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AN EASILY COMPUTABLE ERROR ESTIMATOR IN SPACE AND TIME FOR THE WAVE EQUATION

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Abstract. We propose a cheaper version of *a posteriori* error estimator from Gorynina *et al.* (*Numer. Anal.* (2017)) for the linear second-order wave equation discretized by the Newmark scheme in time and by the finite element method in space. The new estimator preserves all the properties of the previous one (reliability, optimality on smooth solutions and quasi-uniform meshes) but no longer requires an extra computation of the Laplacian of the discrete solution on each time step.

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1. Introduction

In this paper, we are interested in *a posteriori* time-space error estimates for finite element discretizations of the wave equation. Such lestimates were designed, for instance, in [9, 12] for the case of implicit Euler discretization in time, in [13] for the case of the second order discretization in time by Cosine (or, equivalently, Newmark) scheme, and in [15] for a particular variant of the Newmark scheme $\beta = 1/4$, $\gamma = 1/2$ (the advantage of the approach from [15] being its suitability for non constant time steps while the estimator from [13] is restricted to uniform meshes in time). In both [13, 15], the error is measured in a physically natural norm: H^1 in space, L^∞ in time. Another common feature of these two papers is that the time error estimators proposed there contain the Laplacian of the discrete solution which should be computed *via* an auxiliary finite element problem at each time step. This requires thus a non-negligible extra work in comparison with computing the discrete solution itself. In the present paper, we propose an alternative time error estimator for the particular Newmark scheme considered in [15] that avoids these additional computations.

Note that we have cited above only the articles on explicit residual based error bounds in space and time. The litterature on the error control of finite element methods for second order hyperbolic problems, although much less abundant than that for eliptic and parabolic problems, also contains different approaches. We can cite the goal-oriented error estimators by Bangerth *et al.* [6–8] where the error is measured with respect to some functional of the solution, and the work by Adjerid *et al.* [1–4] proposing asymptotically accurate error estimates at the expense of a workload which is generally bigger than that of explicit estimators. We also note

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that the work of Adjerid *et al.* is related to some space-time Galerkin discretizations, which are different from the time marching schemes considered in the present work as well as in other papers cited above.

In deriving our *a posteriori* estimates, we follow first the approach of [15]. First of all, we recognize that the Newmark method can be reinterpreted as the Crank–Nicolson discretization of the reformulation of the governing equation as the first-order system, as in [5]. We then use the techniques stemming from *a posteriori* error analysis for the Crank–Nicolson discretization of the heat equation in [17], based on a piecewise quadratic polynomial in time reconstruction of the numerical solution. Finally, in a departure from [15], we replace the second derivatives in space (Laplacian of the discrete solution) in the error estimate with the forth derivatives in time by reusing the governing equation. This leads to the new *a posteriori* error estimate in time and also allows us to easily recover the error estimates in space that turn out to be the same as those of [15]. The resulting estimate is referred to as the 5-point estimator since it contains the fourth order finite differences in time and thus involves the discrete solution at 5 points in time at each time step. On the other hand, the estimate [15] involves only 3 points in time at each time step and will be thus referred to as the 3-point estimator.

Like in the case of the 3-point estimator, we are able to prove that the new 5-point estimator is reliable on general regular meshes in space and non-uniform meshes in time (with constants depending on the regularity of meshes in both space and time). Moreover, the 5-point estimator is proved to be of optimal order at least on sufficiently smooth solutions, quasi-uniform meshes in space and uniform meshes in time, again reproducing the results known for the 3-point estimator. Numerical experiments demonstrate that 3-point and 5-point error estimators produce very similar results in the majority of test cases. Both turn out to be of optimal order in space and time, even in situations not accessible to the current theory (non quasi-uniform meshes, not constant time steps). It should be therefore possible to use the new estimator for mesh adaptation in space and time. In fact, the best strategy in practice may be to combine both estimators to take benefit from the strengths of each of them: the relative cheapness of the 5-point one, and the better numerical behavior of the 3-point estimator under abrupt changes of the mesh.

The outline of the paper is as follows. We present the governing equations and the discretization in Section 2. Since our work is based on techniques from [15], Section 3 recalls the *a posteriori* bounds in time and space from there. In Section 4, the 5-point *a posteriori* error estimator for the fully discrete wave problem is derived. Numerical experiments on several test cases are presented in Section 5.

2. The Newmark scheme for the wave equation

We consider initial-boundary-value problem for the wave equation. Let Ω be a bounded domain in $\mathbb{R}^2$ with boundary $\partial\Omega$ and $T > 0$ be a given final time. Let $u = u(x,t) : \Omega \times [0,T] \to \mathbb{R}$ be the solution to

$$\begin{cases} \dfrac{\partial^2 u}{\partial t^2} - \Delta u = f, & \text{in } \Omega \times \left]0,T\right], \\ u = 0, & \text{on } \partial\Omega \times \left]0,T\right], \\ u(\cdot,0) = u_0, & \text{in } \Omega, \\ \dfrac{\partial u}{\partial t}(\cdot,0) = v_0, & \text{in } \Omega, \end{cases} \tag{2.1}$$

where f, u_0, v_0 are given functions. Note that if we introduce the auxiliary unknown $v = \frac{\partial u}{\partial t}$ then model (2.1) can be rewritten as the following first-order in time system

$$\begin{cases} \dfrac{\partial u}{\partial t} - v = 0, & \text{in } \Omega \times \left]0,T\right], \\ \dfrac{\partial v}{\partial t} - \Delta u = f, & \text{in } \Omega \times \left]0,T\right], \\ u = v = 0, & \text{on } \partial\Omega \times \left]0,T\right], \\ u(\cdot,0) = u_0, \;\; v(\cdot,0) = v_0, & \text{in } \Omega. \end{cases} \tag{2.2}$$

The above problem (2.1) has the following weak formulation [11]: for given $f \in L^2(0,T;L^2(\Omega))$, $u_0 \in H_0^1(\Omega)$ and $v_0 \in L^2(\Omega)$ find a function

$$u \in L^2\left(0,T;H_0^1(\Omega)\right), \ \frac{\partial u}{\partial t} \in L^2\left(0,T;L^2(\Omega)\right), \ \frac{\partial^2 u}{\partial t^2} \in L^2\left(0,T;H^{-1}(\Omega)\right), \tag{2.3}$$

such that $u(x,0) = u_0$ in $H_0^1(\Omega)$, $\dfrac{\partial u}{\partial t}(x,0) = v_0$ in $L^2(\Omega)$ and

$$\left\langle \frac{\partial^2 u}{\partial t^2}, \varphi \right\rangle + (\nabla u, \nabla \varphi) = (f, \varphi), \ \forall \varphi \in H_0^1(\Omega), \tag{2.4}$$

where $\langle \cdot,\cdot \rangle$ denotes the duality pairing between $H^{-1}(\Omega)$ and $H_0^1(\Omega)$ and the parentheses $(\cdot,\cdot)$ stand for the inner product in $L^2(\Omega)$. Following Chapter 7, Section 2, Theorem 5 of [11], we observe that in fact

$$u \in C^0\left(0,T;H_0^1(\Omega)\right), \ \frac{\partial u}{\partial t} \in C^0\left(0,T;L^2(\Omega)\right), \ \frac{\partial^2 u}{\partial t^2} \in C^0\left(0,T;H^{-1}(\Omega)\right).$$

Higher regularity results with more regular data are also available in [11].

