Error estimation for the time to a threshold value in evolutionary partial differential equations

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Abstract
We develop an a posteriori error analysis for a numerical estimate of the time at which a functional of the solution to a partial differential equation (PDE) first achieves a threshold value on a given time interval. This quantity of interest (QoI) differs from classical QoIs which are modeled as bounded linear (or nonlinear) functionals of the solution. Taylor’s theorem and an adjoint-based a posteriori analysis is used to derive computable and accurate error estimates in the case of semi-linear parabolic and hyperbolic PDEs. The accuracy of the error estimates is demonstrated through numerical solutions of the one-dimensional heat equation and linearized shallow water equations (SWE), representing parabolic and hyperbolic cases, respectively.

Keywords Threshold event · Adjoint-based error estimation · Partial differential equations · Shallow Water Equations

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1 Introduction

Numerical solutions of parabolic and hyperbolic differential equations are essential to the study of physical phenomena that evolve over space and time. To meet the requirements of uncertainty quantification, adjoint-based methods for estimating the error in a quantity of interest that can be expressed as a linear or nonlinear functional of the solution are well developed. However, the time at which a functional of the solution achieves a threshold value, which we refer to as the time to an “event”, is often the primary problem for a computational study of a physical system. Examples include: the time at which the concentration of a chemical species reaches a threshold value at a particular location, the time at which the temperature at a particular location drops below a threshold value, and the time at which a traveling wave reaches a certain location given specific initial values and topography. Unfortunately, the error in an estimated time to a particular event cannot be quantified using standard approaches.

Consider a semi-linear evolutionary PDE of the form

\[ u_t(x, t) + Lu(x, t) = f(u, x, t), \quad x \in \Omega, \quad t \in (0, T], \]
\[ u(x, 0) = g(x), \quad x \in \Omega \tag{1} \]

with appropriate initial and boundary conditions. Here \( u_t = \frac{du}{dt} \), \( L \) is a differential operator in \( x \) that is linear in \( u \), and \( f(u, x, t) \) is a differentiable function. While \( u, L \) and \( f \) may be scalar or vector valued, these cases are not distinguished in our analyses since this will be obvious from the context.

Classical a posteriori error analysis considers quantities of interest (QoIs) that can be expressed as bounded functionals of the solution and utilizes variational analysis, generalized Green’s functions and computable residuals [1–4, 6, 21, 23, 27, 30, 32, 34]. Recent extensions to multiscale and multiphysics systems include [7, 10, 22, 25, 31]. Finite difference and volume methods, and explicit time integration schemes may be analyzed by reformulating these schemes as equivalent finite element methods, see e.g., [11–15, 18, 19, 28]. Nonlinear QoIs are typically handled by linearization around a computed solution, e.g., [4, 33]. The key point motivating this paper is that the time a functional of the solution of a PDE first achieves a threshold value cannot be expressed as a bounded linear functional of \( u \), nor can it be trivially linearized.

Let \( G(u; t) \) be a linear functional of \( u(x, t) \) which is implicitly dependent on \( t \) through \( u \), and let \( R \) be a threshold value of \( G(u; t) \). Assume there are one or more times \( t^* \) during the interval \((0, T]\) for which \( G(u; t^*) = R \) is satisfied and define the time \( H(u, \tau) \) as

\[ H(u, \tau) = \min_{t \in (\tau, T]} \arg(G(u; t) = R). \tag{2} \]

Here \( \tau \) is specified in order to obtain different occurrences of the event \( G(u; t) = R \). For example, \( H(u, 0) \) is the time on the interval \((0, T]\) of the first occurrence of the event of the \( G(u; t) = R \). Similarly, the time to the second occurrence of the event \( G(u; t) = R \) is \( H(u, \tau) \), where \( H(u, 0) \leq \tau < H(u, H(u, 0)) \), i.e., for any \( \tau \) between the times of first and second occurrence of the event. The quantity of interest \( Q(u) \) for a fixed \( \tau \) is defined as
\( Q(u) = H(u, \tau). \) 

(3)

In recent work Chaudry et al. [16], an \textit{a posteriori} error analysis was performed in order to estimate the error in the time to an event (the time of the first occurrence of a functional achieving a threshold value), in the context of ordinary differential equations (ODEs). In the current work, the analysis of Chaudry et al. [16] is extended to evolutionary PDEs and to the QoI specified by (3). An error estimate is derived using Taylor series linearized around the approximate (computed) value of the QoI. The error estimate, which contains terms involving the unknown error of the solution to the PDE, is made computable through the use of solutions to certain adjoint problems. In comparison with the earlier work of Chaudry et al. [16], the current analysis requires the solution of an additional adjoint problem arising due to the presence of the spatial operator \( L \). We apply the analysis to the one-dimensional heat equation and to the one-dimensional linearized shallow water equations (SWE).

A quantity of interest closely related to \( H(u, 0) \) as defined by (2) is examined in [17, 29]. These authors, motivated by safety assessments of underground nuclear waste repositories, seek to determine the time at which a passive tracer released from a specified location and transported by a Darcy flow, crosses the boundary of a given domain. The flow field, while complicated due to the spatially heterogeneous hydraulic conductivity within the flow domain, is independent of time, but an “initial” value problem solved backwards in time along the particle trajectory is required to compute the Gateaux derivative of the travel time functional [29].

Numerical schemes to solve the semi-linear evolutionary PDE (1) are developed in Sect. 2. A variational formulation is introduced in Sect. 2.1 and a space-time Galerkin finite element discretization in Sect. 2.2. The error in QoI (3) is defined in Sect. 3 and the \textit{a posteriori} error analysis for this QoI is presented in Sect. 3.1. A computable estimate is developed in Sect. 3.3 by taking advantage of classical error estimates which are reviewed in Sect. 3.2. Error estimates for two model problems are developed in Sect. 4, the one-dimensional heat equation in Sect. 4.1 and the one-dimensional linearized shallow water equations in Sect. 4.2, respectively. Numerical results for both the linear and nonlinear heat equations and for the linearized shallow water equations with a range of different bottom topographies are presented in Sect. 5.

2 Numerical methods

Adjoint-based, \textit{a posteriori} error estimates utilize the variational (or weak) form of PDEs. A variational formulation for the semi-linear evolutionary PDE (1) is introduced in Sect. 2.1 and a space-time Galerkin finite element discretization is presented in Sect. 2.2.

2.1 Variational formulation

Let \( W \) be a generic Hilbert space over the domain \( \Omega \) with inner product \((\cdot, \cdot)_W\) and the induced W-norm \( \|\cdot\|_W \). Let \( L^2(0, T; W) \) denote the space of (possibly vector-valued)
functions $w$ whose $W$-norm is square integrable $\forall t \in [0, T]$. The variational form of (1) is: Find $u \in L^2(0, T; W)$ such that

$$(u_t(\cdot, t), v(\cdot, t)) + (L_1 u(\cdot, t), L_2 v(\cdot, t)) = (f(\cdot, \cdot, t), v(\cdot, t)), \quad \forall v \in W, \quad \forall t \in (0, T],$$

where $f(\cdot, \cdot, t) \in W$ for any $t \in (0, T]$ and $(a, b) = \int_\Omega a \cdot b \, d\Omega$ is the spatial $L^2$ inner product over $\Omega$. The two operators $L_1, L_2$ are linear differential operators such that

$$L_2^* L_1 u = Lu,$$

where $L_2^*$ denotes the formal adjoint of $L_2$. That is, the formal adjoint $L^*$ of a given operator $L$ is the operator which satisfies

$$(u, L v) = (L^* u, v), \quad \forall u \in W, v \in W.$$

Under suitable conditions on the operators $L_1$ and $L_2$ (and hence $L$), (4) is well-posed; the reader is referred to Lawrence [26] for more details. Although the differential operator $L_1$ may be of lower order than $L$, if a solution $u$ to (4) is sufficiently differentiable, it also satisfies (1).

