differentiation matrix is the matrix which maps the Fourier coefficients of \( p_N(x) \) to the Fourier coefficients of \( p_N'(x) \), and has entries \((0, ik)\) with \(|k| \leq N/2 - 1\) for \( N \) even and \( ik \) with \(|k| \leq (N - 1)/2\) for \( N \) odd. (Note that for \( N \) even, the first entry is 0, as opposed to \(-iN/2\). It is related to the derivative of the sawtooth wave on the grid being zero and not a complex exponential [57, Chapter 3].) More generally, for \( N \) odd and any \( m \geq 1 \), the \( m^{th} \)-order Fourier differentiation matrix has entries \((ik)^m\) with \(|k| \leq (N - 1)/2\). For \( N \) even and \( m \) odd, it has entries \((0, (ik)^m)\) with \(|k| \leq N/2 - 1\) while for \( m \) even it has entries \((i(ik)^m)\) with \(-N/2 \leq k \leq N/2 - 1\).

At every time-step, we look for a solution of the form (5.1)–(5.2), so that the Fourier coefficients become functions of time \( t \), as in (1.3)–(1.4).

Appendix B: Trigonometric interpolation and Fourier spectral methods in 2D and 3D. In 2D, we look for solutions of the form

\[
    u(t, x, y) \approx \sum_{k=-N/2}^{N/2} \sum_{l=-N/2}^{N/2} \hat{u}_{k,l}(t)e^{ikx}e^{ily}, \quad (x, y) \in [0, 2\pi]^2,
\]

with \( N \) points \( \{x_j = 2\pi j/N_x\}_{j=0}^{N_x-1} \) in the \( x \)-direction and \( N \) points \( \{y_j = 2\pi j/N_y\}_{j=0}^{N_y-1} \) in the \( y \)-direction, and appropriate rescaling for different domains. The unknowns, at each time \( t \), are the \( N \times N \) Fourier coefficients \( \hat{u}_{k,l}(t) \), stored as a \( N_x N_y \times 1 \) vector. In 3D, we look for solutions of the form

\[
    u(t, x, y, z) \approx \sum_{k=-N/2}^{N/2} \sum_{l=-N/2}^{N/2} \sum_{m=-N/2}^{N/2} \hat{u}_{k,l,m}(t)e^{ikx}e^{ily}e^{imz}, \quad (x, y, z) \in [0, 2\pi]^3,
\]

with the same \( N_x \) and \( N_y \) points in the \( x \) and \( y \) directions, \( N_z \) points \( \{z_j = 2\pi j/N_z\}_{j=0}^{N_z-1} \) in the \( z \)-direction, and appropriate rescaling for different domains. The unknowns, at each time \( t \), are the \( N_x N_y N_z \) Fourier coefficients \( \hat{u}_{k,l,m}(t) \), stored as a \( N_x N_y N_z \times 1 \) vector. Again, the primes on the summation signs in (5.3)–(5.4) signify that the extreme terms are halved.

To construct the matrix \( \mathbf{L} \), we use Kronecker products and the Fourier differentiation matrices of Appendix A. For example, in 2D, the Laplacian operator

\[
    \mathbf{L}u = \Delta u = uu_{xx} + uu_{yy},
\]

is discretized by the \( N_x N_y \times N_x N_y \) matrix

\[
    \mathbf{L} = \mathbf{I} \otimes \mathbf{D}^{(2)} + \mathbf{D}^{(2)} \otimes \mathbf{I},
\]

We describe in this section Fourier spectral methods in coefficient space. See [57] for details about Fourier spectral methods in value space.
where $I$ is the identity matrix and $D^{(2)}$ is the second-order Fourier differentiation matrix. Note that the first $I$ and the second $D^{(2)}$ are $N_y \times N_y$ while the first $D^{(2)}$ and the second $I$ are $N_x \times N_x$. Similarly, the two-dimensional biharmonic operator,

$$L u = \Delta^2 u = u_{xxxx} + u_{yyyy} + 2u_{xxyy}, \quad (5.7)$$

is discretized by the $N_xN_y \times N_xN_y$ matrix

$$L = I \otimes D^{(4)} + D^{(4)} \otimes I + 2(D^{(2)} \otimes I)(I \otimes D^{(2)}), \quad (5.8)$$

where $D^{(4)}$ is the fourth-order Fourier differentiation matrix, i.e., the matrix with entries $k^4$. Again, ones has to be careful with the dimensions of the matrices. In 3D, the Laplacian operator,

$$L u = \Delta u = u_{xx} + u_{yy} + u_{zz}, \quad (5.9)$$

is discretized by the $N_xN_yN_z \times N_xN_yN_z$ matrix

$$L = I \otimes I \otimes D^{(2)} + I \otimes D^{(2)} \otimes I + D^{(2)} \otimes I \otimes I, \quad (5.10)$$