Let us now discretize (2.1) or, equivalently, (2.2) in space using the finite element method and in time using an appropriate marching scheme. We thus introduce a regular mesh $\mathcal{T}_h$ on Ω with triangles K, diam $K = h_K$, $h = \max_{K \in \mathcal{T}_h} h_K$, internal edges $E \in \mathcal{E}_h$, where $\mathcal{E}_h$ represents the internal edges of the mesh $\mathcal{T}_h$ and the standard finite element space $V_h \subset H_0^1(\Omega)$ of piecewise polynomials of degree $k \geq 1$:

$$V_h = \left\{ v_h \in C(\bar{\Omega}) : v_h|_K \in \mathbb{P}_k \ \forall K \in \mathcal{T}_h \text{ and } v_h|_{\partial\Omega} = 0 \right\}.$$

Let us also introduce a subdivision of the time interval $[0,T]$

$$0 = t_0 < t_1 < \cdots < t_N = T,$$

with non-uniform time steps $\tau_k = t_{n+1} - t_k$ for $n = 0, \ldots, N-1$ and $\tau = \max\limits_{0 \leq n \leq N-1} \tau_k$.

The Newmark scheme [18,19] with coefficients $\beta = 1/4, \gamma = 1/2$ as applied to the wave equation (2.1): given approximations $u_h^0, v_h^0 \in V_h$ of u_0, v_0 compute $u_h^1 \in V_h$ from

$$\left(\frac{u_h^1 - u_h^0}{\tau_0}, \varphi_h \right) + \left(\nabla \frac{\tau_0 (u_h^1 + u_h^0)}{4}, \nabla \varphi_h \right) = \left(v_h^0 + \frac{\tau_0}{4}(f^1 + f^0), \varphi_h \right), \quad \forall \varphi_h \in V_h, \tag{2.5}$$

and then compute $u_h^{n+1} \in V_h$ for $n = 1, \ldots, N-1$ from equation

$$\begin{aligned} \left(\frac{u_h^{n+1} - u_h^n}{\tau_k} - \frac{u_h^n - u_h^{n-1}}{\tau_{n-1}}, \varphi_h \right) &+ \left(\nabla \frac{\tau_k (u_h^{n+1} + u_h^n) + \tau_{n-1}(u_h^n + u_h^{n-1})}{4}, \nabla \varphi_h \right) \\ &= \left(\frac{\tau_k (f^{n+1} + f^n) + \tau_{n-1}(f^n + f^{n-1})}{4}, \varphi_h \right), \quad \forall \varphi_h \in V_h. \end{aligned} \tag{2.6}$$

where f^n is an abbreviation for $f(\cdot, t_k)$.

Following [5,15], we observe that this scheme is equivalent to the Crank–Nicolson discretization of the governing equation written in the form (2.2): taking $u_h^0, v_h^0 \in V_h$ as some approximations to u_0, v_0 compute $u_h^n, v_h^n \in V_h$ for $n = 0, \ldots, N-1$ from the system

$$\frac{u_h^{n+1} - u_h^n}{\tau_k} - \frac{v_h^n + v_h^{n+1}}{2} = 0, \tag{2.7}$$

$$\left(\frac{v_h^{n+1} - v_h^n}{\tau_k}, \varphi_h \right) + \left(\nabla \frac{u_h^{n+1} + u_h^n}{2}, \nabla \varphi_h \right) = \left(\frac{f^{n+1} + f^n}{2}, \varphi_h \right), \quad \forall \varphi_h \in V_h. \tag{2.8}$$

Note that the additional unknowns v_k^h are the approximations are not present in the Newmark scheme (2.5)–(2.6). If needed, they can be recovered on each time step by the following easy computation

$$v_h^{n+1} = 2\frac{u_h^{n+1} - u_h^n}{\tau_k} - v_h^n. \tag{2.9}$$

From now on, we shall use the following notations

$$\begin{aligned} u_h^{n+1/2} &:= \frac{u_h^{n+1} + u_h^n}{2}, \quad \partial_{n+1/2} u_h := \frac{u_h^{n+1} - u_h^n}{\tau_k}, \quad \partial_n u_h := \frac{u_h^{n+1} - u_h^{n-1}}{\tau_k + \tau_{n-1}}, \\ \partial_n^2 u_h &:= \frac{1}{\tau_{n-1/2}} \left(\frac{u_h^{n+1} - u_h^n}{\tau_k} - \frac{u_h^n - u_h^{n-1}}{\tau_{n-1}} \right) \text{ with } \tau_{n-1/2} := \frac{\tau_k + \tau_{n-1}}{2}. \end{aligned} \tag{2.10}$$

We apply this notations to all quantities indexed by a superscript, so that, for example, $f^{n+1/2} = (f^{n+1} + f^n)/2$. We also denote $u(x,t_k)$, $v(x,t_k)$ by u^n, v^n so that, for example, $u^{n+1/2} = \left(u^{n+1} + u^n\right)/2 = \left(u(x,t_{n+1}) + u(x,t_k)\right)/2$.

We shall measure the error in the following norm

$$u \mapsto \max_{t\in[0,T]} \left(\left\| \frac{\partial u}{\partial t}(t) \right\|_{L^2(\Omega)}^2 + |u(t)|_{H^1(\Omega)}^2 \right)^{1/2}. \tag{2.11}$$

Here and in what follows, we use the notations $u(t)$ and $\dfrac{\partial u}{\partial t}(t)$ as a shorthand for, respectively, $u(\cdot,t)$ and $\dfrac{\partial u}{\partial t}(\cdot,t)$. The norms and semi-norms in Sobolev spaces $H^k(\Omega)$ are denoted, respectively, by $\|\cdot\|_{H^k(\Omega)}$ and $|\cdot|_{H^k(\Omega)}$. We call (2.11) the energy norm referring to the underlying physics of the studied phenomenon. Indeed, the first term in (2.11) may be assimilated to the kinetic energy and the second one to the potential energy.

3. The 3-point time error estimator

The aim of this section is to recall *a posteriori* bounds in time and space from [15] for the error measured in the norm (2.11). Their derivation is based on the following piecewise quadratic (in time) 3-point reconstruction of the discrete solution.

Definition 3.1. Let u_h^n be the discrete solution given by the scheme (2.6). Then, the piecewise quadratic reconstruction $\tilde{u}_{h\tau}(t) : [0,T] \to V_h$ is constructed as the continuous in time function that is equal on $[t_k, t_{n+1}]$, $n \geq 1$, to the quadratic polynomial in t that coincides with u_h^{n+1} (respectively u_h^n, u_h^{n-1}) at time t_{n+1} (respectively t_k, t_{n-1}). Moreover, $\tilde{u}_{h\tau}(t)$ is defined on $[t_0, t_1]$ as the quadratic polynomial in t that coincides with u_h^2 (respectively u_h^1, u_h^0) at time t_2 (respectively t_1, t_0). Similarly, we introduce piecewise quadratic reconstruction $\tilde{v}_{h\tau}(t) : [0,T] \to V_h$ based on v_h^n defined by (2.9) and $\tilde{f}_\tau(t) : [0,T] \to L^2(\Omega)$ based on $f(t_k,\cdot)$.

The quadratic reconstructions $\tilde{u}_{h\tau}$, $\tilde{v}_{h\tau}$ are thus based on three points in time (normally looking backwards in time, with the exemption of the initial time slab $[t_0,t_1]$). This is also the case for the time error estimator (3.3), recalled in the following Theorem and therefore referred to as the 3-point estimator.

