

THE DISCRETE ADJOINT METHOD FOR EXPONENTIAL INTEGRATION

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Abstract. The implementation of the discrete adjoint method for exponential time differencing (ETD) schemes is considered. This is important for parameter estimation problems that are constrained by stiff time-dependent PDEs when the discretized PDE system is solved using an exponential integrator. We also discuss the closely related topic of computing the action of the sensitivity matrix on a vector, which is required when performing a sensitivity analysis. The PDE system is assumed to be semi-linear and can be the result of a linearization of a nonlinear PDE, leading to exponential Rosenbrock-type methods. We discuss the computation of the derivatives of the φ -functions that are used by ETD schemes and find that the derivatives strongly depend on the way the φ -functions are evaluated numerically. A general adjoint exponential integration method, required when computing the gradients, is developed and its implementation is illustrated by applying it to the Krogstad scheme. The applicability of the methods developed here to pattern formation problems is demonstrated using the Swift-Hohenberg model.

Key words. Exponential integration, parameter estimation, sensitivity analysis, inverse problems, adjoint method, semi-linear PDE, Rosenbrock method, gradient-based optimization, high-order time-stepping methods, pattern formation, Swift-Hohenberg equation

AMS subject classifications. Partial Differential Equations, Numerical Analysis, Optimization

1. Introduction. Large-scale distributed parameter estimation is an important type of inverse problem dealing with the recovery or approximation of the model parameters appearing in partial differential equations (PDEs). The PDE system models some real-life process and observations of this process, which usually contain noise, are compared to numerically computed solutions of the PDEs. Parameter estimation problems, often referred to as model calibration, are very common in engineering, many branches of science, economics, and elsewhere.

In this paper we consider such inverse problems in the context of stiff, time-dependent, semi-linear PDEs. Using the method of lines approach, the PDE is discretized in space by applying a finite difference, finite volume or finite element method, where the (known) boundary and initial conditions are assumed to have already been incorporated. This results in a large system of ordinary differential equations (ODEs) that can be written in generic first-order form as

$$(1.1) \quad \begin{aligned} \frac{\partial \mathbf{y}(t; \mathbf{m})}{\partial t} &= \mathbf{f}(\mathbf{y}(t; \mathbf{m}), t, \mathbf{m}) \\ &= \mathbf{L}(\mathbf{m})\mathbf{y}(t; \mathbf{m}) + \mathbf{n}(\mathbf{y}(t; \mathbf{m}), t, \mathbf{m}) \\ \mathbf{y}(0) &= \mathbf{y}_0, \end{aligned}$$

on an underlying discrete spatial grid, with $0 \leq t \leq T$. The vector $\mathbf{m} \in \mathbb{R}^{N_m}$ is the set of discretized model parameters that could, for instance, represent some physical properties of the underlying material that we want to estimate. We refer to $\mathbf{y} = \mathbf{y}(t; \mathbf{m})$ in this context as the *forward solution*. It is a time-dependent vector of length N and depends on \mathbf{m} indirectly through the discretized operators \mathbf{L} and \mathbf{n} . The operator \mathbf{L} contains the leading derivatives and is linear, while \mathbf{n} is generally nonlinear in \mathbf{y} . Many interesting PDEs have this form.

The problem of estimating the parameters in (1.1) based on a given set of measurements is often tackled using gradient-based optimization procedures. For large-scale problems, the adjoint method is a well-known efficient approach to computing the required gradients. The

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goal of this study is to systematically implement the discrete adjoint method for the case where a fully discretized version of (1.1) is solved using an exponential time differencing (ETD) scheme [13, 3, 17], also known as an exponential integrator. These methods have come to form an important approach for numerically solving PDEs, particularly when the PDE system exhibits stiffness in time; yet they pose several challenges in carrying out their corresponding adjoint method. Our results are also relevant to the problem of sensitivity analysis, where the efficient computation of the action of the sensitivity matrix on a vector is required.

1.1. PDE-Constrained Optimization. The parameter estimation problem is to recover a feasible set of parameters \mathbf{m} that approximately solves the PDE-constrained optimization problem

$$(1.2) \quad \mathbf{m}^* = \arg \min_{\mathbf{m}} \Omega(\mathbf{m}) \quad \text{s.t. (1.1) holds,}$$

where the *objective function*

$$\Omega(\mathbf{m}) = \Omega(\mathbf{d}, \mathbf{d}^{\text{obs}}; \mathbf{m}, \mathbf{m}^{\text{ref}}) = M(\mathbf{d}, \mathbf{d}^{\text{obs}}) + \beta R(\mathbf{m}, \mathbf{m}^{\text{ref}})$$

has two components. The *regularization function* $R(\mathbf{m}, \mathbf{m}^{\text{ref}})$ penalizes straying too far away from the prior knowledge we have of the true parameter values (which is incorporated in \mathbf{m}^{ref}). Common examples are Tikhonov-type regularization [6, 34], including least squares and total variation (TV) [35]. The *data misfit function* $M(\mathbf{d}, \mathbf{d}^{\text{obs}})$ in some way quantifies the difference between \mathbf{d} and \mathbf{d}^{obs} , with \mathbf{d}^{obs} a given set of observations of the true solution and $\mathbf{d} = \mathbf{d}(\mathbf{m}) = \mathbf{d}(\mathbf{y}(\mathbf{m}))$ the observation of the current simulated solution, depending on \mathbf{m} implicitly through the forward solution.

The most popular choice for M , corresponding to the assumption that the noise in the data is simple and white, is the least-squares function $M = \frac{1}{2} \|\mathbf{d} - \mathbf{d}^{\text{obs}}\|_2^2$; but we will not restrict our discussion to any particular misfit function. The relative importance of the data misfit and prior is adjusted using the regularization parameter β .

Several classes of optimization procedures can be used to solve (1.2), see for instance [6, 35, 34]. Typically, all reduced space methods for PDE-constrained optimization require the gradient of Ω with respect to \mathbf{m} , $\nabla_{\mathbf{m}}\Omega = \nabla_{\mathbf{m}}M + \beta\nabla_{\mathbf{m}}R$ [25, 4]. The derivatives of the regularization function are known and are independent of the time-stepping scheme, so in this paper we focus exclusively on computing the gradient of the misfit function M .

1.2. The Adjoint Method. The gradient of the misfit function requires computing the action of \mathbf{J}^T , where $\mathbf{J} = \frac{\partial \mathbf{d}}{\partial \mathbf{m}}$ is the sensitivity matrix. This matrix function stores the first-order derivatives of the predicted data with respect to the model parameters and can be calculated explicitly in small-scale applications. However, in cases such as those considered here it is far more feasible to compute the action of the sensitivity matrix on a vector using the adjoint method. Originally developed in the optimal control community, the adjoint method was introduced in [2] to the theory of inverse problems to efficiently compute the gradient of a function. See [26] for a review of the method applied to geophysical problems.

There are two frameworks that one can take when computing derivatives of the misfit function, discretize-then-optimize (DO) or optimize-then-discretize (OD). In OD one forms the adjoint differential problem, for either the given PDE or its semi-discretized form (1.1), which is subsequently discretized, thus decoupling the discretization process of the problem from that of its adjoint. A disadvantage of this approach is that the gradients of the discretized problem are not obtained exactly, because a discretization error gets introduced when moving from the continuous setting [9]. We therefore prefer the DO approach, where one applies

the adjoint method to the fully discretized form (1.1). The time-stepping method is therefore of central importance and this article addresses the implementation of the discrete adjoint method where the time-stepping method is an ETD scheme.

An alternative approach to computing the gradient that falls inside the DO framework is automatic differentiation (AD) [8, 24]. AD is a great tool for many purposes, but for large-scale problems where efficiency and memory allocation are essential, the adjoint method approach is advantageous when performance is crucial. In such circumstances it is preferable to have hard-coded and optimizable gradient and sensitivity computations. Having an explicit algorithm for the adjoint time-stepping method, as we develop here, allows one to exploit opportunities to increase the computational efficiency, such as parallelization and the precomputation of repeated quantities. Furthermore, it would require a very sophisticated AD code to compute the derivatives of the φ -functions that arise in ETD schemes, further elaborated upon in Sections 2 and 3.

1.3. Main Contributions and Structure of this Article. Exponential integration methods are reviewed in Section 2. It is shown how to abstractly represent them in the form $\mathbf{t}(\mathbf{y}, \mathbf{m}) = \mathbf{0}$, which we need when applying the discrete adjoint method. We also review Rosenbrock-type methods, since our techniques can be applied to them as well [15, 14, 20, 22].

ETD schemes require the use of φ -functions that are introduced in Section 2 and whose numerical evaluation is briefly reviewed in Section 3.

In Section 4 we apply the discrete adjoint method to the abstract time-stepping representation derived in Section 2. Derivatives of \mathbf{t} with respect to both the solution and the model parameters \mathbf{m} are required, and we derive expressions for them in Section 5. These expressions require the derivatives of the φ -functions when the discretized linear operator \mathbf{L} depends on the solution or the model parameters, and we discuss their differentiation in Section 6.

Section 7 discusses the linearized forward problem that must be solved when computing the action of the sensitivity matrix on some vector. In Section 8 we present the solution of the adjoint problem needed when computing the action of the transpose of the sensitivity matrix, thereby also playing a central role in the calculation of the gradient $\nabla_{\mathbf{m}}\mathbf{M}$. We give general algorithms applicable to any ETD scheme in these sections, and also illustrate their implementation using the ETD scheme of [17].

The results of this work are used in Section 9 to solve a simple parameter estimation problem involving the Swift-Hohenberg model, a PDE problem with solutions exhibiting the interesting phenomenon of pattern formation. Some final thoughts and avenues for future work are provided in Section 10.

2. Exponential Time Differencing. When considering time discretizations for the semi-discretized PDE (1.1), it is often convenient to suppress the dependence on \mathbf{m} in the notation.

Exponential time differencing methods, also referred to as exponential integrators, were originally developed in the 1960s [1, 27] and have attracted much recent attention [13, 19, 18, 21, 32, 31]. This has become an important approach to numerically solving PDEs, particularly when the PDE system exhibits stiffness. Let us discretize the time interval as $0 = t_0 < t_1 < \dots < t_K = T$, with a possibly variable time-step size $\tau_k = t_{k+1} - t_k$. Consider (1.1) and let \mathbf{y}_k denote the approximation of its solution $\mathbf{y}(t_k)$ at time t_k .

Before we review exponential integration, we first give a quick overview of Rosenbrock-type methods. Here, an ODE system resulting from a spatial semi-discretization of a fully nonlinear time-dependent PDE $\frac{\partial}{\partial t}\mathbf{y}(t) = \mathbf{f}(\mathbf{y}(t), t)$ is written in semi-linear form, after

which an exponential integrator can be applied. This can be done by writing

$$\mathbf{f}(\mathbf{y}(t), t) = \mathbf{L}_k \mathbf{y}(t) + \mathbf{n}_k(\mathbf{y}(t), t),$$

where $\mathbf{n}_k(\mathbf{y}(t), t) = \mathbf{f}(\mathbf{y}(t), t) - \mathbf{L}_k \mathbf{y}(t)$. ETD schemes are applied to this linearization, involving exponentiation of the matrix \mathbf{L}_k and leading to exponential Rosenbrock-type methods [15, 14]. The matrix \mathbf{L}_k is meant to approximate the Jacobian $\frac{\partial \mathbf{f}}{\partial \mathbf{y}}(\mathbf{y}_k, t_k)$ at the k th time-step. Occasionally it is sufficient to select $\mathbf{L}_k = \mathbf{L}$ independently of time, but when the dynamical system trajectory varies significantly and rapidly we may have to set $\mathbf{L}_k = \mathbf{L}_k(\mathbf{y}_k) = \frac{\partial \mathbf{f}}{\partial \mathbf{y}}(\mathbf{y}_k, t_k)$. The case where the linear operator \mathbf{L}_k depends on \mathbf{y}_k adds a significant amount of complexity to the adjoint computations considered later in this paper.

Exponential integration is briefly reviewed in Section 2.1 and we give examples of particular schemes in Section 2.2. The discrete adjoint method discussed in Section 4 requires that the time-stepping method be abstractly represented in the form of a *discrete time-stepping equation*

$$(2.1) \quad \mathbf{t}(\mathbf{y}_\tau, \mathbf{m}) = \mathbf{0},$$

where \mathbf{t} is a vector representing the time-stepping method and \mathbf{y}_τ denotes the approximate solution vector composed of all the \mathbf{y}_k 's. In Section 2.3 we show how to represent an arbitrary ETD scheme in the form (2.1).