### 2.2 Space-time Galerkin finite element method

Let $T_h$ be a shape-regular triangulation of the spatial domain $\Omega$ where $h$ denotes the diameter of the largest element. For the numerical examples in Sect. 5, $\Omega$ is one-dimensional and $T_h$ is a uniform set of $N_e$ subintervals of the domain where $h$ denotes the width of the subintervals. Let $V^{qs}$ be the standard space of continuous piecewise polynomials of degree $qs$ on $T_h$. This space may be scalar or vector valued depending upon the context.

The time domain $[0, T]$ is discretized into $N_t$ uniform subintervals of width $p$ denoted $T_p$, i.e., $T_p = \{I_0, \ldots, I_{n}, \ldots, I_{N_t-1}\}$ where $I_n = [t_n, t_{n+1}]$. Let $l_j(t)$ be the $j$th degree Lagrange polynomial in time on the interval $I_n$. For the space-time slab $S_n = \Omega \times I_n$ the solution space is defined as

$$W^{q_t, qs}_{N_t} = \left\{ w(x, t) \mid w(x, t) = \sum_{j=0}^{q_t} l_j(t) v_j(x), \ v_j(x) \in V^{qs}, \ (x, t) \in S_n \right\}.$$

We define the continuous Galerkin method, cG$(q_t, qs)$ as: Find a continuous in time $U \in W^{q_t, qs}_{N_t}$ for $n = 0, \ldots, N_t - 1$, such that

$$\int_{I_n}^{I_{n+1}} \left[ (U_t(\cdot, t), v(\cdot, t)) + (L_1 U(\cdot, t), L_2 v(\cdot, t)) \right] \, dt.$$
\[ = \int_{t_n}^{t_{n+1}} (f(u, \cdot, t), v(\cdot, t)) \, dt, \quad \forall v \in W^{r-1,q}_{n}. \]  

(8)

3 A posteriori error estimation

Let \( u(x, t) \) be the true solution of (1) and \( G(u; t) \) be a time-dependent linear functional of \( u(x, t) \) that may be expressed in terms of the inner product,

\[ G(u; t) = \int_{\Omega} w(x) \cdot u(x, t) \, dx = (w(\cdot), u(\cdot, t)), \]  

(9)

where \( w(x) \) is some differentiable weight function. Assume that \( w(x)|_{\partial \Omega} = 0 \). For a chosen threshold \( R \) and fixed value of \( \tau \) in (2), denote the true value of the QoI

\[ t_i := Q(u). \]  

(10)

Let \( U(x, t) \) be an approximation of the solution satisfying (8) and

\[ t_c := Q(U), \]  

(11)

the corresponding computed value of the QoI. Figure 1 illustrates these definitions. We denote the error in the approximate solution as \( e(x, t) = u(x, t) - U(x, t) \). As noted in Sect. 1, the a posteriori error analysis for functionals of \( e(x, t) \) is well established. However, we seek to estimate the error

\[ e_Q = t_i - t_c, \]  

(12)

and specifically, to calculate a computable estimate \( \nu \approx e_Q \). We define the affectivity ratio of this estimate to be

\[ \rho_{eff} = \frac{\nu}{e_Q}, \]  

(13)

where clearly the goal is to construct an error estimate for which \( \rho_{eff} \approx 1 \). We first derive an error representation in Sect. 3.1. Standard a posteriori techniques (see Sect. 3.2) are then employed to approximate the error in three linear functionals of \( e(x, t) \). The errors in these three functionals are calculated as the inner product of solutions to three distinct adjoint problems and computable residuals as described in Sect. 3.3.

3.1 Error estimation for the time to an event \( G(u; t) = R \)

An adjoint-based a posteriori error estimate for \( e_Q \) as defined in (12) is presented in Theorem 1 below.
Fig. 1  a Reference values of the functional $G(u; t)$ for Sect. 5.4. The QoI is the time for the third occurrence of the event $G(u; t) = R$. b Detail near the time of third occurrence of the event $G(u; t) = R$ showing the true and approximate values of the functional, $G(u; t)$ and $G(U; t)$ respectively, and the corresponding true and approximate values of the QoI, $Q(u)$ and $Q(U)$. The error is $e_Q = Q(u) - Q(U)$. 
Theorem 1 Consider the QoI defined by (3), where the functional \( G \) is defined by (9), and \( t_t, t_c \), and the error in the QoI, \( e_Q \), are defined by (10), (11) and (12) respectively. Let

\[
\mathcal{D}(U, t_c) = (L_2 w(\cdot), L_1 U(\cdot, t_c)) - (w(\cdot), f(U, \cdot, t_c)) \\
- \left( \nabla u_f^\top(U, \cdot, t_c) w(\cdot), e(\cdot, t_c) \right) + (L_2 w(\cdot), L_1 e(\cdot, t_c)), \tag{14}
\]

where \( e(x, t) = u(x, t) - U(x, t) \), and \( \nabla u_f \) is a square matrix with entries \( [\nabla u_f]_{ij} = \partial f_i / \partial u_j \). For semi-linear time evolution PDEs (1), the error in the QoI is given by

\[
e_Q = t_t - t_c = \frac{(w(\cdot), e(\cdot, t_c)) + (w(\cdot), R_1(\cdot, t_c, t_t))}{\mathcal{D}(U, t_c) - (w(\cdot), R_2(u, U, \cdot, t_c))}, \tag{15}
\]

where the two remainder terms are \( R_1(x, t_c, t_t) = O((t_t - t_c)^2) \) and \( R_2(u, U, x, t_c) = O((u - U)^2) \).

Proof Using the definitions of \( t_t \) and \( t_c \),

\[
G(u(t_t)) - G(U(t_c)) = R - R = 0. \tag{16}
\]

From (16) and (9)

\[
(w(\cdot), u(\cdot, t_t) - U(\cdot, t_c)) = 0.
\]

Expanding the functional \( G(u(t_t)) \) about \( t_c \) by expanding \( u(x, t_t) \) around \( t_c \) using Taylor Series,

\[
0 = (w(\cdot), u(\cdot, t_c) + (t_t - t_c)u_t(\cdot, t_c) + R_1(\cdot, t_c, t_t) - U(\cdot, t_c)) \\
= (w(\cdot), e(\cdot, t_c)) + (t_t - t_c) (w(\cdot), u_t(\cdot, t_c)) + (w(\cdot), R_1(\cdot, t_c, t_t)) \tag{17},
\]

where \( e(x, t) = u(x, t) - U(x, t) \) and the remainder \( R_1(x, t_c, t_t) \) is \( O((t_t - t_c)^2) \). Rearranging (17),

\[
t_t - t_c = -\frac{(w(\cdot), e(\cdot, t_c)) + (w(\cdot), R_1(\cdot, t_c, t_t))}{(w(\cdot), u_t(\cdot, t_c))}. \tag{18}
\]

From the weak formulation of the PDE (4),

\[
(w(\cdot), u_t(\cdot, t_c)) = - (L_2 w(\cdot), L_1 u(\cdot, t_c)) + (w(\cdot), f(u, \cdot, t_c)) \\
= - (L_2 w(\cdot), L_1 U(\cdot, t_c)) - (L_2 w(\cdot), L_1 e(\cdot, t_c)) + (w(\cdot), f(u, \cdot, t_c)). \tag{19}
\]
Using Taylor’s Theorem once more to expand \( f(u, x, t_c) \) around \( U(x, t_c) \),

\[
(w(\cdot), f(u, \cdot, t_c)) = (w(\cdot), f(U, \cdot, t_c)) + \left( \nabla_u f^T(U, \cdot, t_c) w(\cdot), e(\cdot, t_c) \right) + (w(\cdot), R_2(u, U, \cdot, t_c)),
\]

(20)

where the remainder \( R_2(u, U, x, t_c) \) is of order \( O((u - U)^2) \). Substituting (20) into (19) and then into (18) yields the final result.