Theorem 3.2. *The following a posteriori error estimate holds between the solution u of the wave equation (2.1) and the discrete solution u_h^n given by (2.5) and (2.6) for all t_k, $0 \leq n \leq N$ with v_h^n given by (2.9):*

$$\begin{aligned} \left(\left\| v_h^n - \frac{\partial u}{\partial t}(t_n) \right\|_{L^2(\Omega)}^2 + |u_h^n - u(t_n)|_{H^1(\Omega)}^2 \right)^{1/2} &\leq \left(\|v_h^0 - v_0\|_{L^2(\Omega)}^2 + |u_h^0 - u_0|_{H^1(\Omega)}^2 \right)^{1/2} \\ &\quad + \eta_S(t_n) + \sum_{k=0}^{n-1} \tau_k \eta_T(t_k) + \int_0^{t_n} \|f - \tilde{f}_\tau\|_{L^2(\Omega)} \mathrm{d}t, \end{aligned} \tag{3.1}$$

where the space indicator is defined by

$$\eta_S(t_n) = C_1 \max_{0\leqslant t\leqslant t_n} \left[\sum_{K\in\mathcal{T}_h} h_K^2 \left\| \frac{\partial \tilde{v}_{h\tau}}{\partial t} - \Delta \tilde{u}_{h\tau} - f \right\|^2_{L^2(K)} + \sum_{E\in\mathcal{E}_h} h_E \left|[n\cdot\nabla \tilde{u}_{h\tau}]\right|^2_{L^2(E)} \right]^{1/2} \tag{3.2}$$
$$+ C_2 \sum_{m=0}^{n-1} \int_{t_m}^{t_{m+1}} \left[\sum_{K\in\mathcal{T}_h} h_K^2 \left\| \frac{\partial^2 \tilde{v}_{h\tau}}{\partial t^2} - \Delta\frac{\partial \tilde{u}_{h\tau}}{\partial t} - \frac{\partial f}{\partial t} \right\|^2_{L^2(K)} + \sum_{E\in\mathcal{E}_h} h_E \left\| \left[n\cdot\nabla \frac{\partial \tilde{u}_{h\tau}}{\partial t} \right] \right\|^2_{L^2(E)} \right]^{1/2} \mathrm{d}t,$$

here $C_1,\ C_2$ are constants depending only on the mesh regularity, $[\cdot]$ stands for a jump on an edge $E\in\mathcal{E}_h$, and $\tilde{u}_{h\tau},\ \tilde{v}_{h\tau}$ are given by Definition 3.1.

The error indicator in time for $k=1,\dots,N-1$ is

$$\eta_T(t_k) = \left(\frac{1}{12}\tau_k^2 + \frac{1}{8}\tau_{k-1}\tau_k\right)\left(\left|\partial_k^2 v_h\right|^2_{H^1(\Omega)} + \left\|\partial_k^2 f_h - z_h^k\right\|^2_{L^2(\Omega)}\right)^{1/2}, \tag{3.3}$$

where z_h^k is such that

$$\left(z_h^k, \varphi_h\right) = (\nabla\partial_k^2 u_h, \nabla\varphi_h), \quad \forall\varphi_h\in V_h, \tag{3.4}$$

and

$$\eta_T(t_0) = \left(\frac{5}{12}\tau_0^2 + \frac{1}{2}\tau_1\tau_0\right)\left(\left|\partial_1^2 v_h\right|^2_{H^1(\Omega)} + \left\|\partial_1^2 f_h - z_h^1\right\|^2_{L^2(\Omega)}\right)^{1/2}. \tag{3.5}$$

We also recall an optimality result for the 3-point time error estimator. We introduce to this end the H_0^1-orthogonal projection $\Pi_h : H_0^1(\Omega)\to V_h$ so that

$$(\nabla\Pi_h v, \nabla\varphi_h) = (\nabla v, \nabla\varphi_h)\,, \quad \forall v\in H_0^1(\Omega), \quad \forall\varphi_h\in V_h, \tag{3.6}$$

Theorem 3.3. *Let u be the solution of wave equation (2.1) and $\dfrac{\partial^3 u}{\partial t^3}(0)\in H^1(\Omega)$, $\dfrac{\partial^2 u}{\partial t^2}(0)\in H^2(\Omega)$, $\dfrac{\partial^2 f}{\partial t^2}(t)\in L^\infty(0,T;L^2(\Omega))$, $\dfrac{\partial^3 f}{\partial t^3}(t)\in L^2(0,T;L^2(\Omega))$. Suppose that mesh $\mathcal{T}_h$ is quasi-uniform, the mesh in time is uniform ($t_k = k\tau$), and the initial approximations are chosen as*

$$u_h^0 = \Pi_h u_0, \quad v_h^0 = \Pi_h v_0. \tag{3.7}$$

Then, the 3-point time error estimator $\eta_T(t_k)$ defined by (3.3, 3.5) is of order τ^2, i.e.

$$\eta_T(t_k) \leq C\tau^2.$$

with a positive constant C depending only on u, f, and the regularity of mesh $\mathcal{T}_h$.

Remark 3.4. Note that the particular choice for the approximation of initial conditions in (3.7) using the H_0^1-orthogonal projection (3.6) is crucial to obtain the optimal order of the 3-point time error estimator, as confirmed both theoretically and numerically in [15].

4. The 5-point *a posteriori* error estimator

As already mentioned in the Introduction, the time error estimator (3.3) contains a finite element approximation to the Laplacian of u_h^k, *i.e.* z_h^k given by (3.4). This is unfortunate because z_h^k should be computed by solving an additional finite element problem that implies additional computational effort. Having in mind that the term $\partial_n^2 f_h - z_h^n$ in (3.3) is a discretization of $\partial^2 f/\partial t^2 + \Delta u = \partial^4 u/\partial t^4$ at time t_n our goal now is to avoid the second derivatives in space in the error estimates and replace them with the forth derivatives in time.

We introduce a "fourth order finite difference in time" ∂_n^4 defined by

$$\partial_n^4 w_h = \frac{8}{\tau_n + \tau_{n-1} + \tau_{n-2} + \tau_{n-3}} \left(\frac{\partial_n^2 w_h - \partial_{n-1}^2 w_h}{\tau_n + \tau_{n-2}} - \frac{\partial_{n-1}^2 w_h - \partial_{n-2}^2 w_h}{\tau_{n-1} + \tau_{n-3}} \right) \tag{4.1}$$

on any sequence $\{w_h^n\}_{n=0,1,\ldots} \in V_h$. This can be rewritten as a composition of two second order finite difference operators

$$\partial_n^4 w_h = \hat{\partial}_n^2 \partial^2 w_h, \tag{4.2}$$

where $\partial^2 w_h$ is the standard finite difference (2.10) applied to w_h, and $\hat{\partial}_n^2$ is a modified second order finite difference defined by

$$\begin{aligned} \hat{\partial}_n^2 \omega_h &= \frac{2}{(\hat{t}_n - \hat{t}_{n-2})} \left(\frac{\omega_h^n - \omega_h^{n-1}}{\hat{t}_n - \hat{t}_{n-1}} - \frac{\omega_h^{n-1} - \omega_h^{n-2}}{\hat{t}_{n-1} - \hat{t}_{n-2}} \right), \\ \hat{t}_n &= \frac{t_{n+1} + t_{n-1}}{2} \end{aligned} \tag{4.3}$$

on any sequence $\{\omega_h^n\}_{n=0,1,\ldots} \in V_h$. Note that a lower subscript "n" is lacking from $\partial^2 w_h$ in (4.2) consistent with the fact that $\hat{\partial}_n^2$ is applied there to the sequence $\{\partial_n^2 w_h\}_{n=0,1,\ldots}$ rather than to a single instance of $\partial_n^2 w_h$. In full detail, (4.2) should be interpreted as $\partial_n^4 w_h = \hat{\partial}_n^2 \omega_h$ with $\omega_h^n = \partial_n^2 w_h$.