2.1. Derivation of ETD RK methods. Recall the semi-discretized, semi-linear system (1.1) which we write as

$$(2.2) \quad \frac{\partial \mathbf{y}(t)}{\partial t} = \mathbf{L}_k \mathbf{y}(t) + \mathbf{n}_k(\mathbf{y}(t), t).$$

Integrating (2.2) exactly from time level t_k to $t_{k+1} = t_k + \tau_k$ gives

$$(2.3) \quad \mathbf{y}_{k+1} = e^{\tau_k \mathbf{L}_k} \mathbf{y}_k + \int_{t_k}^{t_{k+1}} e^{(t_{k+1}-t) \mathbf{L}_k} \mathbf{n}_k(\mathbf{y}(t_k+t), t_k+t) dt.$$

The *exponential Euler method* is obtained by interpolating the integrand at the known value $\mathbf{n}_k(\mathbf{y}_k, t_k)$ only,

$$(2.4) \quad \mathbf{y}_{k+1} = e^{\tau_k \mathbf{L}_k} \mathbf{y}_k + \tau_k \varphi_1(\tau_k \mathbf{L}_k) \mathbf{n}_k(\mathbf{y}_k, t_k)$$

where $\varphi_1(z) = \frac{e^z - 1}{z}$. This is the simplest numerical method that can be obtained for solving (2.3).

The integral in (2.3) can be approximated using some quadrature rule, leading to a class of s -stage explicit *exponential time differencing Runge-Kutta* (ETDRK) methods with matrix coefficients $a_{i,j}(\tau_k \mathbf{L}_k)$, weights $b_i(\tau_k \mathbf{L}_k)$ and nodes c_i , so for $1 \leq i, j \leq s$ we obtain

$$(2.5a) \quad \mathbf{y}_{k+1} = e^{\tau_k \mathbf{L}_k} \mathbf{y}_k + \tau_k \sum_{i=1}^s b_i(\tau_k \mathbf{L}_k) \mathbf{Y}_{k+1,i},$$

with the internal stages

$$(2.5b) \quad \mathbf{Y}_{k+1,i} = \mathbf{n}_k \left(e^{c_i \tau_k \mathbf{L}_k} \mathbf{y}_k + \tau_k \sum_{j=1}^{i-1} a_{ij}(\tau_k \mathbf{L}_k) \mathbf{Y}_{k+1,j}, t_k + c_i \tau_k \right) \quad 1 \leq i \leq s.$$

The procedure starts from a known initial condition \mathbf{y}_0 . There are several alternate ways of writing (2.5a), but for our purposes the representation given here is most useful.

The Butcher tableau for these methods is

$$\begin{array}{c|ccc} c_1 & & & \\ c_2 & a_{21}(\tau \mathbf{L}_k) & & \\ \vdots & \vdots & \ddots & \\ c_s & a_{s1}(\tau_k \mathbf{L}_k) & \cdots & a_{s,s-1}(\tau_k \mathbf{L}_k) \\ \hline & b_1(\tau_k \mathbf{L}_k) & \cdots & b_{s-1}(\tau_k \mathbf{L}_k) \quad b_s(\tau_k \mathbf{L}_k) \end{array}.$$

The coefficients a_{ij} and b_i are linear combinations of the entire functions

$$\varphi_0(z) = e^z \quad \varphi_\ell = \int_0^1 e^{(1-\theta)z} \frac{\theta^{\ell-1}}{(\ell-1)!} d\theta, \quad \ell \geq 1.$$

It is not hard to see that the φ -functions satisfy the recurrence relation

$$(2.6) \quad \varphi_\ell(z) = \frac{\varphi_{\ell-1}(z) - \varphi_{\ell-1}(0)}{z}, \quad \ell > 0,$$

and that $\varphi_\ell(z) = \sum_{i=0}^{\infty} \frac{z^i}{(i+\ell)!}$. Notice that the expansion of $\varphi_\ell(z)$ is that of the exponential function with the coefficients shifted forward.

As is evident by the structure of φ_ℓ for $\ell > 0$, for small z the evaluation of $\varphi_\ell(z)$ will be subject to cancellation error, and this could become a problem when evaluating $\varphi_\ell(\tau_k \mathbf{L}_k)$ if the matrix $\tau_k \mathbf{L}_k$ has small eigenvalues.

From now on, for brevity of notation we use $\varphi_\ell = \varphi_\ell(\tau_k \mathbf{L}_k)$ and $\varphi_{\ell,i} = \varphi_\ell(c_i \tau_k \mathbf{L}_k)$.

2.2. Examples. The four-stage ETD4RK method of Cox and Matthews [3] has the following Butcher tableau:

$$(2.7) \quad \begin{array}{c|ccc} 0 & & & \\ \frac{1}{2} & \frac{1}{2}\varphi_{1,2} & & \\ \frac{1}{2} & \mathbf{0}_{N \times N} & \frac{1}{2}\varphi_{1,3} & \\ 1 & \varphi_{1,4} - \varphi_{1,3} & \mathbf{0}_{N \times N} & \varphi_{1,3} \\ \hline & \varphi_1 - 3\varphi_2 + 4\varphi_3 & 2\varphi_2 - 4\varphi_3 & 2\varphi_2 - 4\varphi_3 \quad 4\varphi_3 - \varphi_2 \end{array}.$$

This method can be fourth-order accurate when certain conditions are satisfied, but in the worst case is only second-order.

Krogstad [17] derived the method given by

$$(2.8) \quad \begin{array}{c|ccc} 0 & & & \\ \frac{1}{2} & \frac{1}{2}\varphi_{1,2} & & \\ \frac{1}{2} & \frac{1}{2}\varphi_{1,3} - \varphi_{2,3} & \varphi_{2,3} & \\ 1 & \varphi_{1,4} - 2\varphi_{2,4} & \mathbf{0}_{N \times N} & 2\varphi_{2,4} \\ \hline & \varphi_1 - 3\varphi_2 + 4\varphi_3 & 2\varphi_2 - 4\varphi_3 & 2\varphi_2 - 4\varphi_3 \quad 4\varphi_3 - \varphi_2 \end{array}.$$

It is usually also fourth-order accurate and has order three in the worst case.

The following five-stage method is due to Hochbruck and Ostermann [12]:

$$(2.9) \quad \begin{array}{c|ccc} 0 & & & \\ \frac{1}{2} & \frac{1}{2}\varphi_{1,2} & & \\ \frac{1}{2} & \frac{1}{2}\varphi_{1,3} - \varphi_{2,3} & \varphi_{2,3} & \\ 1 & \varphi_{1,4} - 2\varphi_{2,4} & \varphi_{2,4} & \varphi_{2,4} \\ \frac{1}{2} & \frac{1}{2}\varphi_{1,5} - \frac{1}{4}\varphi_{2,5} - a_{5,2} & a_{5,2} & a_{5,2} \quad \frac{1}{4}\varphi_{2,5} - a_{5,2} \\ \hline & \varphi_1 - 3\varphi_2 + 4\varphi_3 & \mathbf{0}_{N \times N} & \mathbf{0}_{N \times N} \quad -\varphi_2 + 4\varphi_3 \quad 4\varphi_2 - 8\varphi_3 \end{array},$$

3.1. Krylov Subspace Methods. The M th Krylov subspace with respect to a matrix \mathbf{L} and a vector \mathbf{w} is denoted by $\mathcal{K}_M(\mathbf{L}, \mathbf{w}) = \text{span}\{\mathbf{w}, \mathbf{L}\mathbf{w}, \dots, \mathbf{L}^{M-1}\mathbf{w}\}$. Normalizing $\|\mathbf{w}\| = 1$, the Arnoldi process can be used to construct an orthonormal basis $\mathbf{V}_M \in \mathbb{C}^{N \times M}$ of $\mathcal{K}_M(\mathbf{L}, \mathbf{w})$ and an unreduced upper Hessenberg matrix $\mathbf{H}_M \in \mathbb{C}^{M \times M}$ satisfying the standard Krylov recurrence formula

$$\mathbf{L}\mathbf{V}_M = \mathbf{V}_M\mathbf{H}_M + h_{M+1,M}\mathbf{v}_{M+1}\mathbf{e}_M^T, \quad \mathbf{V}_M^*\mathbf{V}_M = \mathbf{I}_M,$$

with \mathbf{e}_M the M th unit vector in \mathbb{C}^N . Using the orthogonality of \mathbf{V}_M , it can then be shown that

$$(3.1) \quad \varphi(\mathbf{L})\mathbf{w} \approx \mathbf{V}_M\varphi(\mathbf{H}_M)\mathbf{e}_1$$

(see for instance [28]). It is assumed that $M \ll N$, so that $\varphi(\mathbf{H}_M)$ can be computed using standard methods such as diagonalization or Padé approximations.

There has been a lot of work on Krylov subspace methods for evaluating matrix functions, see for instance [5, 10] and the references therein. See in particular [11] for a discussion on Krylov subspace methods for matrix exponentials.

3.2. Polynomial Approximations. Polynomial methods approximate $\varphi(\mathbf{L})$ using some truncated polynomial series, for instance Taylor series (which is rarely used in this context), Chebyshev series for Hermitian or skew-Hermitian \mathbf{L} , Faber series for general \mathbf{L} , or Leja interpolants. See [13] and the references therein for a review of Chebyshev approximations and Leja interpolants in the context of exponential time differencing.

A polynomial approximation can generally be written in the form

$$(3.2) \quad \varphi(\mathbf{L})\mathbf{w} \approx \sum_{j=0}^M c_j \mathbf{L}^j \mathbf{w},$$

although sometimes other forms are more suitable. For instance, in the case of Chebyshev polynomials it makes more sense to write

$$(3.3) \quad \varphi(\mathbf{L})\mathbf{w} \approx \sum_{j=0}^M c_j T_j(\mathbf{L})\mathbf{w}$$

if \mathbf{L} is Hermitian or skew-Hermitian and the eigenvalues of \mathbf{L} all lie inside $[-1, 1]$. The $T_j(\mathbf{L})$ satisfy the recurrence relation

$$T_{j+1}(\mathbf{L}) = 2\mathbf{L}T_j(\mathbf{L}) - T_{j-1}(\mathbf{L}), \quad j = 1, 2, \dots$$

initialized by $T_0(\mathbf{L}) = \mathbf{I}$ and $T_1(\mathbf{L}) = \mathbf{L}$.

3.3. Rational Approximations. The function $\varphi(z)$ can be estimated to arbitrary order using rational approximations

$$\varphi(z) \approx \varphi_{[m,n]}(z) = \sum_{i=0}^m a_i z^i / \sum_{k=0}^n b_k z^k = p_m(z)/q_n(z).$$

The polynomials $p_m(z)$ and $q_n(z)$ can be found using either Padé approximations or by using the Carathéodory-Fejér (CF) method on the negative real line, which is an efficient method for constructing near-best rational approximations. It has been applied to the problem of approximating φ -functions in [29]. The Padé approximation works for general matrices \mathbf{L} ,

but the CF method used in [29] works only if z is negative and real, so that \mathbf{L} must be symmetric negative definite.

For large N it will generally be too expensive to evaluate $\varphi_{[m,n]}(\mathbf{L})$ in this form. But suppose we have that $m \leq n$, q_n has n distinct roots denoted by s_1, \dots, s_n , and p_m and q_n have no roots in common. Then we can find a partial fraction expansion

$$\varphi_{[m,n]}(z) = c_0 + \sum_{i=1}^n \frac{c_k}{s_i - z},$$

where c_0 is some constant and $c_k = \text{Res}[\varphi_{[m,n]}(z), \rho_k]$. In practice one would find these coefficients simply by clearing the denominators.

The product of $\varphi(\mathbf{L})$ with some vector \mathbf{w} therefore is

$$(3.4) \quad \varphi(\mathbf{L}) \mathbf{w} \approx \varphi_{[m,n]}(\mathbf{L}) \mathbf{w} = c_0 \mathbf{w} + \sum_{i=1}^n c_k (s_i \mathbf{I} - \mathbf{L})^{-1} \mathbf{w}.$$

See [29] for a discussion on how a common set of poles can be used for the evaluation of different φ_j . While this approach requires a higher degree n in the rational approximation to achieve a given accuracy, in the use of exponential integration this would still lead to a more efficient method overall since the same computations can be used to evaluate different φ_ℓ .

3.4. Contour Integration. The last approach we consider is based on the Cauchy integral formula

$$\phi(z) = \frac{1}{2\pi i} \int_{\Gamma} \frac{\phi(s)}{s - z} ds$$

for a fixed value of z , where $\phi(z)$ is some arbitrary function and Γ is a contour in the complex plane that encloses z and is well-separated from 0. This formula still holds when replacing z by some general matrix \mathbf{L} , so that

$$(3.5) \quad \phi(\mathbf{L}) = \frac{1}{2\pi i} \int_{\Gamma} \phi(s) (s\mathbf{I} - \mathbf{L})^{-1} ds,$$

where Γ can be any contour that encloses all the eigenvalues of \mathbf{L} . The integral is then approximated using some quadrature rule.