\( \square \)

**Corollary 1** If the differential equation (1) is linear, so that \( f = f(x, t) \) does not depend on \( u \), then the error representation is

\[
t_t - t_c = \frac{(w(\cdot), e(\cdot, t_c)) + (w(\cdot), R_1(\cdot, t_c, t))}{(L_2 w(\cdot), L_1 U(\cdot, t_c)) - (w(\cdot), f(\cdot, t_c)) + (L_2 w(\cdot), L_1 e(\cdot, t_c))}.
\]

(21)

### 3.2 Error estimation for a linear functional

In order to define a computable error estimate, standard adjoint-based *a posteriori* error analysis is employed to approximate the three terms in (15) that are linear functionals of \( e(x, t) \). The standard analysis is presented for completeness in Theorem 2 below.

**Theorem 2** Given a numerical solution \( U(x, t) \) to (1) and data \( \psi(x) \), for any \( \hat{t} \in (0, T] \) the error \( (\psi(\cdot), e(\cdot, \hat{t})) \) is given by

\[
(\psi(\cdot), e(\cdot, \hat{t})) = (\phi(\cdot, 0), e(\cdot, 0)) + \int_0^{\hat{t}} (\phi(\cdot, t), f(U(\cdot, t) - U_t(\cdot, t))) \, dt
\]

\[
- \int_0^{\hat{t}} (L_2 \phi(\cdot, t), L_1 U(\cdot, t)) \, dt
\]

(22)

where \( \phi(x, t) \) is the solution of the adjoint problem

\[
- \phi_t(x, t) + L^* \phi(x, t) - A^*_{u, U} \phi(x, t) = 0, \quad x \in \Omega, \quad t \in [0, \hat{t}],
\]

\[
\phi(x, \hat{t}) = \psi(x), \quad x \in \Omega.
\]

The operator \( A^*_{u, U} \) is the adjoint of the linear operator

\[
A_{u, U} = \int_0^1 \frac{df}{dz}(z, x, t) \, ds,
\]

(24)

where \( z = su + (1 - s)U \).
Proof Multiplying the adjoint Eq. (23) by the error $e(x, t) = u(x, t) - U(x, t)$, and integrating over the space-time domain $\Omega \times [0, \hat{t}]$,

$$
0 = \int_0^\hat{t} (\phi(t, \cdot), e(\cdot, t)) \, dt - \int_0^\hat{t} \left( L^* \phi(t, \cdot), e(\cdot, t) \right) \, dt \\
+ \int_0^\hat{t} \left( A_{u, U}^* \phi(t, \cdot), e(\cdot, t) \right) \, dt.
$$

Integrating the first term of (25) by parts in time and enforcing the initial condition $\phi(x, 0) = \psi(x)$,

$$
\int_0^\hat{t} (\phi(t, \cdot), e(\cdot, t)) \, dt = \left( \psi(\cdot), e(\cdot, \hat{t}) \right) - (\phi(\cdot, 0), e(\cdot, 0)) - \int_0^\hat{t} (\phi(\cdot, t), e_t(\cdot, t)) \, dt.
$$

From (5), $L^* = L_1^* L_2$, and the second term of (25) becomes

$$
\int_0^\hat{t} \left( L^* \phi(t, \cdot), e(\cdot, t) \right) \, dt = \int_0^\hat{t} \left( L_1^* L_2 \phi(t, \cdot), e(\cdot, t) \right) \, dt \\
= \int_0^\hat{t} \left( L_2 \phi(t, \cdot), L_1 e(\cdot, t) \right) \, dt.
$$

The operator $A_{u, U}$ has the property

$$
A_{u, U} e(x, t) = f(u, x, t) - f(U, x, t),
$$

hence, using the property of the adjoint (6) and (27), the third term of (25) becomes

$$
\int_0^\hat{t} \left( A_{u, U}^* \phi(t, \cdot), e(\cdot, t) \right) \, dt = \int_0^\hat{t} \left( \phi(t, \cdot), A_{u, U} e(\cdot, t) \right) \, dt \\
= \int_0^\hat{t} \left( \phi(t, \cdot), f(u, \cdot, t) - f(U, \cdot, t) \right) \, dt.
$$

Combining (25), (26), and (28) yields,

$$
0 = \left( \psi(\cdot), e(\cdot, \hat{t}) \right) - (\phi(\cdot, 0), e(\cdot, 0)) - \int_0^\hat{t} (\phi(\cdot, t), e_t(\cdot, t)) \, dt, \\
- \int_0^\hat{t} \left( L_2 \phi(t, \cdot), L_1 e(\cdot, t) \right) \, dt + \int_0^\hat{t} \left( \phi(t, \cdot), f(u, \cdot, t) - f(U, \cdot, t) \right) \, dt.
$$

Since $e(x, t) = u(x, t) - U(x, t)$

$$
(\psi, e(\cdot, \hat{t})) = (\phi(\cdot, 0), e(\cdot, 0)) + \int_0^\hat{t} (\phi(\cdot, t), u_t(\cdot, t) - U_t(\cdot, t)) \, dt \\
+ \int_0^\hat{t} \left( L_2 \phi(\cdot, t), L_1 u(\cdot, t) - L_1 U(\cdot, t) \right) \, dt - \int_0^\hat{t} (\phi(\cdot, t), f(u, \cdot, t) - f(U, \cdot, t)) \, dt.
$$
Noting that the exact solution $u(x, t)$ satisfies (4) produces the desired result. □

In practice, since operator $A_{u,U}$ requires the true solution to (1), it is approximated by

$$A_{u,U} \approx \nabla_u f(U, x, t).$$

With this, the $A_{u,U}^*$ term of the adjoint equation (23) is approximated by

$$A_{u,U}^* \phi(x, t) \approx (\nabla_u f(U, x, t))^\top \phi(x, t).$$

**Remark 1** Theorem 2 is formulated in terms of the strong form of the adjoint problem (23), but clearly it is adequate for $\phi$ to satisfy the weak form of the problem

$$- (\phi(\cdot, t), v(\cdot)) + (L_2 \phi(\cdot, t), L_1 v(\cdot)) = (\phi(\cdot, t), A_{u,U} v(\cdot)) \quad \forall v \in H^1_0(\Omega), \quad \forall t \in (0, \hat{t}).$$

**Remark 2** The boundary conditions of the adjoint problem (23) depend on the boundary conditions of the primal problem (1). The specific boundary conditions used for the two model problems are specified in Sects. 4.1 and 4.2. The proof of Theorem 2 does not directly depend on the boundary conditions as long as property (6) is satisfied.

### 3.3 A computable error estimate for the time to an event $G(u; t) = R$

The magnitudes of the remainders $R_1$ and $R_2$ in the error representation (15) decrease more rapidly than other terms as the accuracy of the numerical solution increases (e.g., by increasing $N_x, N_t, q_t$ or $q_s$ in Sect. 2.2). Setting both $(w(\cdot), R_1(\cdot, t_c, t)) \approx 0$ and $(w(\cdot), R_2(u, U, \cdot, t_c)) \approx 0$ gives a first approximation

$$t_t - t_c \approx \frac{(w(\cdot), e(\cdot, t_c))}{D(U, t_c)},$$

where $D(U, t_c)$ is defined in (14). The terms in the numerator and denominator containing the unknown error $e(x, t)$ may be estimated using Theorem 2. However, each of these expressions have different stability properties, their estimation requires the solution to distinct adjoint problems as given below.