Remark 4.1. In the case of constant time steps $\tau_n = \tau$, (4.1) is reduced to

$$\partial_n^4 w_h = \frac{w_h^{n+1} - 4w_h^n + 6w_h^{n-1} - 4w_h^{n-2} + w_h^{n-3}}{\tau^4}.$$

It is thus indeed a standard finite difference approximation to the fourth derivative. In particular, it is exact on polynomials (in time) of degree up to 4. However, a standard fourth order finite difference in the general case of non constant time steps would be given by the divided differences

$$\begin{aligned} \tilde{\partial}_n^4 w_h &= 4![w_h^{n-3}, \ldots, w_h^{n+1}] \\ &= \frac{12}{\tau_n + \tau_{n-1} + \tau_{n-2} + \tau_{n-3}} \left(\frac{\partial_n^2 w_h - \partial_{n-1}^2 w_h}{\tau_n + \tau_{n-1} + \tau_{n-2}} - \frac{\partial_{n-1}^2 w_h - \partial_{n-2}^2 w_h}{\tau_{n-1} + \tau_{n-2} + \tau_{n-3}} \right). \end{aligned}$$

Clearly, the formulas for $\partial_n^4 w_h$ and $\tilde{\partial}_n^4 w_h$, although similar, do not coincide in general, and consequently $\partial_n^4 w_h$ is not necessarily consistent with the fourth derivative in time of w_h. Definition (4.1) may seem thus artificial and counter-intuitive. We shall see however that it arises naturally in the analysis of Newmark scheme, *cf.* forthcoming Lemma 4.2. Indeed, in order to "differentiate" in time the averaged quantities $\bar{w}_h^n$ defined by (4.4) and present in the scheme (2.6), *cf.* also (4.13), one needs to employ the modified second order finite difference $\hat{\partial}_n^2$, which shall be composed further with ∂_n^2 to give rise to ∂_n^4.

For any sequence $\{w_h^n\}_{n=0,1,\ldots} \in V_h$, we denote

$$\bar{w}_h^n = \frac{\tau_n(w_h^{n+1} + w_h^n) + \tau_{n-1}(w_h^n + w_h^{n-1})}{4\tau_{n-1/2}}. \tag{4.4}$$

Consistently with the conventions above, $\bar{w}_h$ will stand for the collection of any sequence $\{\bar{w}_h^n\}_{n=0,1,\ldots}$. The following technical lemma establishes a connection between second order discrete derivatives $\hat{\partial}_n^2$ and ∂_n^2.

Lemma 4.2. *For all integer $n = 3, \dots N-1$ there exist coefficients α_k, $k = n-2, n-1, n$ such that for all $\{w_h^n\}_{n=0,1,\dots}$*

$$\hat{\partial}_n^2 \bar{w}_h = \sum_{k=n-2}^{n} \alpha_k \partial_k^2 w_h, \tag{4.5}$$

Moreover

$$|\alpha_k| \le c, \text{ for } k = n-2, n-1, n, \text{ and } \sum_{k=n-2}^{n} \alpha_k \ge C,$$

where c and C are positive constants depending only on the mesh regularity in time, i.e. on $\max_{k\ge 0}\left(\frac{\tau_{k+1}}{\tau_k} + \frac{\tau_k}{\tau_{k+1}}\right)$.

Proof. We first note that relation (4.5) does not contain any derivatives in space and thus it should hold at any point $x \in \Omega$. Consequently, it is sufficient to prove this Lemma assuming that w_h^n, $\partial_k^2 w_h$, etc. are real numbers, *i.e.* replacing V_h by $\mathbb{R}$. This is the assumption adopted in this proof. We shall thus drop the sub-indexes h everywhere. Furthermore, it will be convenient to reinterpret w^n in (4.2), (4.3) and (4.4) as the values of a real valued function $w(t)$ at $t = t_n$. We shall also use the notations like $\bar{w}^n$, $\partial_n^2 w$, and so on, where w is a continuous function on $\mathbb{R}$, always assuming $w^n = w(t_n)$.

Observe that $\hat{\partial}_n^2 \bar{w}$ is a linear combination of 5 numbers $\{w^{n-3}, \dots, w^{n+1}\}$. Thus, it is enough to check equality (4.5) on any 5 continuous functions $\phi_{(k)}(t)$, $k = n-3, \dots, n+1$, such that the vector of values of $\phi_{(k)}$ at times t_l, $l = n-3, \dots, n+1$, form a basis of $\mathbb{R}^5$. For fixed n, let us choose these functions as

$$\phi_{(k)}(t) = \begin{cases} \dfrac{t - t_{k-1}}{\tau_{k-1}}, & \text{if } t < t_k, \\ \dfrac{t_{k+1} - t}{\tau_k}, & \text{if } t \ge t_k, \end{cases} \qquad k = n-3, \dots, n+1. \tag{4.6}$$

First we notice that for every linear function $u(t)$ on $[t_{n-3}, t_{n+1}]$ we have $\hat{\partial}_n^2 \bar{u} = \partial_n^2 u = 0$. Thus, we get immediately $\hat{\partial}_n^2 \bar{\phi}_{(n-3)} = \partial_n^2 \phi_{(n-3)} = 0$ and $\hat{\partial}_k^2 \bar{\phi}_{(n+1)} = \partial_k^2 \phi_{(n+1)} = 0$ so that (4.5) is fulfilled on functions $\phi_{(n-3)}$, $\phi_{(n+1)}$ with any coefficients α_k, $k = n-2, n-1, n$. Now we want to provide coefficients α_k, $k = n-2, n-1, n$ for which (4.5) is fulfilled on functions $\phi_{(n-2)}$, $\phi_{(n-1)}$ and $\phi_{(n)}$. For brevity, we demonstrate the idea only for function $\phi_{(n)}(t)$. Function $\phi_{(n)}(t)$ is linear on $[t_{n-3}, t_n]$ and thus

$$\partial_{n-2}^2 \phi_{(n)} = 0, \ \partial_{n-1}^2 \phi_{(n)} = 0.$$

From direct computations it is easy to show that

$$\partial_n^2 \phi_{(n)} \sim \frac{1}{\tau_k^2}, \ \bar{\phi}_{(n)} \sim 1, \ \hat{\partial}_k^2 \bar{\phi}_{(n)} \sim \frac{1}{\tau_k^2},$$

where $\sim$ hides some factors that can be bounded by constants depending only on the mesh regularity. Thus we are able to establish expression for coefficient $\alpha_n = \dfrac{\hat{\partial}_k^2 \bar{\phi}_{(n)}}{\partial_n^2 \phi_{(n)}} \le C$. Similar reasoning for function $\phi_{(n-1)}$ and $\phi_{(n-2)}$ shows that $\alpha_{n-1} = \dfrac{\hat{\partial}_n^2 \bar{\phi}_{(n-1)}}{\partial_{n-1}^2 \phi_{(n-1)}} \le C$ and $\alpha_{n-2} = \dfrac{\hat{\partial}_n^2 \bar{\phi}_{(n-2)}}{\partial_{n-2}^2 \phi_{(n-2)}} \le C$.