There is some freedom in choosing the contour integral and the quadrature rule. Kassam and Trefethen [16] proposed the contour integral approach to circumvent the cancellation error in (2.6). For convenience, they let Γ simply be a circle in the complex plane that is large enough to enclose all the eigenvalues of \mathbf{L} , and then used the trapezoidal rule for the approximation. If \mathbf{L} is real, then one can additionally simplify the calculations by considering only points on the upper half of a circle with its center on the real axis, and taking the real part of the result. Discretizing the contour using M points s_i and using the trapezoidal rule to evaluate (3.5), we have

$$(3.6) \quad \phi(\mathbf{L}) \approx \frac{1}{M} \Re \left(\sum_{i=1}^M s_i \phi(s_i) (s_i \mathbf{I} - \mathbf{L})^{-1} \right),$$

where M must be chosen large enough to give a good approximation. Then let $\phi = \varphi$ and multiply by \mathbf{w} to get an approximation of the product $\varphi(\mathbf{L})\mathbf{w}$. This is important in the context of multi-stage ETDRK.

Since the same contour integral will be used throughout the procedure, the quadrature points s_i remain the same for all φ -functions and one can therefore use the same solutions $\mathbf{v}_i = (s_i \mathbf{I} - \mathbf{L})^{-1} \mathbf{w}$ of the resolvent systems when computing the product of different φ -functions with some vector \mathbf{w} .

A contour integral that specifically applies to φ -functions is

$$\varphi_\ell(z) = \frac{1}{2\pi i} \int_{\Gamma} \frac{e^s}{s^\ell} \frac{1}{s-z} ds.$$

Again, different contour integrals and quadrature rules can be used. If z is on the negative real line or close to it, then we can use a Hankel contour (see also [33]). Letting $z = \mathbf{L}$ and using the trapezoidal rule, we get

$$(3.7) \quad \varphi_\ell(\mathbf{L}) \approx \frac{1}{M} \Re \left(\sum_{i=1}^M \frac{e^{s_i}}{s_i^\ell} (s_i \mathbf{I} - \mathbf{L})^{-1} \right),$$

for quadrature points s_i on Γ . This integral representation has the advantage that the integrand is exponentially decaying and therefore fewer quadrature points need to be used [29, 13].

Incidentally, (3.6), (3.7) and (3.4) all require an efficient procedure for solving linear systems of the form

$$(s_i \mathbf{I} - \mathbf{L}) \mathbf{v}_i = \mathbf{w}.$$

This can be achieved, for instance, using sparse direct solvers or preconditioned Krylov subspace methods. Solving M different linear systems might seem prohibitive, but when using Krylov methods one has the advantage that $\mathcal{K}_M(\mathbf{L}, \mathbf{w}) = \mathcal{K}_M(s \mathbf{I} - \mathbf{L}, \mathbf{w})$ for all $s \in \mathbb{C}^N$, so that the same Krylov subspace can theoretically be used for all s_i . The computation also allows for parallelization since each system can be solved independently.

4. The Discrete Adjoint Method. To save on notation, we omit throughout the next five sections the subscript τ and write the abstract representation (2.12) of the discrete linear time-stepping system as

$$\mathbf{t}(\mathbf{y}, \mathbf{m}) = \mathbf{0}.$$

It is now used in conjunction with the adjoint method to systematically find the procedures for computing the action of the sensitivity matrix

$$\mathbf{J} = \frac{\partial \mathbf{d}}{\partial \mathbf{m}} = \frac{\partial \mathbf{d}}{\partial \mathbf{y}} \frac{\partial \mathbf{y}}{\partial \mathbf{m}}.$$

We emphasize that here $\mathbf{y} = \mathbf{y}(\mathbf{m})$ is a discrete vector which is the solution of the discrete forward problem. To find an expression for $\frac{\partial \mathbf{y}}{\partial \mathbf{m}}$, we start by differentiating $\mathbf{t}(\mathbf{y}(\mathbf{m}), \mathbf{m}) = \mathbf{0}$ with respect to \mathbf{m} :

$$\frac{\partial}{\partial \mathbf{m}} \mathbf{t}(\mathbf{y}(\mathbf{m}), \mathbf{m}) = \frac{\partial \mathbf{t}}{\partial \mathbf{m}} + \frac{\partial \mathbf{t}}{\partial \mathbf{y}} \frac{\partial \mathbf{y}}{\partial \mathbf{m}} = \mathbf{0}_{N \times N_m}.$$

It follows that

$$(4.1) \quad \frac{\partial \mathbf{y}}{\partial \mathbf{m}} = - \left(\frac{\partial \mathbf{t}}{\partial \mathbf{y}} \right)^{-1} \frac{\partial \mathbf{t}}{\partial \mathbf{m}}, \quad \text{hence } \mathbf{J} = - \frac{\partial \mathbf{d}}{\partial \mathbf{y}} \left(\frac{\partial \mathbf{t}}{\partial \mathbf{y}} \right)^{-1} \frac{\partial \mathbf{t}}{\partial \mathbf{m}}.$$

It is neither desirable nor necessary to compute the Jacobian \mathbf{J} explicitly: what one really needs is to be able to quickly compute the action of \mathbf{J} and its transpose on appropriately-sized arbitrary vectors \mathbf{w} . Notice that the computation of the product of \mathbf{J} with some vector \mathbf{w} of length N_m requires the solution of the *linearized forward problem* $\frac{\partial \mathbf{t}}{\partial \mathbf{y}} \mathbf{v} = \mathbf{q}$ (with $\mathbf{q} = \frac{\partial \mathbf{t}}{\partial \mathbf{m}} \mathbf{w}$ here); we will discuss the structure of $\frac{\partial \mathbf{t}}{\partial \mathbf{y}}$ in the following section. The computation of the product of \mathbf{J}^\top with some vector \mathbf{w} of length N requires the solution of the *adjoint problem* $\left(\frac{\partial \mathbf{t}}{\partial \mathbf{y}}\right)^\top \boldsymbol{\lambda} = \boldsymbol{\theta}$, where $\boldsymbol{\lambda}$ is the *adjoint solution* and $\boldsymbol{\theta}$ is the *adjoint source*. In this context $\boldsymbol{\theta} = \left(\frac{\partial \mathbf{d}}{\partial \mathbf{y}}\right)^\top \mathbf{w}$.

Now, to compute the gradient of the misfit function, we use the chain rule to write

$$\nabla_{\mathbf{m}} M = \left(\frac{\partial \mathbf{d}}{\partial \mathbf{m}}\right)^\top \nabla_{\mathbf{d}} M = \mathbf{J}^\top \nabla_{\mathbf{d}} M.$$

The gradient $\nabla_{\mathbf{m}} M$ is therefore easily obtained by letting $\mathbf{w} = \nabla_{\mathbf{d}} M$ above. In addition to the forward solution \mathbf{y} , one must compute the adjoint solution in order to get the gradient.

The gradient is used by all iterative gradient-based optimization methods, including steepest descent, nonlinear conjugate gradient, quasi-Newton such as BFGS, Gauss-Newton and Levenberg-Marquardt. The latter two methods, in particular, require the computation of a solution to the linearized forward problem as well as an adjoint solution, in addition to the computation of \mathbf{y} .

5. The derivatives of \mathbf{t} . We now focus on deriving expressions of the derivatives for $\frac{\partial \mathbf{t}}{\partial \mathbf{y}}$ and $\frac{\partial \mathbf{t}}{\partial \mathbf{m}}$ required by the sensitivity matrix. Recall equations (2.12) and (2.13), and let \mathbf{A}_k^s be the $s \times s$ block matrix where the (i, j) th entry is $a_{ij}(\tau_k \mathbf{L}_k)$. To ease the notation further, let

$$(5.1a) \quad t_{k,i} = t_k + c_i \tau_k,$$

$$(5.1b) \quad \underline{\mathbf{y}}_{k+1,i} = e^{c_i \tau_k \mathbf{L}_k(\mathbf{y}_k, \mathbf{m})} \mathbf{y}_k + \tau_k \sum_{j=1}^{i-1} a_{ij}(\tau_k \mathbf{L}_k(\mathbf{y}_k, \mathbf{m})) \mathbf{Y}_{k+1,j},$$

and¹

$$(5.1c) \quad \frac{\partial \mathbf{N}_{k+1}}{\partial \mathbf{y}} = \text{diag} \left(\frac{\partial \mathbf{n}_{k,1}}{\partial \mathbf{y}}, \dots, \frac{\partial \mathbf{n}_{k,s}}{\partial \mathbf{y}} \right).$$

The solution procedure at the $(k+1)$ th time-step is represented by

$$(5.2) \quad \mathbf{t}_{k+1} = \begin{bmatrix} \mathbf{Y}_{k+1} - \mathbf{N}_{k+1} \\ -e^{\tau_k \mathbf{L}_k} \mathbf{y}_k - \mathbf{B}_{k+1,s}^\top \mathbf{Y}_{k+1} + \mathbf{y}_{k+1} \end{bmatrix}.$$

We will now take the derivative of \mathbf{t} with respect to \mathbf{y} and \mathbf{m} in turn.

5.1. Computing $\frac{\partial \mathbf{t}}{\partial \mathbf{y}}$. We compute the derivative of $\frac{\partial \mathbf{t}}{\partial \mathbf{y}} = \mathbf{T} - \frac{\partial \mathbf{n}}{\partial \mathbf{y}}$ at the $(k+1)$ th time-step. Letting $\widehat{\mathbf{y}}_{k+1} = [\mathbf{Y}_{k+1}^\top \quad \mathbf{y}_{k+1}^\top]^\top$, this derivative is

$$\frac{\partial \mathbf{t}_{k+1}}{\partial \mathbf{y}} = \begin{bmatrix} \frac{\partial \mathbf{t}_{k+1}}{\partial \widehat{\mathbf{y}}_1} & \frac{\partial \mathbf{t}_{k+1}}{\partial \widehat{\mathbf{y}}_2} & \dots & \frac{\partial \mathbf{t}_{k+1}}{\partial \widehat{\mathbf{y}}_K} \end{bmatrix},$$

¹The Jacobian $\frac{\partial \mathbf{n}_{k,i}}{\partial \mathbf{y}}$ is taken with respect to the semi-discretized $\mathbf{y}(t)$.

with

$$(5.3) \quad \frac{\partial \mathbf{t}_{k+1}}{\partial \hat{\mathbf{y}}_j} = \begin{bmatrix} \frac{\partial}{\partial \hat{\mathbf{y}}_j} (\mathbf{Y}_{k+1} - \mathbf{N}_{k+1}) \\ \frac{\partial}{\partial \hat{\mathbf{y}}_j} (-e^{\tau_k \mathbf{L}_k} \mathbf{y}_k - \mathbf{B}_{k+1}^\top \mathbf{Y}_{k+1} + \mathbf{y}_{k+1}) \end{bmatrix}.$$

Looking at the terms in (5.3) individually and using the chain rule, we have for $j = k + 1$

$$\begin{aligned} \frac{\partial \mathbf{Y}_{k+1}}{\partial \hat{\mathbf{y}}_{k+1}} &= [\mathbf{I}_{sN \times sN} \quad \mathbf{0}_{sN \times N}] & \frac{\partial \mathbf{N}_{k+1}}{\partial \hat{\mathbf{y}}_{k+1}} &= \tau_k \frac{\partial \mathbf{N}_{k+1}}{\partial \mathbf{y}} [\mathbf{A}_k^s \quad \mathbf{0}_{sN \times N}] \\ \frac{\partial \mathbf{y}_{k+1}}{\partial \hat{\mathbf{y}}_{k+1}} &= [\mathbf{0}_{N \times sN} \quad \mathbf{I}_{N \times N}] & \frac{\partial (\mathbf{B}_{k+1}^\top \mathbf{Y}_{k+1})}{\partial \hat{\mathbf{y}}_{k+1}} &= [\mathbf{B}_{k+1}^\top \quad \mathbf{0}_{N \times N}] \end{aligned}$$

and for $j = k$

$$\begin{aligned} \frac{\partial \mathbf{N}_{k+1}}{\partial \hat{\mathbf{y}}_k} &= \begin{bmatrix} \mathbf{0}_{sN \times sN} & \frac{\partial \mathbf{N}_{k+1}}{\partial \mathbf{y}_k} \end{bmatrix} & \frac{\partial (e^{\tau_k \mathbf{L}_k} \mathbf{y}_k)}{\partial \hat{\mathbf{y}}_k} &= \begin{bmatrix} \mathbf{0}_{N \times sN} & \frac{\partial (e^{\tau_k \mathbf{L}_k} \mathbf{y}_k)}{\partial \mathbf{y}_k} \end{bmatrix} \\ & & \frac{\partial (\mathbf{B}_{k+1}^\top \mathbf{Y}_k)}{\partial \hat{\mathbf{y}}_k} &= \begin{bmatrix} \mathbf{0}_{N \times sN} & \frac{\partial (\mathbf{B}_{k+1}^\top \mathbf{Y}_{k+1})}{\partial \mathbf{y}_k} \end{bmatrix}. \end{aligned}$$