**First adjoint problem** To estimate $(w(\cdot), e(\cdot, t_c))$, (23) is solved backwards from $t_c$ with initial condition $\psi(x) = \psi^{(1)}(x) = w(x)$. Substituting the solution $\phi^{(1)}$ in (22) provides a computable estimate for

$$E_1 \approx \left(\psi^{(1)}(\cdot), e(\cdot, t_c)\right) = (w(\cdot), e(\cdot, t_c)).$$

**Second adjoint problem** To estimate $(L_2 w(\cdot), L_1 e(\cdot, t_c))$, we assume $w(x)$ is smooth enough for $L^* w$ to be well-defined and solve (23) backwards from $t_c$ with initial
condition $\psi(x) = \psi^{(2)}(x) = L^*w(x)$. Substituting the solution $\phi^{(2)}$ in (22) provides a computable estimate for
\[ E_2 \approx \left( \psi^{(2)}(\cdot), e(\cdot, t_c) \right) = \left( L^*w(\cdot), e(\cdot, t_c) \right) = (L_2w(\cdot), L_1e(\cdot, t)). \]

Third adjoint problem To estimate $\left( \nabla u f^\top(U, \cdot, t_c)w(\cdot), e(\cdot, t_c) \right)$, (23) is solved backwards with initial condition $\psi(x) = \psi^{(3)}(x) = \nabla u f^\top(U, x, t_c)w(x)$. Substituting the solution $\phi^{(3)}$ in (22) provides a computable estimate for
\[ E_3 \approx \left( \psi^{(3)}(\cdot), e(\cdot, t_c) \right) = \left( \nabla u f^\top(U, \cdot, t_c)w(\cdot), e(\cdot, t_c) \right). \]

The third adjoint problem is only required for nonlinear problems. If the right-hand-side of (1) is $f = f(x,t)$, the gradient is $\nabla u f = 0$ and $E_3 \equiv 0$.

Remark 3 If the numerical solution $U$ is not sufficiently accurate, the $n$-th event for the approximate solution $U$ may be closest to the $m$-th event for the true solution $u$ where $n \neq m$. If this is the case, approximation by Taylor series around $t_c$ and $U(x, t_c)$ is inappropriate and the error estimator may not be accurate. See Remark 2 in [16].

4 Model problems

We apply the abstract theory developed in Sect. 3 to the heat equation and the 1D linearized shallow water equations.

4.1 Heat equation

The heat equation models the diffusion of heat or chemical species. We consider the heat equation in a domain $\Omega \subset \mathbb{R}^n$,

\[ \begin{align*}
  u_t(x, t) - \nabla^2 u(x, t) &= f(u, x, t), \quad x \in \Omega, \quad t \in (0, T], \\
  u(x, t) &= 0, \quad x \in \partial \Omega, \quad t \in (0, T], \\
  u(x, 0) &= u_0(x), \quad x \in \Omega,
\end{align*} \]

where $u(x, t)$ is the temperature of the medium or concentration of a chemical species.

Weak form

The weak form is: Find $u \in L^2(0, T; H^1_0(\Omega))$ such that

\[ (u_t, v) + (\nabla u, \nabla v) = (f, v) \quad \forall v \in H^1_0(\Omega), \quad t \in (0, T]. \]

When written in standard form as $u_t + Lu = f$, the operator $L$ is
\[ L = -\nabla^2. \]
For any function $v \in H_0^1(\Omega)$,

$$(Lu, v) = (-\nabla^2 u, v) = (\nabla u, \nabla v),$$

implying

$$L_1 = L_2 = \nabla.$$

**Error estimate**

The error estimate (30) applied to the heat Eq. (31) becomes

$$t_f - t_c \approx \frac{(w(\cdot), e(\cdot, t_c)) - (w(\cdot), f(U(\cdot, \cdot), t_c)) - (\nabla_u f^\top(U(\cdot, \cdot), t_c) w(\cdot), e(\cdot, t_c)) + (\nabla w(\cdot), \nabla e(\cdot, t_c))}{(\nabla w(\cdot), \nabla U(\cdot, \cdot, t_c) w(\cdot), e(\cdot, t_c))}.$$ 

The three adjoint problems presented in Sect. 3.3 all have the same form,

$$\begin{aligned}
-\phi_i^{(i)}(x, t) - \nabla^2 \phi_i^{(i)}(x, t) - \nabla_u f^\top \phi_i^{(i)} = 0, & \quad x \in \Omega, \quad t \in (t_c, 0] \\
\phi_i^{(i)}(x, t_c) = \psi_i^{(i)}(x), & \quad x \in \Omega, \quad t \in (t_c, 0] \\
\phi_i^{(i)}(x, t_c) = \psi_i^{(i)}(x), & \quad x \in \Omega, \quad t \in (t_c, 0] \\
\end{aligned}$$

but different initial conditions

$$\begin{aligned}
\psi_1^{(i)}(x) &= w(x), \\
\psi_2^{(i)}(x) &= -\nabla^2 w(x), \\
\psi_3^{(i)}(x) &= \nabla_u f^\top(U(x), t_c) w(x). \\
\end{aligned}$$

Note that for this example we have

$$L^* = -\nabla^2, \quad \text{and} \quad L_1^* = L_2^* = \nabla.$$

**4.2 1D linearized shallow water equation (SWE)**

The shallow water equations model wave propagation in a fluid domain in which the horizontal scale is large compared to the vertical scale. Applications of the SWE arise frequently in the study of the ocean and atmosphere. In particular, the linearized SWE model has been used to model tsunami wave propagation and inundation in coastal areas, flooding from a dam break, and flows and waves in the atmosphere, see e.g., [5, 8]. A posteriori error analysis for QoIs that are functionals of the solution to the linearized SWE has been conducted previously in [20].

The nonlinear shallow water equations in one dimension on a domain $\Omega = [0, D]$ are (see [20])

$$\begin{aligned}
\mu_t(x, t) + \frac{\eta_t(x, t) + \mu_x(x, t)}{\eta(x, t)} + \frac{1}{2} g \eta(x, t)^2_x + g \eta B_x(x) = f_2(x, t), & \quad x \in \Omega, \quad t \in (0, T]. \\
\end{aligned}$$

(32)
where $\eta(x,t)$ corresponds to the water surface elevation and $\mu(x,t)$ corresponds to the momentum of the fluid. The constant $g$ is the gravitational acceleration constant, $f(x,t) = (f_1(x,t), f_2(x,t))^T$ is the forcing (typically 0) and $B(x)$ is the bathymetry (bottom surface profile).

Linearizing (32) around a flat fluid surface with elevation $\bar{\eta}$ and momentum $\bar{\mu} = 0$,

\[
\begin{align*}
\eta_t(x,t) + \mu_x(x,t) = f_1(x,t), \\
\mu_t(x,t) + g\bar{h}(x)\eta_x(x,t) = f_2(x,t), \\
\mu(x,t) = 0, \\
\eta(x,0) = \eta_0(x), \\
\mu(x,0) = \mu_0(x),
\end{align*}
\]

$x \in \Omega$, $t \in (0, T]$, (33)

where $\bar{h}(x) = \bar{\eta} - B(x)$, $\eta_0(x)$ is the initial surface profile, $\mu_0(x)$ is the initial momentum profile, and $\eta$ satisfies reflective boundary conditions (see [20]).

**Weak form**

The weak form of (33) is: Find $\eta \in L^2(0, T; H^1(\Omega))$ and $\mu \in L^2(0, T; H^1_0(\Omega))$ such that

\[
\begin{align*}
(\eta_t, v_1) + (\mu_t, v_2) + (\mu_x, v_1) + g\bar{h}(\eta_x, v_2) &= (f_1, v_1) + (f_2, v_2), \\
\forall v_1 \in H^1(\Omega), v_2 \in H^1_0(\Omega), & t \in (0, T).
\end{align*}
\]

When written in standard form as $u_t + Lu = f$, where $u(x,t) = (\eta(x,t), \mu(x,t))^T$, the operator $L$ is

\[
L = \begin{pmatrix}
0 & \frac{\partial}{\partial x} \\
g\bar{h}(x) & 0
\end{pmatrix},
\]

and since $L$ contains only first order derivatives, the operators $L_1$ and $L_2$ are

$L_1 = L$, $L_2 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$.