The next step is to show boundedness from below of $\displaystyle\sum_{k=n-2}^{n} \alpha_k$. We will show it by applying equality (4.5) to second order polynomial function $s(t) = \dfrac{t^2}{2}$. Using a Taylor expansion of $s(t)$ around $\hat{t}_n$ in the definition of $\bar{s}^n$

gives

$$\bar{s}^n = \frac{\tau_n(\hat{t}_n^2 + \hat{t}_n\tau_{n-1} + \frac{1}{4}(\tau_n^2 + \tau_{n-1}^2)) + \tau_{n-1}(\hat{t}_n^2 - \hat{t}_n\tau_n + \frac{1}{4}(\tau_n^2 + \tau_{n-1}^2))}{2(\tau_n + \tau_{n-1})}$$
$$= \frac{\hat{t}_n^2}{2} + \frac{1}{8}\left(\tau_n^2 + \tau_{n-1}^2\right).$$

Substituting this into the definition of $\hat{\partial}_n^2 \bar{s}$ we obtain

$$\hat{\partial}_n^2 \bar{s} = \frac{\dfrac{\bar{s}^n - \bar{s}^{n-1}}{\hat{t}_n - \hat{t}_{n-1}} - \dfrac{\bar{s}^{n-1} - \bar{s}^{n-2}}{\hat{t}_{n-1} - \hat{t}_{n-2}}}{\left(\hat{t}_n - \hat{t}_{n-2}\right)/2} = 1 + \frac{1}{8}\left(\frac{2\dfrac{\tau_n^2 - \tau_{n-2}^2}{\tau_n + \tau_{n-2}} - 2\dfrac{\tau_{n-1}^2 - \tau_{n-3}^2}{\tau_{n-1} + \tau_{n-3}}}{\frac{1}{4}(\tau_n + \tau_{n-1} + \tau_{n-2} + \tau_{n-3})}\right)$$
$$= 1 + \frac{\tau_n - \tau_{n-1} - \tau_{n-2} + \tau_{n-3}}{\tau_n + \tau_{n-1} + \tau_{n-2} + \tau_{n-3}}.$$

Using (4.5) and the fact that $\partial_n^2 s = 1$ for $k = n-2, n-1, n$ we note that

$$1 + \frac{\tau_n - \tau_{n-1} - \tau_{n-2} + \tau_{n-3}}{\tau_n + \tau_{n-1} + \tau_{n-2} + \tau_{n-3}} = \sum_{k=n-2}^{n} \alpha_k.$$

This implies $\displaystyle\sum_{k=n-2}^{n} \alpha_k \geq C.$ □

Lemma 4.3. *Let $w_h^n, s_h^n \in V_h$ be such that*

$$\frac{w_h^{n+1} - w_h^n}{\tau_k} - \frac{s_h^n + s_h^{n+1}}{2} = 0, \ \forall n \geq 0. \tag{4.7}$$

For all $n \geq 3$ there exist coefficients β_k, $k = n-2, n-1, n$ such that

$$\sum_{k=n-2}^{n} \alpha_k \partial_n^2 w_h = \left(\sum_{k=n-2}^{n} \alpha_k\right) \partial_k^2 w_h - \tau_k \sum_{k=n-2}^{n} \beta_k \partial_k^2 s_h, \tag{4.8}$$

where coefficients α_k, $k = n-2, n-1, n$ are introduced in Lemma 4.2. Moreover

$$|\beta_k| \leq C, \ k = n-2, n-1, n,$$

where C is a positive constant depending only on the mesh regularity in time, i.e. on $\max_{k\geq 0}\left(\frac{\tau_{k+1}}{\tau_k} + \frac{\tau_k}{\tau_{k+1}}\right)$.

Proof. As in proof of Lemma 4.2, we assume $V_h = \mathbb{R}$, drop the sub-indexes h and interpret w^n, s^n as the values of continuous real valued functions $w(t)$, $s(t)$ at $t = t_n$. Using (4.7) and notations (2.10) implies $\partial_k^2 w = \partial_k s$. Now, we are able to rewrite (4.8) in terms of s^n only

$$\sum_{k=n-2}^{n} \alpha_k \partial_k s = \left(\sum_{k=n-2}^{n} \alpha_k\right) \partial_n s - \tau_k \sum_{k=n-2}^{n} \beta_k \partial_k^2 s, \tag{4.9}$$

As in the proof of Lemma 4.2 we take into account the fact that equation (4.9) should hold for every 5 numbers $\{s^{n-3}, \ldots, s^{n+1}\}$ and therefore it's enough to check equality (4.9) on 5 linearly independent piecewise linear functions $\phi_{(k)}$ introduced by (4.6). Using the reasoning as in Lemma 4.2 leads to desired result (4.8). □

We can now prove an *a posteriori* error estimate involving $\partial_n^4 u_h$. Since the latter is computed through 5 points in time $\{t_{n-3}, \dots, t_{n+1}\}$, we shall refer to this approach as the 5-point estimator. For the same reason, this estimator is only applicable from time t_4. The error at first 3 time steps should be thus measured differently, for example using the 3-point estimator from Theorem 3.2.

Theorem 4.4. *The following a posteriori error estimate holds between the solution u of the wave equation (2.1) and the discrete solution u_h^n given by (2.5)–(2.6) for all t_n, $4 \le n \le N$ with v_h^n given by (2.9):*

$$\left(\left\| v_h^n - \frac{\partial u}{\partial t}(t_n) \right\|_{L^2(\Omega)}^2 + |u_h^n - u(t_n)|_{H^1(\Omega)}^2 \right)^{1/2} \le \left(\left\| v_h^3 - \frac{\partial u}{\partial t}(t_3) \right\|_{L^2(\Omega)}^2 + \left| u_h^3 - u(t_3) \right|_{H^1(\Omega)}^2 \right)^{1/2}$$
$$+ \eta_S(t_n) + C \sum_{k=3}^{n-1} \tau_k \hat{\eta}_T(t_k) + C \sum_{k=1}^{n-1} \tau_k \hat{\eta}_T^{\text{h.o.t}}(t_k)$$
$$+ \int_{t_3}^{t_n} \|f - \tilde{f}_\tau\|_{L^2(\Omega)} \mathrm{d}t, \tag{4.10}$$

where the space error indicator is defined by (3.2) and the time error indicator is

$$\hat{\eta}_T(t_k) = \left(\frac{1}{12}\tau_k^2 + \frac{1}{8}\tau_{k-1}\tau_k \right) \left(\left| \partial_k^2 v_h \right|_{H^1(\Omega)} + \left\| \partial_k^4 u_h \right\|_{L^2(\Omega)} \right) \tag{4.11}$$

with additional higher order terms

$$\hat{\eta}_T^{\text{h.o.t}}(t_k) = \tau_k^3 \left\| \partial_k^2 \dot{f}_h - A_h \partial_k^2 v_h \right\|_{L^2(\Omega)}$$

where $\dot{f}_h^n$ satisfy

$$\frac{f_h^{n+1} - f_h^n}{\tau_n} = \frac{\dot{f}_h^n + \dot{f}_h^{n+1}}{2}.$$

The constant $C > 0$ depends only on the mesh regularity in time, i.e. on $\max_{k \ge 0} \left(\frac{\tau_{k+1}}{\tau_k} + \frac{\tau_k}{\tau_{k+1}} \right)$.