The terms

$$\begin{aligned} \frac{\partial (\mathbf{B}_{k+1}^\top \mathbf{Y}_{k+1})}{\partial \mathbf{y}_k} &= \tau_k \sum_{i=1}^s \frac{\partial (b_i(\tau_k \mathbf{L}_k(\mathbf{y}_k)) \mathbf{Y}_{k+1,i})}{\partial \mathbf{y}_k} \\ \frac{\partial \mathbf{n}_{k,i}(\mathbf{y}_{k,i}(\mathbf{y}_k), \mathbf{y}_k)}{\partial \mathbf{y}_k} &= \frac{\partial \mathbf{n}_{k,i}}{\partial \mathbf{y}} \frac{\partial \mathbf{y}_{k+1,i}(\mathbf{y}_k)}{\partial \mathbf{y}_k} + \frac{\partial \mathbf{n}_{k,i}(\mathbf{y}_k)}{\partial \mathbf{y}_k} \end{aligned}$$

with

$$\frac{\partial \mathbf{y}_{k+1,i}(\mathbf{y}_k)}{\partial \mathbf{y}_k} = \frac{\partial e^{c_i \tau_k \mathbf{L}_k(\mathbf{y}_k)} \mathbf{y}_k}{\partial \mathbf{y}_k} + \tau_k \sum_{j=1}^{i-1} \frac{\partial (a_{ij}(\tau_k \mathbf{L}_k(\mathbf{y}_k)) \mathbf{Y}_{k+1,j})}{\partial \mathbf{y}_k},$$

where

$$\frac{\partial (e^{c_i \tau_k \mathbf{L}_k(\mathbf{y}_k)} \mathbf{y}_k)}{\partial \mathbf{y}_k} = e^{c_i \tau_k \mathbf{L}_k(\mathbf{y}_k)} + \frac{\partial (e^{c_i \tau_k \mathbf{L}_k(\mathbf{y}_k)} \mathbf{y}_k^{\text{fixed}})}{\partial \mathbf{y}_k},$$

will be discussed in detail in the following section.

Now let

$$(5.4) \quad \begin{aligned} \mathbf{A}_{k+1} &= \mathbf{I}_{sN} - \tau_k \frac{\partial \mathbf{N}_{k+1}}{\partial \mathbf{y}} \mathbf{A}_k^s & \mathbf{C}_{k+1} &= -\frac{\partial \mathbf{N}_{k+1}}{\partial \mathbf{y}_k}, \\ \mathbf{D}_{k+1} &= -\frac{\partial (e^{\tau_k \mathbf{L}_k} \mathbf{y}_k)}{\partial \mathbf{y}_k} - \frac{\partial (\mathbf{B}_{k+1}^\top \mathbf{Y}_{k+1})}{\partial \mathbf{y}_k} \end{aligned}$$

so that the $(k+1, j)$ th $(s+1)N \times (s+1)N$ block of $\frac{\partial \mathbf{t}}{\partial \mathbf{y}}$ is

$$(5.5) \quad \frac{\partial \mathbf{t}_{k+1}}{\partial \hat{\mathbf{y}}_j} = \begin{cases} \begin{bmatrix} \mathbf{A}_{k+1} & \mathbf{0}_{sN \times N} \\ -\mathbf{B}_{k+1}^\top & \mathbf{I}_N \end{bmatrix} & \text{if } j = k+1 \\ \begin{bmatrix} \mathbf{0}_{sN \times sN} & \mathbf{C}_{k+1} \\ \mathbf{0}_{N \times sN} & \mathbf{D}_{k+1} \end{bmatrix} & \text{if } j = k \\ \mathbf{0}_{(s+1)N \times (s+1)N} & \text{otherwise.} \end{cases}$$

where $\mathbf{v}_{k+1,i} = \frac{\partial \mathbf{n}_{k,i}}{\partial \mathbf{y}}^\top \mathbf{W}_{k+1,i}$ and

$$\frac{\partial \mathbf{y}_{k+1,i}}{\partial \mathbf{m}}^\top \mathbf{v}_{k+1,i} = \frac{\partial (e^{c_i \tau_k \mathbf{L}_k(\mathbf{m})} \mathbf{y}_k)^\top}{\partial \mathbf{m}} \mathbf{v}_{k+1,i} + \tau_k \sum_{j=1}^{i-1} \frac{\partial (a_{ij}(\tau_k \mathbf{L}_k(\mathbf{m})) \mathbf{Y}_{k+1,i})^\top}{\partial \mathbf{m}} \mathbf{v}_{k+1,i}.$$

The terms in braces in (5.10) are ignored if \mathbf{L}_k is independent of \mathbf{m} .

6. The Derivatives of φ . If the linear operator \mathbf{L}_k depends on either \mathbf{y}_k or \mathbf{m} we have to be able to take the derivatives of the products $a_{ij}(\tau_k \mathbf{L}_k(\mathbf{y}_k, \mathbf{m})) \mathbf{w}$, $b_i(\tau_k \mathbf{L}_k(\mathbf{y}_k, \mathbf{m})) \mathbf{w}$ and $e^{c_i \tau_k \mathbf{L}_k(\mathbf{y}_k, \mathbf{m})} \mathbf{w}$, where \mathbf{w} is an arbitrary vector of length N , with respect to \mathbf{y}_k or \mathbf{m} .

Since the a_{ij} and b_i are linear combinations of the $\varphi_{\ell,i}$ - and φ_ℓ -functions respectively, we will simply consider the derivatives of $\varphi(\mathbf{L}) \mathbf{w}$ for some arbitrary φ -function and matrix $\mathbf{L} = \tau_k \mathbf{L}_k(\mathbf{y}_k, \mathbf{m})$. Without loss of generality we assume in this section that the differentiation is with respect to \mathbf{y}_k , but all the results also apply when taking the derivative with respect to \mathbf{m} .

The calculation of the derivatives of the products of the φ_ℓ -functions will depend on the way these terms are evaluated numerically. Recall the approaches for evaluating φ_ℓ reviewed in Section 3.

6.1. Krylov Subspace Methods. Using Krylov subspace methods is unfortunately unsuitable for our purposes since if \mathbf{L} depends on \mathbf{y}_k or \mathbf{m} , it is extremely difficult to find the dependence of the right-hand side of (3.1) on these variables. For this reason we will not consider this approach further here, although it can of course be used for parameter estimation problems where \mathbf{L} is independent of \mathbf{y}_k and \mathbf{m} .

6.2. Polynomial Approach. If we represent φ by a truncated polynomial series as in (3.2) and multiply by \mathbf{w} , we have

$$\varphi(\mathbf{L}(\mathbf{y}_k)) \mathbf{w} \approx \sum_{j=0}^M c_j \mathbf{L}^j(\mathbf{y}_k) \mathbf{w}.$$

Let \mathbf{L} depend on a single parameter z first. The derivative of $\mathbf{L}^j(z) \mathbf{w}$ then is

$$\frac{\partial \mathbf{L}^j(z)}{\partial z} \mathbf{w} = \sum_{i=1}^j \mathbf{L}^{i-1} \frac{\partial \mathbf{L}(z)}{\partial z} \mathbf{L}^{j-i} \mathbf{w} = \sum_{i=1}^j \mathbf{L}^{i-1} \frac{\partial \mathbf{L}(z)}{\partial z} \mathbf{v}_{j-i}$$

with $\mathbf{v}_{j-i} = \mathbf{L}^{j-i} \mathbf{w}$. In the case of $\mathbf{L} = \mathbf{L}(\mathbf{y}_k)$ we therefore have

$$\frac{\partial \mathbf{L}^j(\mathbf{y}_k) \mathbf{w}}{\partial \mathbf{y}_k} = \sum_{i=1}^j \mathbf{L}^{i-1} \frac{\partial \mathbf{L}(\mathbf{y}_k) \mathbf{v}_{j-i}}{\partial \mathbf{y}_k}.$$

This implies that we need to have $j-1$ derivatives $\frac{\partial \mathbf{L}(\mathbf{y}_k) \mathbf{v}_{j-i}}{\partial \mathbf{y}_k}$ available for each j , but of course a lot of these derivatives can also be reused for different values of j .

In the special case where the matrices \mathbf{L} and $\frac{\partial \mathbf{L}}{\partial y}$ commute for each element y of \mathbf{y}_k , we can simplify the above by using the matrix analogue of the usual power rule:

$$\frac{\partial \mathbf{L}^j(\mathbf{y}_k)}{\partial \mathbf{y}_k} \mathbf{w} = \mathbf{L}^{j-1} \frac{\partial \mathbf{L}(\mathbf{y}_k) \mathbf{w}}{\partial \mathbf{y}_k}.$$

This is much less cumbersome to implement, but it is hard to think of realistic scenarios where this commutativity property would hold.

The drawback of considering each monomial term on its own is that this does not necessarily reflect how the polynomial approximation of φ is actually computed. For instance, the Chebyshev approximation (3.3) is

$$\varphi(\mathbf{L})\mathbf{w} \approx \sum_{j=0}^M c_j T_j(\mathbf{L})\mathbf{w}$$

assuming $\mathbf{L}(\mathbf{m})$ is Hermitian or skew-Hermitian and the eigenvalues of $\mathbf{L}(\mathbf{y}_k)$ all lie inside $[-1, 1]$. Each $T_j(\mathbf{y}_k)\mathbf{w}$ is computed using the recurrence relation

$$T_{j+1}(\mathbf{L}(\mathbf{y}_k))\mathbf{w} = 2\mathbf{L}T_j(\mathbf{L}(\mathbf{y}_k))\mathbf{w} - T_{j-1}(\mathbf{L}(\mathbf{y}_k))\mathbf{w}, \quad j = 1, 2, \dots$$

initialized by $T_0(\mathbf{L}(\mathbf{y}_k))\mathbf{w} = \mathbf{w}$ and $T_1(\mathbf{L}(\mathbf{y}_k))\mathbf{w} = \mathbf{L}(\mathbf{y}_k)\mathbf{w}$. Taking the derivative of (3.3) with respect to \mathbf{y}_k ,

$$\frac{\partial \varphi(\mathbf{L})\mathbf{w}}{\partial \mathbf{y}_k} \approx \sum_{j=0}^M c_j \frac{\partial T_j(\mathbf{L})\mathbf{w}}{\partial \mathbf{y}_k},$$

with the recurrence relation

$$\frac{\partial T_{j+1}(\mathbf{L})\mathbf{w}}{\partial \mathbf{y}_k} = 2 \frac{\partial (\mathbf{L}\mathbf{v})}{\partial \mathbf{y}_k} + 2\mathbf{L} \frac{\partial T_j(\mathbf{L})\mathbf{w}}{\partial \mathbf{y}_k} - \frac{\partial T_{j-1}(\mathbf{L})\mathbf{w}}{\partial \mathbf{y}_k}, \quad j = 1, 2, \dots$$

where $\mathbf{v} = T_j\mathbf{w}$, $\frac{\partial T_0(\mathbf{L})\mathbf{w}}{\partial \mathbf{y}_k} = \mathbf{0}_{N \times N}$ and $\frac{\partial T_1(\mathbf{L})\mathbf{w}}{\partial \mathbf{y}_k} = \frac{\partial (\mathbf{L}\mathbf{w})}{\partial \mathbf{y}_k}$.

We also need to be able to compute the products of the transposes of $\frac{\partial \varphi(\mathbf{L})\mathbf{w}}{\partial \mathbf{y}_k}$ with some vector; this is straightforward to derive from the equations above.

6.3. Rational Approximations and Contour Integration. We saw in Sections 3.3 and 3.4 that the action of a φ -function can be computed by both rational approximations (under certain conditions) and contour integrals in the form

$$\varphi(\mathbf{L})\mathbf{w} \approx \sum_{i=1}^M c_i (s_i \mathbf{I} - \mathbf{L})^{-1} \mathbf{w},$$

for some complex scalars c_i and s_i , where the s_i do not coincide with the eigenvalues of \mathbf{L} .