**Error estimate**

For the linearized shallow water equations (33), Corollary 1 is applicable and the error estimate (30) becomes

\[
t_t - t_c \approx \frac{(w(\cdot), e(\cdot, t_c))}{(w(\cdot), A(\cdot)U_x(\cdot, t_c)) - (w(\cdot), f(\cdot, t_c)) + (w(\cdot), A(\cdot)e_x(\cdot, t_c))},
\]

where

\[
u = \begin{pmatrix} \eta \\ \mu \end{pmatrix}, \quad f = \begin{pmatrix} f_1 \\ f_2 \end{pmatrix}, \quad A(x) = \begin{pmatrix} 0 & 1 \\ g\bar{h}(x) & 0 \end{pmatrix}.
\]
The two non-trivial adjoint problems take the form

\[
\begin{align*}
-\phi^{(i)}(x, t) + L^*(\phi^{(i)})(x, t) &= 0, \quad x \in \Omega, \quad t \in (t_c, 0], \\
\phi^{(i)}(x, t) &= 0, \quad x \in \partial \Omega, \quad t \in (t_c, 0], \\
\phi^{(i)}(x, t_c) &= \psi^{(i)}(x), \quad x \in \Omega
\end{align*}
\]

where for a given \( \omega = [\omega_1, \omega_2]^T \) the operator \( L^* \) is defined as,

\[
L^*(\omega) = -\frac{\partial}{\partial x} \left( g\bar{h}(x)\omega_2 \right)_{\omega_1},
\]

Since \( L^* \) contains only first order derivatives, the operators \( L_1^* \) and \( L_2^* \) are

\[
L_1^*(\omega) = L^*(\omega), \quad L_2^* = L_2
\]

with initial conditions

\[
\psi^{(1)}(x) = w(x), \\
\psi^{(2)}(x) = -(A^\top(x)w(x))_x.
\]

5 Numerical results

All numerical examples were computed using a uniform one-dimensional spatial mesh of length \( D \) with \( N_x \) finite elements and a uniform temporal mesh of length \( T \) with \( N_t \) elements. The forward problems were solved using a space-time Galerkin method as described Sect. 2.2. Unless otherwise noted, the same degree of approximation was used for the basis functions in both space and time. In all examples, the adjoint problems were solved using the same space-time mesh as the forward problem, but with a Galerkin finite element method two degrees higher in both space and time. We choose to solve the adjoint problem with this precision in order to demonstrate the accuracy of the estimates. In practice, when estimates are used to drive an adaptive strategy, lower accuracy may be acceptable.

5.1 1D linear heat equation

Consider the heat equation in one dimension,

\[
\begin{align*}
\frac{u_t}{u_{xx}} - \sin(\pi x)(\pi^2 \cos(t) - \sin(t)) &= 0, \quad x \in [0, 1], \quad t \in (0, 0.5], \\
u(0, t) = u(1, t) &= 0, \quad t \in (0, 0.5], \\
u(x, 0) &= \sin(\pi x), \quad x \in [0, 1].
\end{align*}
\]
Table 1  Computed time $t_c$ to the first occurrence of the event $G(u; t) = R$, error in the QoI $e_Q$, and effectivity ratio $\rho_{eff}$, for Sect. 5.1, using cG(1,1) to solve the forward problem and cG(2,2) to solve the adjoint problems.

| $N$  | $t_c$          | $e_Q$          | $\rho_{eff}$ |
|------|----------------|----------------|--------------|
| 50   | 0.347229       | $9.367 \times 10^{-4}$ | 1.001        |
| 100  | 0.347931       | $2.354 \times 10^{-4}$ | 1.000        |
| 200  | 0.348108       | $5.832 \times 10^{-5}$ | 1.000        |
| 400  | 0.348166       | $1.472 \times 10^{-5}$ | 1.000        |

The exact time to the first occurrence of the event is $t_f = 0.34815698$.

The right-hand-side forcing function has been chosen so that (34) has the analytical solution $u(x, t) = \cos(t) \sin(\pi x)$. Let the functional $G(u; t)$ be

$$ G(u; t) = (w(\cdot), u(\cdot, t)) = (\sin(\pi(\cdot)), u(\cdot, t)), $$

and the threshold value be $R = 0.47$. The true values of the functional $G(u; t)$ are provided in Fig. 2a and the threshold value $R$ appears as a dashed horizontal line. The QoI is the first occurrence of the event $G(u; t) = R$, that is, $t_f = H(u, 0)$.

The “initial” conditions for the adjoint problems in Sect. 4.1 are

$$
\psi^{(1)}(x) = w(x) = \sin(\pi x),
\psi^{(2)}(x) = -w_{xx}(x) = \pi^2 \sin(\pi x),
\psi^{(3)}(x) = \nabla u f^T(U, x, t_c)w(x) = 0.
$$

The problem (34) was solved using the cG(1,1) method on a sequence of increasingly refined uniform meshes. The computed time $t_c$ to the first occurrence of the event $G(u; t) = R$, the error in the QoI $e_Q$, and the effectivity ratio $\rho_{eff}$, of the a posteriori error estimator are presented in Table 1. The error decreases as the mesh is refined as expected, and the effectivity ratios are close to 1 in all cases.

5.2 1D nonlinear heat equation

Consider the nonlinear heat equation in one dimension

$$ u_t - u_{xx} = -u^2 + \sin(\pi x)(-\sin(t) + \pi^2 \cos(t) + \cos^2(t) \sin(\pi x)), $$

$$ x \in (0, 1], \quad t \in (0, 0.5], $$

$$ u(0, t) = u(1, t) = 0 \quad t \in (0, 0.5], $$

$$ u(x, 0) = \sin(\pi x) \quad x \in [0, 1]. $$

The right-hand-side “forcing” function has been chosen so that the nonlinear heat equation (35) has the same analytical solution as the linear heat equation (34) in Sect. 5.1, namely $u(x, t) = \cos(t) \sin(\pi x)$. The functional $G(u; t)$ is again chosen to be

$$ G(u; t) = (w(\cdot), u(\cdot, t)) = (\sin(\pi(\cdot)), u(\cdot, t)). $$
and the threshold value to be $R = 0.47$. The QoI is the first occurrence of the event $G(u; t) = R$, that is, $t_t = H(u, 0)$. The true values of the functional are graphed in Fig. 2a.
Table 2 Computed time $t_c$ to the first occurrence of the event $G(u; t) = R$, error in the QoI $e_Q$, and effectivity ratio $\rho_{\text{eff}}$, for Sect. 5.2, using cG(1,1) to solve the forward problem and cG(2,2) to solve the adjoint problems

| $N$ | $t_c$       | $e_Q$      | $\rho_{\text{eff}}$ |
|-----|-------------|------------|----------------------|
| 50  | 0.347362    | $8.036 \times 10^{-4}$ | 1.001                |
| 100 | 0.347964    | $2.023 \times 10^{-4}$ | 1.000                |
| 200 | 0.348166    | $5.006 \times 10^{-5}$ | 1.000                |
| 400 | 0.348166    | $1.265 \times 10^{-5}$ | 1.000                |

The exact time to the first occurrence of the event is $t_t = 0.34816598$.

The “initial” conditions for the adjoint problems in Sect. 4.1 are

\[ \psi(1)(x) = w(x) = \sin(\pi x), \]
\[ \psi(2)(x) = -w_{xx}(x) = \pi^2 \sin(\pi x), \]
\[ \psi(3)(x) = \nabla_u f^\top (U, x, t_c)w(x) = -2 \sin(\pi x)U(x, t_c). \]

Note in particular, that unlike for the previous, linear case in Sect. 5.1, the third adjoint problem is non-trivial. The problem (35) was solved using the cG(1,1) methods using a sequence of increasingly refined uniform meshes. The computed time $t_c$ to the first occurrence of the event $G(u; t) = R$, the error in the QoI $e_Q$, and the effectivity ratio $\rho_{\text{eff}}$, of the a posteriori error estimator are presented in Table 2 which clearly indicates that the error decreases as the mesh is refined and the effectivity ratios remains close to 1 in all cases.