Proof. We note first of all that it is sufficient to prove the Theorem for the final time, *i.e.* $n = N$ because the statement for the general case $n < N$ will follow by resetting the final time N to n. Introducing the L^2-orthogonal projection $P_h : H_0^1(\Omega) \to V_h$ and operator $A_h : V_h \to V_h$ such that

$$(A_h w_h, \varphi_h) = (\nabla w_h, \nabla \varphi_h), \quad \forall \varphi_h \in V_h, \tag{4.12}$$

we can rewrite scheme (2.6) as

$$\partial_n^2 u_h + A_h \bar{u}_h^n = \bar{f}_h^n, \tag{4.13}$$

for $n = 0, \dots, N-1$ where $\bar{f}_h^n$ is defined through averaging (4.4) from $f_h^n = P_h f(t_n, \cdot)$. Taking a linear combination of instances of (4.13) at steps $n, n-1, n-2$ with appropriate coefficients gives

$$\partial_n^4 u_h + A_h \hat{\partial}_n^2 \bar{u}_h = \hat{\partial}_n^2 \bar{f}_h. \tag{4.14}$$

Using the definition of operator $\hat{\partial}_n^2$ and re-introducing v_h^n by (2.7) leads to

$$\hat{\partial}_n^2 \bar{u}_h = \sum_{k=n-2}^{n} \alpha_k \partial_k^2 u_h = \left(\sum_{k=n-2}^{n} \alpha_k \right) \partial_k^2 u_h - \tau_n \sum_{k=n-2}^{n} \beta_k \partial_k^2 v_h,$$

with coefficients α_k, β_k introduced in Lemmas 4.2 and 4.3. Moreover, by Lemma 4.2 $\gamma = \left(\sum_{k=n-2}^{n} \alpha_k\right)^{-1}$ is positive and bounded so that

$$\partial_n^2 u_h = \gamma \hat{\partial}_n^2 \bar{u}_h + \tau_n \sum_{k=n-2}^{n} \gamma_k \partial_k^2 v_h,$$

with $\gamma_k = \gamma\beta_k$ that are all uniformly bounded on regular meshes in time. Similarly,

$$\partial_n^2 f_h = \hat{\partial}_n^2 \bar{f}_h + \tau_n \sum_{k=n-2}^{n} \gamma_k \partial_k^2 \dot{f}_h.$$

Thus,

$$\begin{aligned}\partial_n^2 f_h - A_h \partial_n^2 u_h &= \hat{\partial}_n^2 \bar{f}_h - A_h \hat{\partial}_n^2 \bar{u}_h + \tau_n \sum_{k=n-2}^{n} \gamma_k \left(\partial_k^2 \dot{f}_h - A_h \partial_k^2 v_h\right)\\ &= \partial_n^4 u_h + \tau_n \sum_{k=n-2}^{n} \gamma_k \left(\partial_k^2 \dot{f}_h - A_h \partial_k^2 v_h\right).\end{aligned}$$

The rest of the proof follows closely that of Theorem 3.2, *cf.* [15]. We adopt the vector notation $U(t,x) = \begin{pmatrix} u(t,x) \\ v(t,x) \end{pmatrix}$ where $v = \partial u/\partial t$. Note that the first equation in (2.2) implies that

$$\left(\nabla \frac{\partial u}{\partial t}, \nabla\varphi\right) - (\nabla v, \nabla\varphi) = 0, \quad \forall \varphi \in H_0^1(\Omega),$$

by taking its gradient, multiplying it by $\nabla\varphi$ and integrating over Ω. Thus, system (2.2) can be rewritten in the vector notations as

$$b\left(\frac{\partial U}{\partial t}, \Phi\right) + (\mathcal{A}\nabla U, \nabla\Phi) = b(F, \Phi), \quad \forall \Phi \in (H_0^1(\Omega))^2, \tag{4.15}$$

where $\mathcal{A} = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$, $F = \begin{pmatrix} 0 \\ f \end{pmatrix}$ and

$$b(U, \Phi) = b\left(\begin{pmatrix} u \\ v \end{pmatrix}, \begin{pmatrix} \varphi \\ \psi \end{pmatrix}\right) := (\nabla u, \nabla\varphi) + (v, \psi).$$

Similarly, Newmark scheme (2.7) and (2.8) can be rewritten as

$$b\left(\frac{U_h^{n+1} - U_h^n}{\tau_n}, \Phi_h\right) + \left(\mathcal{A}\nabla \frac{U_h^{n+1} + U_h^n}{2}, \nabla\Phi_h\right) = b\left(F^{n+1/2}, \Phi_h\right), \quad \forall \Phi_h \in V_h^2, \tag{4.16}$$

where $U_h^n = \begin{pmatrix} u_h^n \\ v_h^n \end{pmatrix}$ and $F^{n+1/2} = \begin{pmatrix} 0 \\ f^{n+1/2} \end{pmatrix}$.

The *a posteriori* analysis relies on an appropriate residual equation for the quadratic reconstruction $\tilde{U}_{h\tau} = \begin{pmatrix} \tilde{u}_{h\tau} \\ \tilde{v}_{h\tau} \end{pmatrix}$. We have thus for $t \in [t_n, t_{n+1}]$, $n = 1, \ldots, N-1$

$$\tilde{U}_{h\tau}(t) = U_h^{n+1} + (t - t_{n+1})\partial_{n+1/2} U_h + \frac{1}{2}(t - t_{n+1})(t - t_n)\partial_n^2 U_h, \tag{4.17}$$

so that, after some simplifications,

$$b\left(\frac{\partial \tilde{U}_{h\tau}}{\partial t}, \Phi_h\right) + (\mathcal{A}\nabla \tilde{U}_{h\tau}, \nabla\Phi_h) = b\left((t-t_{n+1/2})\partial_n^2 U_h + F^{n+1/2}, \Phi_h\right)$$
$$+\left((t-t_{n+1/2})\mathcal{A}\nabla\partial_{n+1/2}U_h + \frac{1}{2}(t-t_{n+1})(t-t_n)\mathcal{A}\nabla\partial_n^2 U_h, \nabla\Phi_h\right). \tag{4.18}$$

Consider now (4.16) at time steps n and $n-1$. Subtracting one from another and dividing by $\tau_{n-1/2}$ yields

$$b\left(\partial_n^2 U_h, \Phi_h\right) + (\mathcal{A}\nabla\partial_n U_h, \nabla\Phi_h) = b\left(\partial_n F, \Phi_h\right),$$

or

$$b\left(\partial_n^2 U_h, \Phi_h\right) + \left(\mathcal{A}\nabla\left(\partial_{n+1/2}U_h - \frac{\tau_{n-1}}{2}\partial_n^2 U_h\right), \nabla\Phi_h\right) = b\left(\partial_n F, \Phi_h\right),$$

so that (4.18) simplifies to

$$b\left(\frac{\partial \tilde{U}_{h\tau}}{\partial t}, \Phi_h\right) + \left(\mathcal{A}\nabla \tilde{U}_{h\tau}, \Phi_h\right) = \left(p_n\mathcal{A}\nabla\partial_n^2 U_h, \nabla\Phi_h\right) + b\left(\left(t-t_{n+1/2}\right)\partial_n F + F^{n+1/2}, \Phi_h\right)$$
$$= \left(p_n\mathcal{A}\nabla\partial_n^2 U_h, \nabla\Phi_h\right) + b\left(\tilde{F}_\tau - p_n\partial_n^2 F, \Phi_h\right), \tag{4.19}$$

where

$$p_n = \frac{\tau_{n-1}}{2}(t-t_{n+1/2}) + \frac{1}{2}(t-t_{n+1})(t-t_n),$$
$$\tilde{F}_\tau(t) = F_h^{n+1} + (t-t_{n+1})\partial_{n+1/2}F + \frac{1}{2}(t-t_{n+1})(t-t_n)\partial_n^2 F.$$