To find the derivative of $\varphi(\mathbf{L})\mathbf{w}$ in this case, let $\mathbf{v}_i = (s_i \mathbf{I} - \mathbf{L})^{-1} \mathbf{w}$, so that

$$(6.1) \quad \frac{\partial \varphi(\mathbf{L})\mathbf{w}}{\partial \mathbf{y}_k} \approx \sum_{i=1}^M c_i \frac{\partial \mathbf{v}_i}{\partial \mathbf{y}_k}.$$

To find an expression for $\frac{\partial \mathbf{v}_i}{\partial \mathbf{y}_k}$, consider $(s_i \mathbf{I} - \mathbf{L})\mathbf{v}_i = \mathbf{w}$ and take the derivative with respect to \mathbf{y}_k on both sides,

$$\begin{aligned} \frac{\partial}{\partial \mathbf{y}_k} (s_i \mathbf{I} - \mathbf{L})\mathbf{v}_i = \mathbf{0}_{N \times N} &\quad \Rightarrow \quad (s_i \mathbf{I} - \mathbf{L}) \frac{\partial \mathbf{v}_i}{\partial \mathbf{y}_k} - \frac{\partial (\mathbf{L}\mathbf{v}_i)}{\partial \mathbf{y}_k} = \mathbf{0}_{N \times N} \\ &\quad \Rightarrow \quad \frac{\partial \mathbf{v}_i}{\partial \mathbf{y}_k} = (s_i \mathbf{I} - \mathbf{L})^{-1} \frac{\partial (\mathbf{L}\mathbf{v}_i)}{\partial \mathbf{y}_k}, \end{aligned}$$

for $k = 0, \dots, K - 1$ and internal stages

$$\mathbf{A}_{k+1} \mathbf{V}_{k+1} = \mathbf{Q}_{k+1} - \mathbf{C}_{k+1} \mathbf{v}_k,$$

with $\mathbf{v}_0 = \mathbf{0}_{N \times 1}$.

Substituting (5.4) then gives

$$\mathbf{v}_{k+1} = \mathbf{q}_{k+1} + \mathbf{B}_{k+1}^\top \mathbf{V}_{k+1} + \frac{\partial (e^{\tau_k \mathbf{L}_k} \mathbf{y}_k)}{\partial \mathbf{y}_k} \mathbf{v}_k + \frac{\partial (\mathbf{B}_{k+1}^\top \mathbf{Y}_{k+1})}{\partial \mathbf{y}_k} \mathbf{v}_k$$

for $k = 0, \dots, K - 1$ and internal stages

$$\mathbf{V}_{k+1} = \mathbf{Q}_{k+1} + \frac{\partial \mathbf{N}_{k+1}}{\partial \mathbf{y}_k} \mathbf{v}_k + \tau_k \frac{\partial \mathbf{N}_{k+1}}{\partial \mathbf{y}} \mathbf{A}_k^s \mathbf{V}_{k+1}.$$

The detailed solution procedure is summarized in Algorithm 7.1.

ALGORITHM 7.1. The Linearized ETD RK Method

Let $\mathbf{v}_0 = \mathbf{0}_{N \times 1}$ and ignore the terms in braces if \mathbf{L}_k does not depend on \mathbf{y}_k .

For $k = 0, \dots, K - 1$:

- For $i = 1, \dots, s$, compute the internal stages

$$(7.3a) \quad \begin{aligned} \mathbf{V}_{k+1,i} = & \mathbf{Q}_{k+1,i} + \frac{\partial \mathbf{n}_{k,i}}{\partial \mathbf{y}} \left(e^{c_i \tau_k \mathbf{L}_k} \mathbf{v}_k + \tau_k \sum_{j=1}^{i-1} a_{ij}(\tau_k \mathbf{L}_k) \mathbf{V}_{k+1,j} \right) + \\ & + \left\{ \frac{\partial \mathbf{n}_{k,i}}{\partial \mathbf{y}_k} \mathbf{v}_k + \frac{\partial \mathbf{n}_{k,i}}{\partial \mathbf{y}} \left(\frac{\partial (e^{c_i \tau_k \mathbf{L}_k(\mathbf{y}_k)} \mathbf{y}_k^{\text{fixed}})}{\partial \mathbf{y}_k} \mathbf{v}_k + \right. \right. \\ & \left. \left. + \tau_k \sum_{j=1}^{i-1} \frac{\partial (a_{ij}(\tau_k \mathbf{L}_k(\mathbf{y}_k)) \mathbf{Y}_{k+1,j})}{\partial \mathbf{y}_k} \mathbf{v}_k \right) \right\}. \end{aligned}$$

- Compute the update:

$$(7.3b) \quad \begin{aligned} \mathbf{v}_{k+1} = & \mathbf{q}_{k+1} + e^{\tau_k \mathbf{L}_k} \mathbf{v}_k + \tau_k \sum_{i=1}^s b_i(\tau_k \mathbf{L}_k) \mathbf{V}_{k+1,i} + \\ & + \left\{ \frac{\partial (e^{\tau_k \mathbf{L}_k(\mathbf{y}_k)} \mathbf{y}_k^{\text{fixed}})}{\partial \mathbf{y}_k} \mathbf{v}_k + \tau_k \sum_{i=1}^s \frac{\partial (b_i(\tau_k \mathbf{L}_k(\mathbf{y}_k)) \mathbf{Y}_{k+1,i})}{\partial \mathbf{y}_k} \mathbf{v}_k \right\}. \end{aligned}$$

□

The derivatives in the braces in (7.3) can be evaluated by writing a_{ij} and b_i in terms of φ -functions and then differentiating the φ -functions as in Section 6. Notice that without the terms in braces we simply have the standard ETD RK method where the nonlinear term has been linearized, except that we allow for the possibility of a source term in the update formula.

7.2. Application to Krogstad's scheme. We show the above algorithm applied to the scheme proposed in [17]. Recall that the matrix coefficients a_{ij} and b_i are given in (2.8) in terms of the φ -functions. The linearized scheme is presented in Algorithm 7.2.

ALGORITHM 7.2. The Linearized Scheme

Let $\mathbf{v}_0 = \mathbf{0}_{N \times 1}$, $\varphi_\ell = \varphi_\ell(\tau_k \mathbf{L}_k(\mathbf{y}_k))$ and $\varphi_{\ell,i} = \varphi_{\ell,i}(\tau_k \mathbf{L}_k(\mathbf{y}_k))$, and ignore the terms in braces if \mathbf{L}_k does not depend on \mathbf{y}_k . For $k = 0, \dots, K - 1$:

- *Compute the internal stages*

$$\mathbf{V}_{k+1,1} = \mathbf{Q}_{k+1,1} + \frac{\partial \mathbf{n}_{k,1}}{\partial \mathbf{y}} \mathbf{v}_k + \left\{ \frac{\partial \mathbf{n}_{k,1}}{\partial \mathbf{y}_k} \mathbf{v}_k \right\}$$

$$\begin{aligned} \mathbf{V}_{k+1,2} = & \mathbf{Q}_{k+1,2} + \frac{\partial \mathbf{n}_{k,2}}{\partial \mathbf{y}} \left(\varphi_{0,2} \mathbf{v}_k + \frac{\tau_k}{2} \varphi_{1,2} \mathbf{V}_{k+1,1} \right) + \\ & + \left\{ \frac{\partial \mathbf{n}_{k,2}}{\partial \mathbf{y}} \left(\frac{\partial(\varphi_{0,2} \mathbf{y}_k^{\text{fixed}})}{\partial \mathbf{y}_k} + \frac{\tau_k}{2} \frac{\partial(\varphi_{1,2} \mathbf{Y}_{k+1,1})}{\partial \mathbf{y}_k} \right) \mathbf{v}_k + \frac{\partial \mathbf{n}_{k,2}}{\partial \mathbf{y}_k} \mathbf{v}_k \right\} \end{aligned}$$

$$\begin{aligned} \mathbf{V}_{k+1,3} = & \mathbf{Q}_{k+1,3} + \frac{\partial \mathbf{n}_{k,3}}{\partial \mathbf{y}} \left(\varphi_{0,3} \mathbf{v}_k + \frac{\tau_k}{2} \varphi_{1,3} \mathbf{V}_{k+1,1} + \tau_k \varphi_{2,3} (\mathbf{V}_{k+1,2} - \mathbf{V}_{k+1,1}) \right) + \\ & + \left\{ \frac{\partial \mathbf{n}_{k,3}}{\partial \mathbf{y}_k} \mathbf{v}_k + \frac{\partial \mathbf{n}_{k,3}}{\partial \mathbf{y}} \left(\frac{\partial(\varphi_{0,3} \mathbf{y}_k^{\text{fixed}})}{\partial \mathbf{y}_k} + \frac{\tau_k}{2} \frac{\partial(\varphi_{1,3} \mathbf{Y}_{k+1,1})}{\partial \mathbf{y}_k} \right) \mathbf{v}_k \right\} \\ & + \left\{ \tau_k \frac{\partial \mathbf{n}_{k,3}}{\partial \mathbf{y}} \left(\frac{\partial(\varphi_{2,3} (\mathbf{Y}_{k+1,2} - \mathbf{Y}_{k+1,1}))}{\partial \mathbf{y}_k} \right) \mathbf{v}_k \right\} \end{aligned}$$

$$\begin{aligned} \mathbf{V}_{k+1,4} = & \mathbf{Q}_{k+1,4} + \frac{\partial \mathbf{n}_{k,4}}{\partial \mathbf{y}} \left(\varphi_0 \mathbf{v}_k + \tau_k \varphi_{1,4} \mathbf{V}_{k+1,1} + 2\tau_k \varphi_{2,4} (\mathbf{V}_{k+1,3} - \mathbf{V}_{k+1,1}) \right) + \\ & + \left\{ \frac{\partial \mathbf{n}_{k,4}}{\partial \mathbf{y}_k} \mathbf{v}_k + \frac{\partial \mathbf{n}_{k,4}}{\partial \mathbf{y}} \left(\frac{\partial(\varphi_0 \mathbf{y}_k^{\text{fixed}})}{\partial \mathbf{y}_k} + \tau_k \frac{\partial(\varphi_{1,4} \mathbf{Y}_{k+1,1})}{\partial \mathbf{y}_k} \right) \mathbf{v}_k \right\} + \\ & + \left\{ 2\tau_k \frac{\partial \mathbf{n}_{k,4}}{\partial \mathbf{y}} \left(\frac{\partial(\varphi_{2,4} (\mathbf{Y}_{k+1,3} - \mathbf{Y}_{k+1,1}))}{\partial \mathbf{y}_k} \right) \mathbf{v}_k \right\} \end{aligned}$$

- *Compute the update:*

$$\begin{aligned} \mathbf{v}_{k+1} = & \mathbf{q}_{k+1} + \varphi_0 \mathbf{v}_k + \tau_k \varphi_2 (-3\mathbf{V}_{k+1,1} + 2\mathbf{V}_{k+1,2} + 2\mathbf{V}_{k+1,3} - \mathbf{V}_{k+1,4}) + \\ & + \tau_k \varphi_1 \mathbf{V}_{k+1,1} + 4\tau_k \varphi_3 (\mathbf{V}_{k+1,1} - \mathbf{V}_{k+1,2} - \mathbf{V}_{k+1,3} + \mathbf{V}_{k+1,4}) + \\ & + \left\{ \frac{\partial(\varphi_0 \mathbf{y}_k^{\text{fixed}})}{\partial \mathbf{y}_k} \mathbf{v}_k + \tau_k \frac{\partial(\varphi_1 \mathbf{Y}_{k+1,1})}{\partial \mathbf{y}_k} \mathbf{v}_k + \right. \\ & + \tau_k \frac{\partial(\varphi_2 (-3\mathbf{Y}_{k+1,1} + 2\mathbf{Y}_{k+1,2} + 2\mathbf{Y}_{k+1,3} - \mathbf{Y}_{k+1,4}))}{\partial \mathbf{y}_k} \mathbf{v}_k + \\ & \left. + 4\tau_k \frac{\partial(\varphi_3 (\mathbf{Y}_{k+1,1} - \mathbf{Y}_{k+1,2} - \mathbf{Y}_{k+1,3} + \mathbf{Y}_{k+1,4}))}{\partial \mathbf{y}_k} \mathbf{v}_k \right\}. \end{aligned}$$

□

The way the scheme is written here may of course not represent the most computationally efficient implementation: for instance, there are some opportunities for parallelization and one should also exploit the fact that $c_2 = c_3 = 1/2$.

8. Solving the Adjoint Problem. The major ingredient needed when calculating the action of the transpose of the sensitivity matrix, and therefore especially important for the gradient computation, is the solution of the adjoint problem,

$$(8.1) \quad \boldsymbol{\lambda} = \left(\frac{\partial \mathbf{t}}{\partial \mathbf{y}} \right)^{-\top} \boldsymbol{\theta},$$

where $\boldsymbol{\lambda} = [\boldsymbol{\Lambda}_1^\top \quad \boldsymbol{\lambda}_1^\top \quad \cdots \quad \boldsymbol{\Lambda}_K^\top \quad \boldsymbol{\lambda}_K^\top]^\top$ is the adjoint solution (with internal stages $\boldsymbol{\Lambda}_k$) and $\boldsymbol{\theta} = [\boldsymbol{\Theta}_1^\top \quad \boldsymbol{\theta}_1^\top \quad \cdots \quad \boldsymbol{\Theta}_K^\top \quad \boldsymbol{\theta}_K^\top]$ is taken in this section to be some arbitrary adjoint source; for the gradient computation we will have $\boldsymbol{\theta} = \frac{\partial \mathbf{d}}{\partial \mathbf{y}}^\top \nabla_{\mathbf{d}} \mathcal{M}$.