5.3 1D linearized SWE: manufactured solution

Consider the linearized SWEs (33) over the space-time domain $(x, t) \in [0, 10] \times [0, 1]$ with right-hand-side

\[ f = \begin{pmatrix} f_1 \\ f_2 \end{pmatrix} = \begin{pmatrix} -\sin(t) \sin(\pi x) + \pi \cos(t) \cos(\pi x) \\ -\sin(t) \sin(\pi x) + \pi \bar{g} \bar{h}(x) \cos(t) \cos(\pi x) \end{pmatrix}. \]  \hfill (36)

In order to construct an analytical exact solution, the bathymetry was chosen to be a constant, $B(x) = -10$ as shown in Fig. 3a and Dirichlet boundary conditions were imposed at the boundaries of the domain, specifically $u(0, t) = u(10, t) = (2, 0)^\top$. The initial surface elevation and momentum were chosen as $u(x, 0) = (\eta_0(x), \mu_0(x))^\top = (2 + \sin(\pi x), \sin(\pi x))^\top$. The initial surface elevation $\eta_0(x)$ is shown in Fig. 3b. The rest-state elevation was $\bar{\eta} = 2$.

Finally, the forcing term (36) was chosen so that (33) has the analytical solution

\[ u(x, t) = \begin{pmatrix} \eta(x, t) \\ \mu(x, t) \end{pmatrix} = \begin{pmatrix} 2 + \cos(t) \sin(\pi x) \\ \cos(t) \sin(\pi x) \end{pmatrix}. \]
Fig. 3 The bathymetry $B(x)$, initial wave height $\eta_0(x)$, and nonzero component of the weight function $w_2(x)$ for Sect. 5.3

Table 3 Computed time $t_c$ to the first occurrence of the event $G(u; t) = R$, error in the QoI $e_Q$, and effectivity ratio $\rho_{\text{eff}}$, for Sect. 5.3, using cG(2,2) to solve the forward problem and cG(4,4) to solve the adjoint problems

| $N$  | $t_c$       | $e_Q$            | $\rho_{\text{eff}}$ |
|------|-------------|------------------|----------------------|
| 50   | 0.821197    | $-1.321 \times 10^{-3}$ | 0.997                |
| 100  | 0.819938    | $-6.126 \times 10^{-5}$ | 1.000                |
| 200  | 0.819885    | $-8.257 \times 10^{-6}$ | 1.000                |
| 400  | 0.819878    | $-1.933 \times 10^{-6}$ | 1.000                |

The exact time to the first occurrence of the event is $t_f = 0.81987644$

In order to define the functional $G(u; t)$, let the weight function be $w(x) = (0, w_2(x))$ where

$$w_2(x) = \begin{cases} 
0 & x \leq 5, \\
10(x - 5)^2(x - 6)^2 & 5 < x < 6, \\
0 & x \geq 6.
\end{cases}$$

The non-zero component of the weight function $w_2(x)$ is depicted in Fig. 3c. The true values of the functional $G(u; t) = (w(\cdot), u(\cdot), t)$ are provided in Fig. 2b, where the threshold value $R = -0.19$ appears as a dashed horizontal line. The QoI is the first occurrence of the event $G(u; t) = R$, that is, $t_f = H(u, 0)$.

The initial conditions for the adjoint problems in Sect. 4.2 are

$$\psi^{(1)}(x) = (0, w_2(x))^\top,$$
$$\psi^{(2)}(x) = (-g(\bar{h}(x)w_2(x))_x, 0)^\top.$$ 

The linear SWE were solved using the cG(2,2) method (Sect. 2.2) on a sequence of increasingly refined uniform meshes. The computed time $t_c$ to the first occurrence of the event $G(u; t) = R$, the error in the QoI $e_Q$, and the effectivity ratio $\rho_{\text{eff}}$, of the a posteriori error estimator are presented in Table 3.

5.4 1D linearized SWE: constant bathymetry

Consider the linearized SWEs (33) over the space-time domain $(x, t) \in [0, 400] \times [0, 200]$, with the more realistic right-hand-side $f = (0, 0)^\top$. The bathymetry was
chosen to be the constant $B(x) = -0.1$ as depicted in Fig. 4a and the rest-state height was $\bar{\eta} = 1$. Dirichlet boundary conditions were imposed on the momentum only, specifically $\mu(0,t) = \mu(D,t) = 0$. The initial conditions were $u(x,0) = (\eta_0(x), 0)^\top$, where

$$
\eta_0(x) = \begin{cases}
0, & x \leq 100, \\
0.4 \times \frac{(x-100)^2(x-150)^2}{390625}, & 100 < x < 150, \\
0, & x \geq 150.
\end{cases}
$$

The initial surface elevation $\eta_0(x)$ is shown in Fig. 4b.

In order to define the functional $G(u; t)$ we set the weight function $w = (w_1(x), 0)^\top$ where

$$
w_1(x) = \begin{cases}
0, & x \leq 160, \\
\frac{1}{200,000} (x-160)^2 (x-200)^2, & 160 < x < 200, \\
0, & x \geq 200.
\end{cases}
$$

The non-zero component of the weight function $w_1(x)$ is shown in Fig. 4c. The linear SWE were solved using the cG(2,2) method (Sect. 2.2), and the surface elevation
Evolution of the surface elevation $\eta(x, t)$ for Sect. 5.4. The initial profile generates left and right traveling waves which eventually reflect off the left-hand and right-hand boundaries. The arrows indicate the direction of propagation.

$\eta(x, t)$ at several times is shown in Fig. 5. Since an analytical solution $u$ is unavailable, a reference solution $u$ was computed using a mesh-size of $N_{\text{ref}} = 800$ with the $cG(3,3)$ method. Reference values of the functional $G(u; t)$ are graphed in Fig. 6a, where the threshold value of $R = 2$ is indicated by the dashed horizontal line.

The QoI defined by the functional $G(u; t)$ is essentially the time at which the surface elevation at a narrow region centered at $x = 180$ achieves a specified value. Recall that by an event we mean $G(\cdot; t)$ achieving the threshold value $R$. The first event occurs when the incident wave arrives near $x = 180$ and $G(u; t)$ increases above the threshold value. The second event occurs when the incident wave travels beyond the narrow region centered at $x = 180$ and $G(u; t)$ drops below the threshold value. The third and fourth events occur when the reflected wave passes through the narrow region centered at $x = 180$ and $G(u; t)$ first increases above and then drops below the threshold value.

The initial conditions for the adjoint problems in Sect. 4.2 are

$$
\psi^{(1)}(x) = (w_1(x), 0)^T,
$$

$$
\psi^{(2)}(x) = (0, -w_{1,x}(x))^T.
$$
The computed times $t_c$ to the first, second and third occurrences of the event $G(u; t) = R$, errors in the QoI $e_Q$, and effectivity ratios $\rho_{eff}$, are presented in Table 4, where the effectivity ratios are all seen to be close to 1 even for the later events.

5.5 1D linearized SWE: continental shelf

Consider the linearized SWEs (33) over the space-time domain $(x, t) \in [0, 400, 000] \times [0, 4200]$. In this example, the bathymetry $B(x)$ was chosen to be

$$B(x) = \begin{cases} 
-200, & x \leq 25000, \\
-0.152x + 3600, & 25000 < x < 50000, \\
-4000, & x \geq 50000,
\end{cases}$$

as depicted in Fig. 7a and represents a continental shelf. The rest-state height $\bar{\eta} = 1$. Dirichlet boundary conditions were applied to the momentum only, specifically...
Table 4: Computed times $t_c$ to the first, second and third occurrences of the event $G(u; t) = R$, error in the QoI $e_Q$, and effectivity ratio $\rho_{eff}$, for Sect. 5.4, using $cG(2,2)$ to solve the forward problem and $cG(4,4)$ to solve the adjoint problems.