Introduce the error between reconstruction $\tilde{U}_{h\tau}$ and solution U to problem (4.15):

$$E = \tilde{U}_{h\tau} - U, \tag{4.20}$$

or, component-wise

$$E = \begin{pmatrix} E_u \\ E_v \end{pmatrix} = \begin{pmatrix} \tilde{u}_{h\tau} - u \\ \tilde{v}_{h\tau} - v \end{pmatrix}.$$

Taking the difference between (4.19) and (4.15) we obtain the residual differential equation for the error valid for $t \in [t_n, t_{n+1}]$, $n = 1, \dots, N-1$

$$b(\partial_t E, \Phi) + (\mathcal{A}\nabla E, \nabla\Phi) = b\left(\frac{\partial \tilde{U}_{\tau h}}{\partial t} - F, \Phi - \Phi_h\right) + \left(\mathcal{A}\nabla\tilde{U}_{\tau h}, \nabla(\Phi - \Phi_h)\right)$$
$$+\left(p_n\mathcal{A}\nabla\partial_n^2 U_h, \nabla\Phi_h\right) + b\left(\tilde{F}_\tau - F - p_n\partial_n^2 F, \Phi_h\right), \quad \forall \Phi_h \in V_h^2. \tag{4.21}$$

Now we take $\Phi = E$, $\Phi_h = \begin{pmatrix} \mathit{\Pi}_h E_u \\ \tilde{I}_h E_v \end{pmatrix}$ where $\mathit{\Pi}_h : H_0^1(\Omega) \to V_h$ is the H_0^1-orthogonal projection operator (3.6) and $\tilde{I}_h : H_0^1(\Omega) \to V_h$ is a Clément-type interpolation operator which is also a projection [10, 20]. Noting that $(\mathcal{A}\nabla E, \nabla E) = 0$ and

$$\left(\nabla\frac{\partial \tilde{u}_{h\tau}}{\partial t}, \nabla(E_u - \mathit{\Pi}_h E_u)\right) = \left(\nabla\tilde{v}_{h\tau}, \nabla\left(E_u - \mathit{\Pi}_h E_u\right)\right) = 0.$$

we get

$$\left(\frac{\partial E_v}{\partial t}, E_v\right) + \left(\nabla E_u, \nabla \frac{\partial E_u}{\partial t}\right) = \left(\frac{\partial \tilde{v}_{\tau h}}{\partial t} - f, E_v - \Pi_h E_v\right) + \left(\nabla \tilde{u}_{\tau h}, \nabla\left(E_v - \tilde{I}_h E_v\right)\right)$$
$$+ \left(p_n\left(A_h \partial_n^2 u_h - \partial_n^2 f_h\right), \tilde{I}_h E_v\right) - \left(p_n \nabla \partial_n^2 v_h, \nabla E_u\right) + \left(\tilde{f}_\tau - f, \tilde{I}_h E_v\right).$$

Integrating (4.21) in time from t_3 to some $t^* \geq t_3$ yields

$$\begin{aligned}\frac{1}{2}\left(|E_u|^2_{H^1(\Omega)} + \|E_v\|^2_{L^2(\Omega)}\right)(t^*) &= \frac{1}{2}\left(|E_u|^2_{H^1(\Omega)} + \|E_v\|^2_{L^2(\Omega)}\right)(t_3)\\ &+ \underbrace{\int_{t_3}^{t^*}\left(\frac{\partial \tilde{v}_{\tau h}}{\partial t} - f, E_v - \tilde{I}_h E_v\right)\mathrm{d}t}_{I} + \underbrace{\int_{t_3}^{t^*}\left(\nabla \tilde{u}_{\tau h}, \nabla(E_v - \tilde{I}_h E_v)\right)\mathrm{d}t}_{II}\\ &+ \underbrace{\int_{t_3}^{t^*}\left[\left(p_n\left(A_h \partial_n^2 u_h - \partial_n^2 f_h\right), \tilde{I}_h E_v\right) - \left(p_n \nabla \partial_n^2 v_h, \nabla E_u\right) + \left(\tilde{f}_\tau - f, \tilde{I}_h E_v\right)\right]\mathrm{d}t}_{III}.\end{aligned} \tag{4.22}$$

Let

$$Z(t) = \sqrt{|E_u|^2_{H^1(\Omega)} + \|E_v\|^2_{L^2(\Omega)}},$$

and assume that $t^* \in [t_3, t_N]$ is the point in time where Z attains its maximum and $t^* \in (t_n, t_{n+1}]$ for some n. We have for the first and second terms in (4.22)

$$\begin{aligned} I + II \leq\ & C_1\left[\sum_{K\in\mathcal{T}_h} h_K^2\left\|\frac{\partial \tilde{v}_{h\tau}}{\partial t} - \Delta\tilde{u}_{h\tau} - f\right\|^2_{L^2(K)} + \sum_{E\in\mathcal{E}_h} h_E\left\|[n\cdot\nabla\tilde{u}_{h\tau}]\right\|^2_{L^2(E)}\right]^{1/2}(t^*)|E_u|_{H^1(\Omega)}(t^*)\\ &+ C_2\sum_{m=1}^{n}\frac{\tau_{m-1}}{2}\left[\sum_{K\in\mathcal{T}_h} h_K^2\left\|\partial_m^2 v_h - \partial_{m-1}^2 v_h\right\|^2_{L^2(K)}\right]^{1/2}|E_u|_{H^1(\Omega)}(t_m)\\ &+ C_3\sum_{m=0}^{n}\int_{t_m}^{\min(t_{m+1},t^*)}\left[\sum_{K\in\mathcal{T}_h} h_K^2\left\|\frac{\partial^2\tilde{v}_{h\tau}}{\partial t^2} - \Delta\frac{\partial\tilde{u}_{\tau h}}{\partial t} - \frac{\partial f}{\partial t}\right\|^2_{L^2(K)}\right.\\ &\left.+ \sum_{E\in\mathcal{E}_h} h_E\left\|\left[n\cdot\nabla\frac{\partial\tilde{u}_{\tau h}}{\partial t}\right]\right\|^2_{L^2(E)}\right]^{1/2}(t)|E_u|_{H^1(\Omega)}(t)\mathrm{d}t.\end{aligned}$$

This follows from an integration by parts with respect to time and the estimates on operators Π_h and $\tilde{I}_h$, *cf.* [15], and gives rise to the space part of the error estimate (4.10). Indeed, we can summarize the bounds above as

$$I + II \leq \eta_s(t_N)Z(t^*).$$

The third term in (4.22) is responsible for the time estimator. It can be written as

$$\begin{aligned} III = \sum_{m=3}^{n-1}\int_{t_m}^{\min(t_{m+1},t^*)}&\left[\left(p_m\left(\partial_m^4 u_h + \tau_m\sum_{k=m-2}^{m}\gamma_k\left(\partial_k^2\dot{f}_h - A_h\partial_k^2 v_h\right)\right), \tilde{I}_h E_v\right)\right.\\ &\left. - \left(p_m\nabla\partial_m^2 v_h, \nabla E_u\right) + \left(\tilde{f}_\tau - f, \tilde{I}_h E_v\right)\right]\mathrm{d}t.\end{aligned} \tag{4.23}$$