- For $i = s, s-1, \dots, 1$, compute

$$(8.5b) \quad \mathbf{\Lambda}_{k,i} = \mathbf{\Theta}_{k,i} + \tau_{k-1} \left(\sum_{j=i+1}^s a_{ji} \tau_{k-1} \mathbf{L}_{k-1}^\top \left(\frac{\partial \mathbf{n}_{k-1,j}}{\partial \mathbf{y}} \right)^\top \mathbf{\Lambda}_{k,j} + b_i \tau_{k-1} \mathbf{L}_{k-1}^\top \boldsymbol{\lambda}_k \right).$$

The derivatives in the braces in (8.5b) are computed as discussed in Section 6. \square

Incidentally, inspecting the different ways in which the φ_ℓ -functions are evaluated reveals that $\varphi_\ell(\tau_k \mathbf{L}_k)^\top = \varphi_\ell(\tau_k \mathbf{L}_k^\top)$, and since in many applications the linear operator is symmetric we will have $\varphi_\ell(\tau_k \mathbf{L}_k)^\top = \varphi_\ell(\tau_k \mathbf{L}_k)$.

8.2. Application to Krogstad's scheme. We continue the example from Section 7.2 and apply the above algorithm to a specific scheme. Recall the matrix coefficients a_{ij} and b_i given in (2.8). The adjoint scheme is given in Algorithm 8.2.

ALGORITHM 8.2. The Adjoint Krogstad Scheme

Let $\widehat{\mathbf{\Lambda}}_{k,i} = \left(\frac{\partial \mathbf{n}_{k-1,i}}{\partial \mathbf{y}} \right)^\top \mathbf{\Lambda}_{k,i}$. For $k = K, \dots, 1$:

- In this step, let $\varphi_\ell = \varphi_\ell(\tau_k \mathbf{L}_k(\mathbf{y}_k))$ and $\varphi_{\ell,i} = \varphi_\ell(c_i \tau_k \mathbf{L}_k(\mathbf{y}_k))$. Compute

$$\begin{aligned} \boldsymbol{\lambda}_k = & \boldsymbol{\theta}_k + e^{\tau_k \mathbf{L}_k^\top} \left(\boldsymbol{\lambda}_{k+1} + \widehat{\mathbf{\Lambda}}_{k+1,4} \right) + e^{\frac{1}{2} \tau_k \mathbf{L}_k^\top} \left(\widehat{\mathbf{\Lambda}}_{k+1,2} + \widehat{\mathbf{\Lambda}}_{k+1,3} \right) + \widehat{\mathbf{\Lambda}}_{k+1,1} + \\ & + \left\{ \sum_{i=1}^4 \frac{\partial \mathbf{n}_{k,i}}{\partial \mathbf{y}_k} \mathbf{\Lambda}_{k+1,i} + \right. \\ & + \frac{\partial e^{\frac{1}{2} \tau_k \mathbf{L}_k(\mathbf{y}_k) \mathbf{y}_k^{\text{fixed}}}}{\partial \mathbf{y}_k} \left(\widehat{\mathbf{\Lambda}}_{k+1,2} + \widehat{\mathbf{\Lambda}}_{k+1,3} \right) + \frac{\partial e^{\tau_k \mathbf{L}_k(\mathbf{y}_k) \mathbf{y}_k^{\text{fixed}}}}{\partial \mathbf{y}_k} \widehat{\mathbf{\Lambda}}_{k+1,4} + \\ & + \frac{\partial (e^{\tau_k \mathbf{L}_k(\mathbf{y}_k) \mathbf{y}_k^{\text{fixed}}})}{\partial \mathbf{y}_k} + \frac{\tau_k}{2} \frac{\partial (\varphi_{1,2} \mathbf{Y}_{k+1,1})}{\partial \mathbf{y}_k} \widehat{\mathbf{\Lambda}}_{k+1,2} + \\ & + \tau_k \left(\left(\frac{1}{2} \frac{\partial (\varphi_{1,3} \mathbf{Y}_{k+1,1})}{\partial \mathbf{y}_k} + \frac{\partial (\varphi_{2,3} (\mathbf{Y}_{k+1,2} - \mathbf{Y}_{k+1,1}))}{\partial \mathbf{y}_k} \right)^\top \widehat{\mathbf{\Lambda}}_{k+1,3} + \right. \\ & + \left. \left(\frac{\partial (\varphi_{1,4} \mathbf{Y}_{k+1,1})}{\partial \mathbf{y}_k} + 2 \frac{\partial (\varphi_{2,4} (\mathbf{Y}_{k+1,3} - \mathbf{Y}_{k+1,1}))}{\partial \mathbf{y}_k} \right)^\top \widehat{\mathbf{\Lambda}}_{k+1,4} + \right. \\ & + \left. \left(\frac{\partial (\varphi_1 \mathbf{Y}_{k+1,1})}{\partial \mathbf{y}_k} - \frac{\partial (\varphi_2 (3\mathbf{Y}_{k+1,1} - 2\mathbf{Y}_{k+1,2} - 2\mathbf{Y}_{k+1,3} + \mathbf{Y}_{k+1,4}))}{\partial \mathbf{y}_k} \right)^\top + \right. \\ & \left. + 4 \frac{\partial (\varphi_3 (\mathbf{Y}_{k+1,1} - \mathbf{Y}_{k+1,2} - \mathbf{Y}_{k+1,3} + \mathbf{Y}_{k+1,4}))}{\partial \mathbf{y}_k} \right)^\top \boldsymbol{\lambda}_{k+1} \Big\} \end{aligned}$$

with $\boldsymbol{\lambda}_{K+1} = \widehat{\mathbf{\Lambda}}_{K+1,i} = \mathbf{0}_{N \times 1}$. Ignore the terms in braces if \mathbf{L}_k is independent of \mathbf{y}_k .

- Now let $\varphi_\ell = \varphi_\ell(\tau_{k-1} \mathbf{L}_{k-1}(\mathbf{y}_{k-1}))$ and $\varphi_{\ell,i} = \varphi_\ell(c_i \tau_{k-1} \mathbf{L}_{k-1}(\mathbf{y}_{k-1}))$. The internal

stages are computed as follows:

$$\begin{aligned}
\Lambda_{k,4} &= \tau_{k-1} b_4^\top \lambda_k = \tau_{k-1} (4\varphi_3^\top - \varphi_2^\top) \lambda_k \\
\Lambda_{k,3} &= \tau_{k-1} b_3^\top \lambda_k + \tau_{k-1} a_{4,3}^\top \widehat{\Lambda}_{k,4} = \tau_{k-1} (2\varphi_2^\top - 4\varphi_3^\top) \lambda_k + \tau_{k-1} 2\varphi_{2,4}^\top \widehat{\Lambda}_{k,4} \\
\Lambda_{k,2} &= \tau_{k-1} b_2^\top \lambda_k + \tau_{k-1} a_{4,2}^\top \widehat{\Lambda}_{k,4} + \tau_{k-1} a_{3,2}^\top \widehat{\Lambda}_{k,3} \\
(8.6) \quad &= \tau_{k-1} (2\varphi_2^\top - 4\varphi_3^\top) \lambda_k + \tau_{k-1} \varphi_{2,3}^\top \widehat{\Lambda}_{k,3} \\
\Lambda_{k,1} &= \tau_{k-1} b_1^\top \lambda_k + \tau_{k-1} a_{4,1}^\top \widehat{\Lambda}_{k,4} + \tau_{k-1} a_{3,1}^\top \widehat{\Lambda}_{k,3} + \tau_{k-1} a_{2,1}^\top \widehat{\Lambda}_{k,2} \\
&= \tau_{k-1} (\varphi_1^\top - 3\varphi_2^\top + 4\varphi_3^\top) \lambda_k + \tau_{k-1} (\varphi_{1,4}^\top - 2\varphi_{2,4}^\top) \widehat{\Lambda}_{k,4} + \\
&\quad + \frac{\tau_{k-1}}{2} (\varphi_{1,3}^\top - 2\varphi_{2,3}^\top) \widehat{\Lambda}_{k,3} + \frac{\tau_{k-1}}{2} \varphi_{1,2}^\top \widehat{\Lambda}_{k,2}.
\end{aligned}$$

□

Other schemes can be handled similarly. We note that the procedure gives ample opportunity for parallelization and precomputing quantities, for instance when computing the products of λ_k with φ_ℓ^\top or the products of $\widehat{\Lambda}_{k,i}$ with $\varphi_{\ell,i}^\top$.

9. Numerical Example. As an interesting and simple application of the methods derived above we consider the parameter estimation problem applied to the following version of the fourth-order Swift-Hohenberg model on the torus $\Omega = \mathbb{T}^2 : [0, L_x) \times [0, L_y)$:

$$(9.1) \quad \frac{\partial y}{\partial t} = r y - (1 + \nabla^2)^2 y + g y^2 - y^3,$$

where $r > 0$ and g are parameter functions that determine the behaviour of the solution. After spatially discretizing in some appropriate way we have

$$(9.2) \quad \frac{\partial \mathbf{y}}{\partial t} = \text{diag}(\mathbf{r}) \mathbf{y} - (\mathbf{I} + \nabla_h^2)^2 \mathbf{y} + \text{diag}(\mathbf{g}) \mathbf{y}^2 - \mathbf{y}^3,$$

with $\mathbf{y} = \mathbf{y}(t)$, \mathbf{r} and \mathbf{g} being the spatial discretizations of r and g respectively, and ∇_h^2 the spatially discretized Laplace operator. The Swift-Hohenberg model is an example of a PDE whose solutions exhibit pattern formation, a phenomenon that occurs in many different branches of science, for instance biology (morphogenesis, vegetation patterns, animal markings, growth of bacterial colonies, etc.), physics (liquid crystals, nonlinear waves, Bénard cells, etc.) and chemical kinetics (e.g. the Belousov-Zhabotinsky, CIMA and PA-MBO relations). The field is enormous; see [7, 23] for some interesting applications, but there are many others. The Swift-Hohenberg model itself was derived from the equations of thermal convection [30], and it is possible to use other nonlinear terms than the one used here.

The fourth-order derivative term implies that this equation is very stiff, making it a good candidate for use with an exponential integrator. The obtained patterns depend on the parameters $\mathbf{m} = (\mathbf{r}, \mathbf{g})$ reshaped as a vector. It is possible to obtain different patterns in different regions of the domain if these parameters exhibit spatial variability, which is the case that we consider here. This is therefore a distributed parameter estimation problem.

We take the linear part to be $\mathbf{L} = -(\mathbf{I} + \nabla_h^2)^2$, hence $\mathbf{n}(\mathbf{y}, \mathbf{m}, t) = \text{diag}(\mathbf{r}) \mathbf{y}(t) + \text{diag}(\mathbf{g}) \mathbf{y}(t)^2 - \mathbf{y}(t)^3$. Notice that we have included the linear term $\text{diag}(\mathbf{r}) \mathbf{y}$ in the nonlinear part of the equation: the dominant differential term is in \mathbf{L} anyway.