while the three-dimensional biharmonic operator,

$$L u = \Delta^2 u = u_{xxxx} + u_{yyyy} + u_{zzzz} + 2u_{xxyy} + 2u_{xxzz} + 2u_{yyzz}, \quad (5.11)$$

is discretized by the $N_xN_yN_z \times N_xN_yN_z$ matrix

$$L = I \otimes I \otimes D^{(4)} + I \otimes D^{(4)} \otimes I + D^{(4)} \otimes I \otimes I + 2(I \otimes D^{(2)} \otimes I)(I \otimes I \otimes D^{(2)}) \quad + 2(D^{(2)} \otimes I \otimes I)(I \otimes I \otimes D^{(2)}) + 2(D^{(2)} \otimes I \otimes I)(I \otimes D^{(2)} \otimes I), \quad (5.12)$$

with matrices of appropriate dimensions. Note that Kronecker products can be computed within MATLAB using the `kron` command, and that the matrices (5.6), (5.8), (5.10), and (5.12) are diagonal.

REFERENCES

[1] A. H. AL-MOHY AND N. J. HIGHAM, Computing the action of the matrix exponential, with an application to exponential integrators, SIAM J. Sci. Comput., 33 (2011), pp. 488–511.

[2] S. M. ALLEN AND J. W. CAHN, A microscopic theory for antiphase boundary motion and its application to antiphase domain coarsening, Acta Metall., 27 (1979), pp. 1085–1095.

[3] 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 (1995), pp. 797–823.

[4] H. BERLAND, B. SCAFLESTAD, AND W. M. WRIGHT, EXPINT—A MATLAB package for exponential integrators, ACM Trans. Math. Softw. (TOMS), 33 (2007), pp. 4:1–4:17.

[5] G. BEYKLIN, J. M. KEISER, AND L. VOZOVII, A new class of time discretization schemes for the solution of nonlinear PDEs, J. Comput. Phys., 147 (1998), pp. 362–387.

[6] N. BOOTLAND, Exponential integrators for stiff PDEs, Master’s thesis, University of Oxford, 2014.

[7] J. W. CAHN AND J. E. HILLIARD, Free energy of a nonuniform system. I. Interfacial free energy, The Journal of Chemical Physics, 28 (1958), pp. 258–267.

[8] M. P. CALVO AND C. PALENCIAS, A class of multistep exponential integrators for semilinear problems, Numer. Math., 102 (2006), pp. 367–381.

[9] B. CANO AND A. GONZÁLEZ-PACHÓN, Exponential time integration of solitary waves of cubic Schrödinger equation, Appl. Numer. Math., 91 (2015), pp. 26–45.

[10] Projected explicit Lawson methods for the integration of Schrödinger equation, Numer. Methods Partial Differential Eq., 31 (2015), pp. 78–104.
EXPONENTIAL INTEGRATORS FOR PERIODIC STIFF PDES

[43] G. Rainwater and M. Tokman, A new class of split exponential propagation iterative methods of Runge-Kutta type (sEPIRK) for semilinear systems of ODEs, J. Comput. Phys., 269 (2014), pp. 40–60.

[44] H. H. Rosenbrock, Some general implicit processes for the numerical solution of differential equations, Computer, 5 (1963), pp. 329–330.

[45] T. Schmelzer and L. N. Trefethen, Evaluating matrix functions for exponential integrators via Carathéodory-Fejér approximation and contour integrals, ETNA, 29 (2007), pp. 1–18.

[46] J. Schnakenberg, Simple chemical reaction systems with limit cycle behaviour, J. Theor. Biol., 81 (1979), pp. 389–400.

[47] G. I. Sivashinsky, Nonlinear analysis of hydrodynamic instability in laminar flames—I. Derivation of basic equations, Acta Astronautica, 4 (1977), pp. 1177–1206.

[48] M. Tokman, Efficient integration of large stiff systems of ODEs with exponential propagation iterative (EPI) methods, J. Comput. Phys., 213 (2006), pp. 748–776.

[49] M. Tokman and J. Loffeld, Efficient design of exponential-Krylov integrators for large scale computing, Procedia Comp. Sci., 1 (2012), pp. 229–237.

[50] A. Townsend and L. N. Trefethen, An extension of Chebfun to two dimensions, SIAM J. Sci. Comput., 35 (2013), pp. C495–C518.

[51] L. N. Trefethen, Spectral Methods in MATLAB, SIAM, Philadelphia, 2000.

[52] L. N. Trefethen and J. A. C. Weideman, The exponentially convergent trapezoidal rule, SIAM Rev., 56 (2014), pp. 385–458.