| N  | First event | Second event | Third event |
|----|-------------|--------------|-------------|
|    | $t_c$ | $e_Q$ | $\rho_{eff}$ | $t_c$ | $e_Q$ | $\rho_{eff}$ | $t_c$ | $e_Q$ | $\rho_{eff}$ |
| 50 | 13.4083 | $-5.849 \times 10^{-2}$ | 1.001 | 20.2736 | $-1.204 \times 10^{-1}$ | 1.008 | 90.0299 | $-5.370 \times 10^{-1}$ | 0.991 |
| 100| 13.3634 | $-1.363 \times 10^{-2}$ | 1.000 | 20.1599 | $-6.778 \times 10^{-3}$ | 1.003 | 89.5458 | $-5.291 \times 10^{-2}$ | 1.000 |
| 200| 13.3495 | $2.779 \times 10^{-4}$ | 1.000 | 20.1529 | $2.538 \times 10^{-4}$ | 0.990 | 89.4961 | $-3.164 \times 10^{-3}$ | 0.988 |
| 400| 13.3499 | $-1.459 \times 10^{-4}$ | 1.000 | 20.1531 | $6.998 \times 10^{-5}$ | 1.002 | 89.4931 | $-2.166 \times 10^{-4}$ | 0.967 |

The first, second, and third events occur at $t_f = 13.349799$, $t_f = 20.153171$, and $t_f = 89.492912$ respectively.
The bathymetry $B(x)$, initial wave height $\eta_0(x)$, and nonzero component of the weight function $w_1(x)$ for Sect. 5.5

$$\mu(0, t) = \mu(D, t) = 0.$$ The initial condition was $u(x, 0) = (\eta_0(x), 0)^\top$, where

$$\eta_0(x) = \begin{cases} 
0, & x \leq 100000, \\
\frac{0.4}{25000^4}(x - 100000)^2(x - 150000)^2, & 100000 < x < 150000, \\
0, & x \geq 150000.
\end{cases}$$

The initial surface elevation $\eta_0(x)$ is depicted in Fig. 7b.

In order to define the functional $G(u; t)$ (9), the weight function $w = (w_1(x), 0)^\top$ was

$$w_1(x) = \begin{cases} 
0, & x \leq 10000, \\
\frac{1}{7500^4}(x - 10000)^2(x - 25000)^2, & 10000 < x < 25000, \\
0, & x \geq 25000.
\end{cases}$$

The non-zero component of the weight function $w_1(x)$ is depicted in Fig. 7c.

A reference solution $u$ was computed using a mesh with $N_{\text{ref}} = 1280$ sub-intervals with the cG(3,3) method. The corresponding values of the functional $G(u; t)$ are plotted in Fig. 6b and the threshold value of $R = 1000$ is presented as a dashed
horizontal line. The QoIs we consider are the times for the first, second and third occurrences of the event $G(u; t) = R$.

The initial conditions for the adjoint problems in Sect. 4.2 are

$$\psi^{(1)}(x) = (w_1(x), 0)^\top,$$
$$\psi^{(2)}(x) = (0, -w_{1,x}(x))^\top.$$ 

The forward problem was solved using the cG(2,2) method (Sect. 2.2) on a sequence of increasingly refined uniform meshes. The computed times $t_c$ to the first, second and third occurrences of the event $G(u; t) = R$, errors in the QoI $e_Q$, and effectivity ratios $\rho_{eff}$, are presented in Table 5.

The effect of the spatial discretization was investigated by repeating the above calculations using cG(2,1). Note that the degree of the spatial basis functions used to solve the adjoint problems was also reduced by one. As anticipated, as is shown in Table 6, the errors $e_Q$ for the times to the first three events $G(u; t) = R$ are much larger than when solving using cG(2,2). However, the effectivity ratios remain close to 1 as desired.

### 5.6 1D linearized SWE: reef

Consider the homogeneous, linearized SWEs (33) over the space-time domain $(x, t) \in [0, 400,000] \times [0, 4200]$. The bathymetry $B(x)$ was a simplified representation of an obstruction on the sea floor, e.g., a reef, and is given as

$$B(x) = \begin{cases} 
-4000, & x \leq 25000 \\
\frac{-50}{25000^2}(x - 200000)(x - 250000) & 200000 < x < 250000 \\
-4000, & x \geq 50000 
\end{cases}$$

which is depicted in Fig. 8a. The rest-state $\bar{\eta} = 1$. The Dirichlet boundary conditions were again $\mu(0, t) = \mu(D, t) = 0$, and the initial condition was $u(x, 0) = (\eta_0(x), 0)^\top$, where

$$\eta_0(x) = \begin{cases} 
0, & x \leq 100000 \\
\frac{0.4}{25000^4}(x - 100000)^2(x - 150000)^2 & 100000 < x < 150000 \\
0, & x \geq 150000. 
\end{cases}$$

The initial wave height $\eta_0(x)$ is presented in Fig. 8b.

In order to define the functional $G(u; t)$, the weight function $w = (w_1(x), 0)^\top$ was given by

$$w_1(x) = \begin{cases} 
0, & x \leq 10000 \\
\frac{1}{7500^2}(x - 10000)^2(x - 25000)^2 & 10000 < x < 15000 \\
0, & x \geq 25000. 
\end{cases}$$

and the non-zero component of the weight function $w_1(x)$ is depicted in Fig. 8c.
Table 5 Computed times $t_c$ to the first, second and third occurrences of the event $G(u; t) = R$, error in the QoI $e_Q$, and effectivity ratio $\rho_{\text{eff}}$, for Sect. 5.5, using $cG(2, 2)$ to solve the forward problem and $cG(4, 4)$ to solve the adjoint problems

| $N$ | First event | Second event | Third event |
|-----|-------------|--------------|------------|
|     | $t_c$ | $e_Q$ | $\rho_{\text{eff}}$ | $t_c$ | $e_Q$ | $\rho_{\text{eff}}$ | $t_c$ | $e_Q$ | $\rho_{\text{eff}}$ |
| 80  | 651.267 | $-3.647 \times 10^{-1}$ | 1.002 | 838.675 | $-2.456 \times 10^{-1}$ | 0.970 | 1438.541 | $9.255 \times 10^{-1}$ | 0.925 |
| 160 | 650.975 | $-7.329 \times 10^{-2}$ | 1.000 | 838.421 | $8.597 \times 10^{-3}$ | 0.929 | 1439.384 | $1.008 \times 10^{-1}$ | 0.979 |
| 320 | 650.907 | $-4.970 \times 10^{-3}$ | 1.000 | 838.428 | $8.944 \times 10^{-4}$ | 1.006 | 1439.479 | $6.161 \times 10^{-3}$ | 0.986 |
| 640 | 650.902 | $3.672 \times 10^{-4}$ | 1.000 | 838.429 | $-2.890 \times 10^{-4}$ | 1.012 | 1439.484 | $1.046 \times 10^{-3}$ | 1.042 |

The first, second, and third events occur at $t_f = 650.79647$, $t_f = 838.42910$, and $t_f = 1439.4849$ respectively.
Table 6  Computed times $t_c$ to the first, second and third occurrences of the event $G(u; t) = R$, error in the QoI $e_Q$, and effectivity ratio $\rho_{\text{eff}}$, for Sect. 5.5, using $cG(2,1)$ to solve the forward problem and $cG(4,3)$ to solve the adjoint problems

| $N$ | First event | Second event | Third event |
|-----|-------------|--------------|-------------|
|     | $t_c$       | $e_Q$        | $\rho_{\text{eff}}$ | $t_c$       | $e_Q$          | $\rho_{\text{eff}}$ | $t_c$       | $e_Q$        | $\rho_{\text{eff}}$ |
| 80  | 643.874     | $6.922 \times 10^0$ | 1.023       | 846.194     | $-7.681 \times 10^0$ | 0.999       | 1465.863     | $-2.648 \times 10^1$ | 1.050       |
| 160 | 650.852     | $-5.536 \times 10^{-2}$ | 1.014       | 840.674     | $-2.161 \times 10^0$ | 0.999       | 1442.571     | $-3.192 \times 10^0$ | 0.994       |
| 320 | 650.802     | $-5.360 \times 10^{-3}$ | 1.002       | 838.683     | $-1.702 \times 10^{-1}$ | 0.998      | 1439.675     | $-2.964 \times 10^{-1}$ | 1.003       |
| 640 | 650.795     | $1.889 \times 10^{-3}$ | 0.997       | 838.521     | $-8.420 \times 10^{-3}$ | 0.995      | 1439.392     | $-1.001 \times 10^{-2}$ | 1.002       |

The first, second, and third events occur at $t_f = 650.79647$, $t_f = 838.51300$, and $t_f = 1439.3789$ respectively
The reference solution was computed on a mesh with $N_{\text{ref}} = 1280$ sub-intervals with the cG(3,3) method. The reference values of the functional $G(u; t)$ are plotted in Fig. 6c where the threshold value of $R = 1000$ is presented as a dashed horizontal line. While this appears more complicated than Fig. 6a, b this is merely because the weight function is located close to a domain boundary and so $G(u; t)$ does not have time to “recover” and drop back to a small value before the reflected wave impinges on the threshold region. The QoIs we consider are the times for the first, second and third occurrences of the event $G(u; t) = R$.