9.1. Experiment setup. Using a finite difference spatial discretization with $N_x \times N_y$ grid points, the periodic boundary conditions allow us to diagonalize the linear term using the

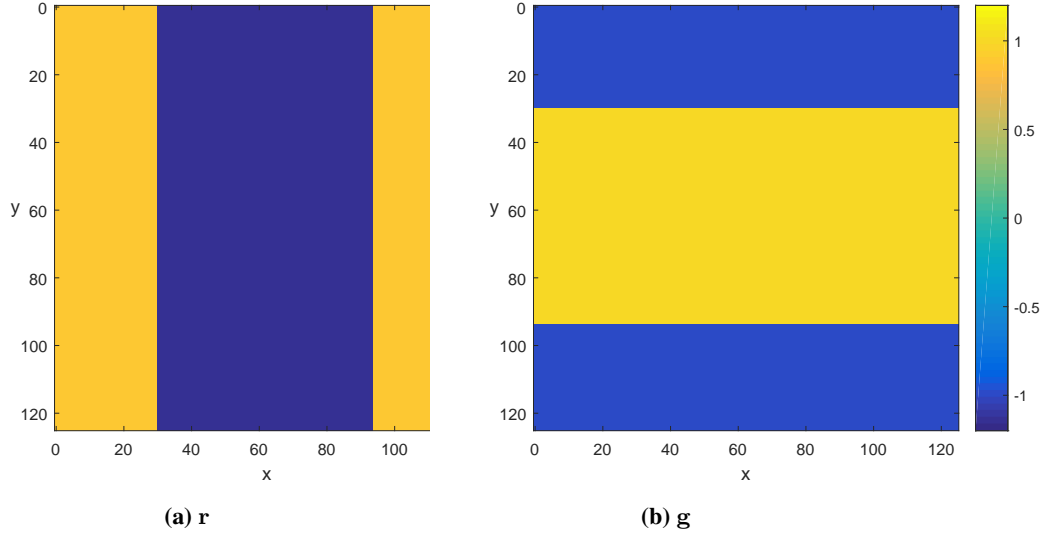


Fig. 1: Actual parameter values

pseudospectral method, where we compute the product with the linear part in the frequency domain and then switch back to the real domain to compute the nonlinear part. Hence

$$(9.3) \quad \frac{\partial \widehat{\mathbf{y}}(t)}{\partial t} = \widehat{\mathbf{L}} \widehat{\mathbf{y}}(t) + \mathbf{F} \left(\text{diag}(\mathbf{r}) \mathbf{F}^{-1} \widehat{\mathbf{y}}(t) + \text{diag}(\mathbf{g}) (\mathbf{F}^{-1} \widehat{\mathbf{y}}(t))^2 - (\mathbf{F}^{-1} \widehat{\mathbf{y}}(t))^3 \right),$$

where \mathbf{F} represents the 2D Fourier transform in space, \mathbf{F}^{-1} is its inverse, $\widehat{\mathbf{y}}(t) = \mathbf{F} \mathbf{y}(t)$ and $\widehat{\mathbf{L}}$ is the diagonalized differential operator. The wave numbers on this grid are $\mathbf{k}_x = \frac{2\pi}{L_x} (-\frac{N_x}{2} : \frac{N_x}{2} - 1)$ and $\mathbf{k}_y = \frac{2\pi}{L_y} (-\frac{N_y}{2} : \frac{N_y}{2} - 1)$, so ∇_h^2 is then diagonalized with each diagonal entry the negative of the sum of the square of an element of \mathbf{k}_x and the square of an element of \mathbf{k}_y . Now $\widehat{\mathbf{y}}(t)$ is taken to be the forward solution instead of $\mathbf{y}(t)$.

In our experiment we let $L_x = L_y = 40\pi$, $N_x = N_y = 2^7$, and the initial condition \mathbf{y}_0 is given by a field of Gaussian noise. We employ contour integration to evaluate the φ -functions, using a parabolic contour with 32 quadrature points. The actual parameter fields \mathbf{r} and \mathbf{g} are taken to be piecewise constant, as shown in Figure 1. The value of \mathbf{r} is 2 in the outer strips and 0.04 in the inner strip. The value of \mathbf{g} is -1 in the outer strips and 1 in the inner strip. The solution $\mathbf{y}(t)$ at time $t = 50s$ is shown in Figure 2. The outer vertical strips in the solution evolve fairly quickly relative to the central vertical strip, which evolves on a much slower time scale due to the small value of \mathbf{r} there.

9.2. Derivatives of \mathbf{n} . The adjoint solution procedure and sensitivity computations require the derivatives of

$$\mathbf{n}(\widehat{\mathbf{y}}, \mathbf{m}, t) = \mathbf{F} \left(\text{diag}(\mathbf{r}) \mathbf{F}^{-1} \widehat{\mathbf{y}}(t) + \text{diag}(\mathbf{g}) (\mathbf{F}^{-1} \widehat{\mathbf{y}}(t))^2 - (\mathbf{F}^{-1} \widehat{\mathbf{y}}(t))^3 \right)$$

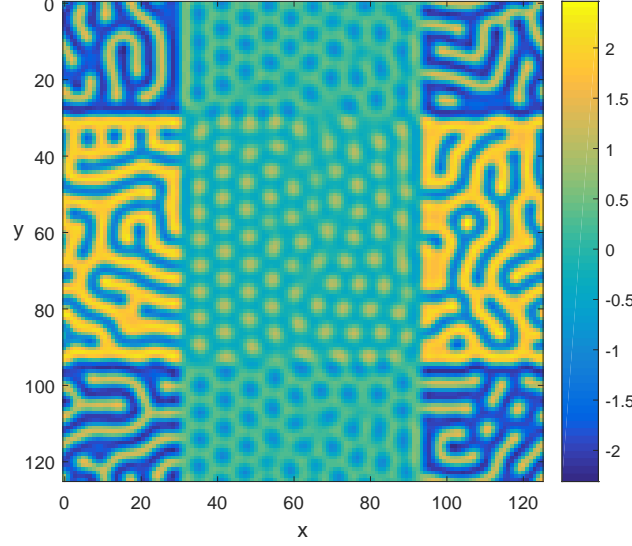


Fig. 2: Ground truth solution at $t = 50s$.

with respect to $\hat{\mathbf{y}}(t)$ and \mathbf{m} , as well as their transposes. We have

$$\begin{aligned}\frac{\partial \mathbf{n}(t)}{\partial \hat{\mathbf{y}}} &= \mathbf{F} \left(\text{diag}(\mathbf{r}) + 2 \text{diag}(\mathbf{g}) (\mathbf{F}^{-1} \hat{\mathbf{y}}(t)) - 3 (\mathbf{F}^{-1} \hat{\mathbf{y}}(t))^2 \right) \mathbf{F}^{-1} \\ \frac{\partial \mathbf{n}(t)}{\partial \mathbf{m}} &= \left[\text{diag}(\hat{\mathbf{y}}(t)) \quad \mathbf{F} \text{diag} \left((\mathbf{F}^{-1} \hat{\mathbf{y}}(t))^2 \right) \right] \\ \frac{\partial \mathbf{n}(t)}{\partial \hat{\mathbf{y}}}^\top &= \mathbf{F}^{-\top} \left(\text{diag}(\mathbf{r}) + 2 \text{diag}(\mathbf{g}) (\mathbf{F}^{-1} \hat{\mathbf{y}}(t)) - 3 (\mathbf{F}^{-1} \hat{\mathbf{y}}(t))^2 \right) \mathbf{F}^\top \\ \frac{\partial \mathbf{n}(t)}{\partial \mathbf{m}}^\top &= \begin{bmatrix} \text{diag}(\hat{\mathbf{y}}(t)) \\ \text{diag} \left((\mathbf{F}^{-1} \hat{\mathbf{y}}(t))^2 \right) \mathbf{F}^\top \end{bmatrix}.\end{aligned}$$

The transposes of \mathbf{F} and \mathbf{F}^{-1} are $\mathbf{F}^\top = N\mathbf{F}^{-1}$ and $\mathbf{F}^{-\top} = \frac{1}{N}\mathbf{F}$, with $N = N_x N_y$, so that

$$\begin{aligned}\frac{\partial \mathbf{n}(t)}{\partial \hat{\mathbf{y}}}^\top &= \mathbf{F} \left(\text{diag}(\mathbf{r}) + 2 \text{diag}(\mathbf{g}) (\mathbf{F}^{-1} \hat{\mathbf{y}}(t)) - 3 (\mathbf{F}^{-1} \hat{\mathbf{y}}(t))^2 \right) \mathbf{F}^{-1} \\ \frac{\partial \mathbf{n}(t)}{\partial \mathbf{m}}^\top &= \begin{bmatrix} \text{diag}(\hat{\mathbf{y}}(t)) \\ N \text{diag} \left((\mathbf{F}^{-1} \hat{\mathbf{y}}(t))^2 \right) \mathbf{F}^{-1} \end{bmatrix}.\end{aligned}$$

Note that $\frac{\partial \mathbf{n}(t)}{\partial \hat{\mathbf{y}}}^\top = \frac{\partial \mathbf{n}(t)}{\partial \hat{\mathbf{y}}}$.

9.3. Order of Accuracy. We numerically illustrate that the adjoint solution and the gradient have the same order of accuracy as the forward solution, meaning that p th-order forward schemes are expected to lead to p th-order adjoint schemes. In this subsection we let $\mathbf{y}(n\tau)$, $\boldsymbol{\lambda}(n\tau)$ and $\nabla(n\tau)$ denote the quantity of interest one gets when performing the computations with a time-step $n\tau$, where we let $\tau = \frac{1}{80}s$. We let $\mathbf{y}_{\text{exact}}$, $\boldsymbol{\lambda}_{\text{exact}}$ and ∇_{exact} denote the "exact" values attained by performing the computations with a fine time-step

	Euler	Cox-Matthews	Krogstad	Hochbruck-Ostermann
$p_{\mathbf{y}}(2\tau, \tau)$	0.9914	4.0644	4.0699	4.0275
$p_{\mathbf{y}}(4\tau, 2\tau)$	0.9908	3.9726	3.9732	3.9719
$p_{\mathbf{y}}(8\tau, 4\tau)$	–	3.9375	3.9378	3.9387
$p_{\mathbf{y}}(16\tau, 8\tau)$	–	3.8849	3.8835	3.8770

Table 9.1: Approximate order of accuracy $p_{\mathbf{y}}$ for the forward solution, computed using $p_{\mathbf{y}}(2^i\tau, 2^{i-1}\tau) = \log_2(\|\epsilon_{\mathbf{y}}(2^i\tau)\|/\|\epsilon_{\mathbf{y}}(2^{i-1}\tau)\|)$ for $i = 1, 2, 3, 4$, with $\epsilon_{\mathbf{y}}(2^i\tau) = \mathbf{y}(2^i\tau) - \mathbf{y}_{\text{exact}}$.

	Euler	Cox-Matthews	Krogstad	Hochbruck-Ostermann
$p_{\lambda}(2\tau, \tau)$	0.9976	4.0383	4.0588	3.9902
$p_{\lambda}(4\tau, 2\tau)$	0.9434	3.9516	3.9568	3.9679
$p_{\lambda}(8\tau, 4\tau)$	–	3.8969	3.9041	3.9343
$p_{\lambda}(16\tau, 8\tau)$	–	3.8027	3.8100	3.8616

Table 9.2: Approximate order of accuracy p_{λ} for the adjoint solution, computed using $p_{\lambda}(2^i\tau, 2^{i-1}\tau) = \log_2(\|\epsilon_{\lambda}(2^i\tau)\|/\|\epsilon_{\lambda}(2^{i-1}\tau)\|)$ for $i = 1, 2, 3, 4$, with $\epsilon_{\lambda}(2^i\tau) = \lambda(2^i\tau) - \lambda_{\text{exact}}$.

$\frac{1}{160}$ s using the Krogstad scheme. The error between the computed and exact forward solution is $\epsilon_{\mathbf{y}}(n\tau) = \mathbf{y}(n\tau) - \mathbf{y}_{\text{exact}}$, and we must have $\|\epsilon_{\mathbf{y}}(n\tau)\| \approx O(n\tau)^p$ for a p th-order method, from which it follows that $(\|\epsilon_{\mathbf{y}}(2^i\tau)\|/\|\epsilon_{\mathbf{y}}(2^{i-1}\tau)\|) \approx 2^p$. Computing $p_{\mathbf{y}}(2^i\tau, 2^{i-1}\tau) := \log_2(\|\epsilon_{\mathbf{y}}(2^i\tau)\|/\|\epsilon_{\mathbf{y}}(2^{i-1}\tau)\|)$ for different values of $i = 1, 2, \dots$ then gives an approximation of the order of accuracy p , with the estimate being more accurate for smaller values of τ and i . The results for the four ETD schemes mentioned in this paper are given in Table 9.1. We note the following:

- The simulations were run from 0s to 20s for the forward solution, and from 20s to 0s for the adjoint solution.
- The initial condition is Gaussian noise and the approximate orders of accuracy actually differ from simulation to simulation because of this. These differences are only slight for the higher-order methods, but can be quite pronounced for the lower-order Euler method. Therefore the results shown are the averages of 10 simulations using different initial conditions.
- The larger time steps are too large for the Euler method, and even the smaller time-steps can lead to inaccurate results on occasion. In computing the average order of accuracy we have therefore only included the computed $p_{\mathbf{y}}$'s that are in the interval $(p - 0.5, p + 0.5)$.
- Incidentally, for the Swift-Hohenberg equation with periodic boundary conditions, we see that Cox-Matthews and Krogstad schemes do indeed attain fourth order accuracy.

The quantities $p_{\lambda}(2^i\tau, 2^{i-1}\tau)$ and $p_{\nabla}(2^i\tau, 2^{i-1}\tau)$ are defined analogously to $p_{\mathbf{y}}$ and are given in Tables 9.2 and 9.3, respectively. We have again averaged the approximate orders of accuracy from 10 simulations.

The crucial observation here is that the orders of accuracy of the adjoint ETD schemes and the resulting gradient are the same as that of the corresponding forward scheme.

9.4. Testing the Rosenbrock Approach. To test the order of accuracy of adjoint exponential Rosenbrock methods, and simultaneously check that our derivations and implementations for these methods are correct, the Swift-Hohenberg equation was reformulated by

	Euler	Cox-Matthews	Krogstad	Hochbruck-Ostermann
$p_{\nabla}(2\tau, \tau)$	1.0260	4.0430	4.0627	3.9947
$p_{\nabla}(4\tau, 2\tau)$	0.9270	3.9546	3.9575	3.9684
$p_{\nabla}(8\tau, 4\tau)$	–	3.9022	3.9056	3.9347
$p_{\nabla}(16\tau, 8\tau)$	–	3.8103	3.8136	3.8622

Table 9.3: Approximate order of accuracy p_{∇} for the gradient, computed using $p_{\nabla}(2^i\tau, 2^{i-1}\tau) = \log_2(\|\epsilon_{\nabla}(2^i\tau)\|/\|\epsilon_{\nabla}(2^{i-1}\tau)\|)$ for $i = 1, 2, 3, 4$, with $\epsilon_{\nabla}(2^i\tau) = \nabla(2^i\tau) - \nabla_{\text{exact}}$.

	Euler	Cox-Matthews	Krogstad	Hochbruck-Ostermann
$p_{\mathbf{y}}(4\tau, 2\tau)$	1.9505	4.1970	4.1967	4.1213
$p_{\mathbf{y}}(8\tau, 4\tau)$	1.9713	4.0774	4.0811	4.0561
$p_{\mathbf{y}}(16\tau, 8\tau)$	1.9846	3.7946	3.7991	3.7884

Table 9.4: Approximate order of accuracy $p_{\mathbf{y}}$ for the forward solution using a Rosenbrock approach, computed using $p_{\mathbf{y}}(2^i\tau, 2^{i-1}\tau) = \log_2(\|\epsilon_{\mathbf{y}}(2^i\tau)\|/\|\epsilon_{\mathbf{y}}(2^{i-1}\tau)\|)$ for $i = 1, 2, 3, 4$, with $\epsilon_{\mathbf{y}}(2^i\tau) = \mathbf{y}(2^i\tau) - \mathbf{y}_{\text{exact}}$.

finding the Jacobian of the right-hand side of (9.3),

$$\frac{\partial \mathbf{f}}{\partial \hat{\mathbf{y}}} = \hat{\mathbf{L}} + \mathbf{F} (\text{diag}(\mathbf{r}) + 2 \text{diag}(\mathbf{g}) \text{diag}(\mathbf{F}^{-1}\hat{\mathbf{y}}(t)) - 3 \text{diag}(\mathbf{F}^{-1}\hat{\mathbf{y}}(t))) \mathbf{F}^{-1},$$

and then setting $\mathbf{L}_k = \frac{\partial \mathbf{f}(\hat{\mathbf{y}}_k)}{\partial \hat{\mathbf{y}}}$ at the k th time-step. Consequently, with $\mathbf{y}_k = \mathbf{F}^{-1}\hat{\mathbf{y}}_k$,

$$\mathbf{L}_k = \hat{\mathbf{L}} + \mathbf{F} \text{diag}(\mathbf{r} + 2\mathbf{g} \odot \mathbf{y}_k - 3\mathbf{y}_k^2) \mathbf{F}^{-1},$$

and hence

$$\mathbf{n}_k = \mathbf{f} - \mathbf{L}_k \hat{\mathbf{y}}(t) = \mathbf{F} \text{diag}(\mathbf{g} \odot (\mathbf{F}^{-1}\hat{\mathbf{y}}(t) - 2\mathbf{y}_k) - (\mathbf{F}^{-1}\hat{\mathbf{y}}(t))^2 - 3\mathbf{y}_k^2) \mathbf{F}^{-1}\hat{\mathbf{y}}(t).$$

The experiment from the previous subsection is repeated, but due to the significant increase in computational effort required by the additional terms in the derivatives we have run the simulations for only 2 different random initial conditions, and for a smallest time-step of 2τ , with the "exact" equations computed using a time-step of τ . We have also run the simulations for just 10s instead of 20s. The results in tables 9.4-9.6 suggest that the adjoint exponential Rosenbrock method does indeed also attain the same (numerical) order of accuracy as the corresponding forward method. Oddly the Euler method seems to have an order of accuracy of around 2 instead of the expected value of 1, but this result should be viewed with reservation. The results for the largest time-step suggest that this time-step was too large, with a noticeable decrease in the order of accuracy especially for the adjoint solution.

9.5. Parameter Estimation. Although outside the stated scope of this paper, we show a possible parameter estimate attained using a gradient-based optimization method, where the gradient is computed using the results from this paper. Recovering estimates that are closer to the ground truth parameters takes a more sophisticated approach than the one used here. In particular, the regularization term $R(\mathbf{m}, \mathbf{m}^{\text{ref}})$ in (1.2), which is not the focus of this paper, may have to be altered, or a level set method may be introduced; this is the subject of a future investigation. The initial guesses for the parameters are shown in Figures 3a and 3b, and the recovered parameters are shown in Figures 3c and 3d. Here are details of the setup:

	Euler	Cox-Matthews	Krogstad	Hochbruck-Ostermann
$p_\lambda(4\tau, 2\tau)$	1.8885	4.2572	4.2482	4.2244
$p_\lambda(8\tau, 4\tau)$	1.9414	4.0531	4.0498	4.0411
$p_\lambda(16\tau, 8\tau)$	1.9702	3.1043	3.1029	3.0998

Table 9.5: Approximate order of accuracy p_λ for the adjoint solution using a Rosenbrock approach, computed using $p_\lambda(2^i\tau, 2^{i-1}\tau) = \log_2(\|\epsilon_\lambda(2^i\tau)\|/\|\epsilon_\lambda(2^{i-1}\tau)\|)$ for $i = 1, 2, 3, 4$, with $\epsilon_\lambda(2^i\tau) = \lambda(2^i\tau) - \lambda_{\text{exact}}$.

	Euler	Cox-Matthews	Krogstad	Hochbruck-Ostermann
$p_\lambda(4\tau, 2\tau)$	1.8730	4.2892	4.2779	4.2580
$p_\lambda(8\tau, 4\tau)$	1.9345	4.0911	4.0839	4.0764
$p_\lambda(16\tau, 8\tau)$	1.9669	3.4815	3.4758	3.4754

Table 9.6: Approximate order of accuracy p_∇ for the gradient using a Rosenbrock approach, computed using $p_\nabla(2^i\tau, 2^{i-1}\tau) = \log_2(\|\epsilon_\nabla(2^i\tau)\|/\|\epsilon_\nabla(2^{i-1}\tau)\|)$ for $i = 1, 2, 3, 4$, with $\epsilon_\nabla(2^i\tau) = \nabla(2^i\tau) - \nabla_{\text{exact}}$.

- The simulations were run using the Krogstad scheme with a time-step of 0.25s.
- Observations were taken every 0.5s up to 25s, and 5% noise was added to each observation.
- The standard least-squares misfit function $M = \|\mathbf{d}(\mathbf{m}) - \mathbf{d}^{\text{obs}}\|$ was employed.
- TV regularization using the smoothed Huber norm was used with $\beta = 10$.
- The parameters were recovered using 400 iterations of L-BFGS (keeping 20 previous updates in storage) with cubic line search. The results after 200 iterations were already very similar to those in Figure 3.
- We used a projected gradient method, where the value of \mathbf{r} at each point was constrained to always lie in the interval $[0.01, 2.3]$ and the value of \mathbf{g} at each point was in $[-1.2, 1.2]$.

We make the following remarks on the results:

- The recovered values of \mathbf{r} are quite acceptable, as are the values of \mathbf{g} on the two outside vertical strips, whereas the estimate of the central vertical strip of \mathbf{g} is poor.
- This is the result of the observations having only been taken for up to 25s, a time after the patterns on the outside vertical strips have formed but before the central pattern, which evolves on a much slower time scale, has formed.

10. Conclusions and Future Work. This paper considers the application of the discrete adjoint method to exponential integration methods for the purposes of (distributed) parameter estimation and sensitivity analysis in time-dependent PDEs. We have derived algorithms for the linearized forward and, more importantly, the adjoint problem, and have applied these algorithms, as an instance of these integration methods, to a specific scheme.

We have found that if the linear operator depends on the solution \mathbf{y}_k at the current time step (as is the case with *some* Rosenbrock-type methods) or the model parameters, the derivatives of the φ -functions with respect to \mathbf{y}_k and \mathbf{m} introduce significant computational overhead. The extra expense introduced in this case could be prohibitive in some applications, and it might then be more reasonable to instead apply an IMEX method to the linearized PDE. The use of IMEX methods in the context of parameter estimation will be the subject of a future investigation.

A simple experiment reveals that the adjoint exponential integrator and the computed gradient of the misfit function have the same order of accuracy as the corresponding exponential integrator. This of course does not constitute a general proof. In case that the linear

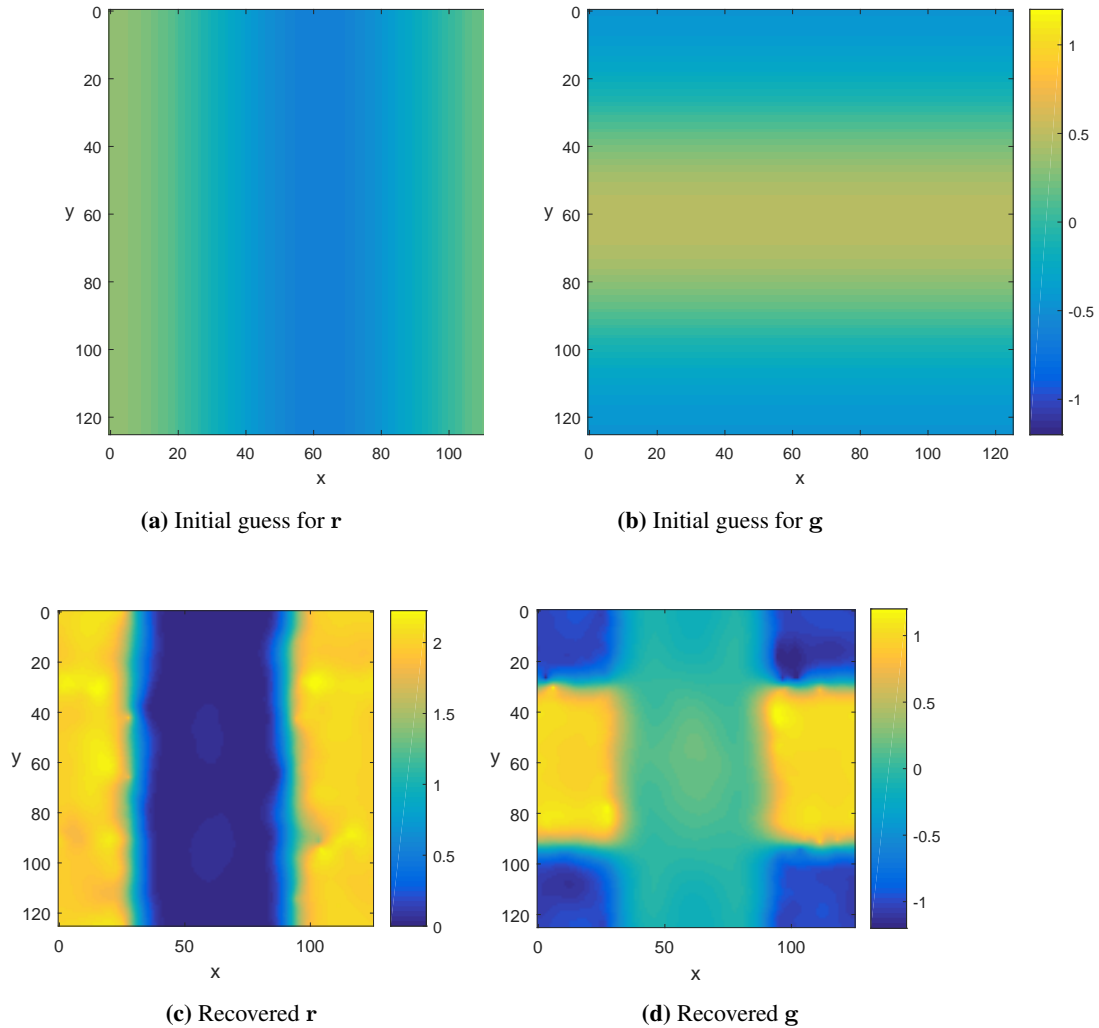


Fig. 3: Recovered parameter values (bottom) and initial guesses (top)

operator \mathbf{L} is independent of the forward solution and the model parameters it appears that one should be able to analytically prove the conjecture that this observation offers. A general proof in the case of Rosenbrock-type methods, however, appears to be a more remote prospect given how dependent the evaluations of the derivatives of the φ -functions are on their numerical implementation.

The results of this work will be of interest in applications where exponential integration is the best choice for solving the forward solution, in particular when the PDE is stiff. One such application of interest to us is pattern formation when the model parameters exhibit spatial variability, and we have applied the techniques from this paper to a simple parameter estimation problem involving Swift-Hohenberg model. A more in-depth examination into parameter estimation of pattern formation problems will be the subject of future work.

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