The initial conditions for the adjoint problems in Sect. 4.2 are

$$\psi^{(1)}(x) = (w_1(x), 0)^\top,$$

$$\psi^{(2)}(x) = (0, -w_{1,x}(x))^\top.$$

The forward problem was solved using the cG(2,2) method (Sect. 2.2) on a series of increasingly fine uniform meshes. The computed times $t_c$ to the first, second and third occurrences of the event $G(u; t) = R$, errors in the QoI $e_Q$, and effectivity ratios $\rho_{\text{eff}}$, are presented in Table 7, where the effectivity ratios are all close to one.
Table 7 Computed times $t_c$ to the first, second and third occurrences of the event $G(u; t) = R$, error in the QoI $e_Q$, and effectivity ratio $\rho_{\text{eff}}$, for Sect. 5.6, using $cG(2,2)$ to solve the forward problem and $cG(4,4)$ to solve the adjoint problems.

| $N$ | First event | Second event | Third event |
|-----|-------------|--------------|-------------|
|     | $t_c$ | $e_Q$ | $\rho_{\text{eff}}$ | $t_c$ | $e_Q$ | $\rho_{\text{eff}}$ | $t_c$ | $e_Q$ | $\rho_{\text{eff}}$ |
| 80  | 489.353 | $-3.398 \times 10^0$ | 1.016 | 615.540 | $-9.503 \times 10^0$ | 1.260 | 663.188 | $-6.692 \times 10^0$ | 0.934 |
| 160 | 485.870 | $8.481 \times 10^{-2}$ | 1.000 | 607.105 | $-1.069 \times 10^0$ | 1.010 | 656.738 | $-2.412 \times 10^{-1}$ | 0.981 |
| 320 | 485.951 | $4.482 \times 10^{-3}$ | 1.000 | 606.055 | $-1.869 \times 10^{-2}$ | 1.043 | 656.478 | $1.899 \times 10^{-2}$ | 0.942 |
| 640 | 485.954 | $7.146 \times 10^{-4}$ | 1.001 | 606.038 | $-1.194 \times 10^{-3}$ | 1.016 | 656.501 | $-4.511 \times 10^{-3}$ | 0.960 |

The first, second, and third events occur at $t_f = 485.95515$, $t_f = 606.03632$, and $t_f = 656.49655$ respectively.
Fig. 9 The reference and numerical values of the function \( G(u; t) \) the SWE examples from Sect. 5.7

Table 8 Computed time \( t_c \) to the third occurrence of the event \( G(u; t) = 1000 \), error in the QoI \( e_Q \), and effectivity ratio \( \rho_{\text{eff}} \), for the SWEs example in Sect. 5.7. The forward problem was solved on a coarse mesh with \( N_x = 80 \) and \( N_t = 40 \) using \( \text{cG}(2,2) \).

| \( N_x \) | \( N_t \) | \( t_c \) | \( e_Q \) | \( \rho_{\text{eff}} \) |
|---|---|---|---|---|
| 80 | 40 | 1449.015 | \(-9.530 \times 10^3\) | 0.879 |

The adjoint problem was solved on the same mesh using \( \text{cG}(4,4) \). The third event occurs at \( t_f = 1439.4849 \).

5.7 Caution on error estimates

While the error estimates are usually quite accurate, they may fail to capture the true error in certain situations. If the temporal or spatial meshes are too coarse, qualitative as well as quantitative features of the solution may be inaccurate, which can result in poor estimates. We provide an example in which the threshold value \( R \) is close to a local maxima. When the threshold value is close to a local maxima or minima, a temporal or spatial mesh that is too course may result in the numerical solution failing to achieve the threshold value, or to spuriously achieve this value. While such effects are highly problem dependent, the closer the threshold value \( R \) is to a local extremum, the greater the likelihood this problem will arise.

An example is provided by reconsidering the problem in Sect. 5.5, calculating the coarse solution using \( \text{cG}(2,2) \) on a mesh with \( N_x = 80 \) and \( N_t = 40 \). The reference solution was computed using the \( \text{cG}(3,3) \) method on a mesh with \( N_{\text{ref}} = 1280 \). The functional \( G(u; t) \) computed using the reference and coarse grid solutions are presented in Fig. 9a, b respectively. For a threshold value of \( R = 1800 \), the numerical approximation is qualitatively inaccurate since only the first two events are captured and the third through sixth events are lost. Clearly any attempt to estimate the error in the time to the third through the sixth events will fail. However, for a threshold value of \( R = 1000 \), the coarse numerical approximation captures all six events. As shown in Table 8, even on such a coarse mesh, the effectivity ratio when estimating the error in the time to the third event suffers only a modest degradation.

The error estimator works well for other problems, even on very coarse meshes, irrespective of the choice of threshold value \( R \). Consider the problem from Sect. 5.1...
The reference and numerical values of the functional $G(u; t)$ for the heat equation example from Sect. 5.7 for $R = 0.47$ and $R = 0.44$

![Fig. 10](image)

**Fig. 10** The reference and numerical values of the functional $G(u; t)$ for the heat equation example from Sect. 5.7 for $R = 0.47$ and $R = 0.44$

**Table 9** Computed time $t_c$ to the only occurrence of the event $G(u; t) = R$ for $R = 0.47$ and $R = 0.44$ for $t \in [0, 0.5]$, error in the QoI $\epsilon_Q$, and effectivity ratio $\rho_{\text{eff}}$, for the heat equation example in Sect. 5.7.

| $R$  | $N_x$ | $N_t$ | $t_c$   | $\epsilon_Q$       | $\rho_{\text{eff}}$ |
|------|-------|-------|---------|---------------------|---------------------|
| 0.47 | 50    | 5     | 0.346099| $2.067 \times 10^{-3}$ | 1.004               |
| 0.44 | 50    | 5     | 0.495497| $-5.630 \times 10^{-4}$| 1.043               |

The adjoint problem was solved on the same mesh using cG(2,2). The event occurs at $t_t = 0.34816598$ for $R = 0.47$ and $t_t = 0.49493410$ for $R = 0.44$

for which the functional $G(u; t)$ is monotonic on $t \in [0, 0.5]$. The exact functional, and the functional computed on a coarse mesh with $N_x = 50$ and $N_t = 5$ are presented in Fig. 10a, b respectively. As shown in Table 9, for threshold values of $R = 0.47$ and $R = 0.44$, the error estimate is accurate even for such a coarse mesh.

### 6 Conclusions

We have developed and implemented an accurate adjoint-based *a posteriori* error estimates for the time to an event, by which we mean the time for a functional of the solution to a time-dependent PDEs to achieve a threshold value. These estimates are based on the use of Taylor’s Theorem on the functional defining the QoI, and multiple applications of standard adjoint-based error analysis, to achieve a computable estimate. Implementations for the 1D heat equation and the linearized shallow water equation provide examples of both parabolic and hyperbolic PDEs. The error estimates provides a basis for developing refinement strategies to reduce the error in the time to the event. A more detailed analysis is required to partition the error into contributions arising from the independent spatial and temporal discretizations (see e.g., [9]) and to determine the overall effect on the error from terms arising in both the numerator and denominator of (30).
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Declarations

Conflict of interest The authors have no conflicts of interest.

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