Recalling that $Z(t^*)$ is the maximum of $Z(t)$ and using the estimate $\|\tilde{I}_h E_v\|_{L^2(\Omega)} \leq C\|E_v\|_{L^2(\Omega)}$ we continue as

$$
\begin{aligned}
III \leq{} & Z(t^*) \sum_{m=3}^{n-1} \int_{t_m}^{\min(t_{m+1},t^*)} |p_m| \mathrm{d}t \\
& \times \left(C\|\partial_m^4 u_h\|_{L^2(\Omega)} + |\nabla \partial_m^2 v_h|_{H^1(\Omega)} + C\tau_m \sum_{k=m-2}^{m} \gamma_k \|\partial_k^2 \dot{f}_h - A_h \partial_k^2 v_h\|_{L^2(\Omega)} \right) \\
& + Z(t^*) \int_{t_3}^{t_n} \|f - \tilde{f}_\tau\|_{L^2(\Omega)} \mathrm{d}t.
\end{aligned}
$$

Noting

$$
\int_{t_m}^{t_{m+1}} |p_m| \mathrm{d}t \leq \frac{1}{12}\tau_m^3 + \frac{1}{8}\tau_{m-1}\tau_m^2,
$$

we can finally bound III as

$$
III \leq \left(C \sum_{k=3}^{N-1} \tau_k \hat{\eta}_T(t_k) + C \sum_{k=1}^{N-1} \tau_k \hat{\eta}_T^{\mathrm{h.o.t}}(t_k) + \int_{t_3}^{t_N} \|f - \tilde{f}_\tau\|_{L^2(\Omega)} \mathrm{d}t \right) Z(t^*).
$$

Summing together the estimates on the terms I, II, III, and recalling $Z(t^*) \geq Z(t_N)$ yields (4.10) at the final time t_N. $\square$

Remark 4.5. The terms $\hat{\eta}_T^{\mathrm{h.o.t}}(t_k)$ in (4.10) are (at least formally) of higher order than $\hat{\eta}_T(t_k)$. We propose therefore to ignore $\hat{\eta}_T^{\mathrm{h.o.t}}(t_k)$ in practice together with the integral of $f - \tilde{f}_\tau$, and to use $\hat{\eta}_T(t_k)$ as the indicator of error due to the discretization in time. The following Theorem shows that the latter is indeed of optimal order τ^2, at least for sufficiently smooth solutions, on quasi-uniform meshes in space and uniform meshes in time.

Theorem 4.6. *Let u be the solution of wave equation (2.1) and $\frac{\partial^3 u}{\partial t^3}(0) \in H^1(\Omega)$, $\frac{\partial^2 u}{\partial t^2}(0) \in H^2(\Omega)$, $\frac{\partial^2 f}{\partial t^2}(t) \in L^\infty(0,T;L^2(\Omega))$, $\frac{\partial^3 f}{\partial t^3}(t) \in L^2(0,T;L^2(\Omega))$. Suppose that mesh $\mathcal{T}_h$ is quasi-uniform, the mesh in time is uniform ($t_k = k\tau$), and the initial approximations are chosen as in (3.7). Then, the 5-point time error estimator $\hat{\eta}_T(t_k)$ defined by (4.11) is of order τ^2, i.e.*

$$
\hat{\eta}_T(t_k) \leq C\tau^2.
$$

with a positive constant C depending only on u, f, and the mesh regularity.

Proof. The result follows from Theorem 3.3 by using (4.14) and Lemma 4.2

$$
\left\|\partial_k^4 u_h\right\|_{L^2(\Omega)} = \left\|\hat{\partial}_k^2 \bar{f}_h - A_h \hat{\partial}_k^2 \bar{u}_h\right\|_{L^2(\Omega)} = \left\| \sum_{k=n-2}^{n} \alpha_k \left(\partial_k^2 f_h - A_h \partial_k^2 u_h \right) \right\|_{L^2(\Omega)}.
$$

$\square$

Remark 4.7. Note, that as in the case for 3-point error estimator, the approximation of initial conditions is crucial for the optimal rate of our time error estimator.

5. Numerical results

5.1. A toy model: a second order ordinary differential equation

Let us consider first the following ordinary differential equation

$$\begin{cases} \dfrac{\mathrm{d}^2 u(t)}{\mathrm{d}t^2} + Au(t) = f(t), \quad t \in [0;T] \\ u(0) = u_0, \\ \dfrac{\mathrm{d}u}{\mathrm{d}t}(0) = v_0. \end{cases} \tag{5.1}$$

with a constant $A > 0$. This problem serves as simplification of the wave equation in which we get rid of the space variable. The Newmark scheme reduces in this case to

$$\begin{aligned} \frac{u^{n+1}-u^n}{\tau_n} - \frac{u^n - u^{n-1}}{\tau_{n-1}} + A\frac{\tau_n(u^{n+1}+u^n)+\tau_{n-1}(u^n+u^{n-1})}{4} \\ = \frac{\tau_n(f^{n+1}+f^n)+\tau_{n-1}(f^n+f^{n-1})}{4}, \quad 1 \le n \le N-1 \\ \frac{u^1-u^0}{\tau_0} = v_0 - \frac{\tau_0}{4}A(u^1+u^0) + \frac{\tau_0}{4}(f^1+f^0), \\ u^0 = u_0, \end{aligned} \tag{5.2}$$

and the error becomes

$$e(t_n) = \max_{0 \le k \le n} \left(\left|v^n - u'(t_n)\right|^2 + A\left|u^n - u(t_n)\right|^2 \right)^{1/2}, \quad 0 \le n \le N. \tag{5.3}$$

The 3-point and the 5-point *a posteriori* error estimates are then defined as follows:

$$\begin{aligned} e(t_n) \le \sum_{k=0}^{n-1} \tau_k \eta_T(t_k) = \tau_0 \left(\frac{5}{12}\tau_0^2 + \frac{1}{2}\tau_0\tau_1\right)\sqrt{A(\partial_1^2 v)^2 + (\partial_1^2 f - A\partial_1^2 u)^2} \\ + \sum_{k=1}^{n-1} \tau_k \left(\frac{1}{12}\tau_k^2 + \frac{1}{8}\tau_{k-1}\tau_k\right)\sqrt{A(\partial_k^2 v)^2 + (\partial_k^2 f - A\partial_k^2 u)^2}, \quad 1 \le n \le N \end{aligned} \tag{5.4}$$

$$e(t_n) \le \sum_{k=3}^{n-1} \tau_k \hat{\eta}_T(t_k) = \sum_{k=3}^{n-1} \tau_k \left(\frac{1}{12}\tau_k^2 + \frac{1}{8}\tau_{k-1}\tau_k\right)\sqrt{A(\partial_k^2 v)^2 + (\partial_k^4 u)^2}, \quad 4 \le n \le N. \tag{5.5}$$

We define the following effectivity indices in order to measure the quality of the 3-point and the 5-point estimators

$$ei_T(t_n) = \frac{\sum_{k=0}^{n-1} \tau_k \eta_T(t_k)}{e(t_k)}, \qquad \hat{ei}_T(t_n) = \frac{\sum_{k=3}^{n-1} \tau_k \hat{\eta}_T(t_k)}{e(t_k)}.$$

We consider problem (5.1) with the exact solution $u = \cos(\sqrt{A}t)$, and the final time $T = 1$. The results of simulations with constant time steps $\tau_n = \tau = T/N$ are presented in Table 1. We observe that 3-point and 5-point estimators are divided by about 100 when the time step τ is divided by 10. The true error $e(t_N)$ also behaves as $O(\tau^2)$ and hence both time error estimators behave as the true error.

In order to check the behavior of time error estimators for variable time step we take the previous example with the following time step $\forall n:\ 0 \le n \le N$

$$\tau_n = \begin{cases} 0.1\tau_*, & \text{if } \mathrm{mod}(n,2) = 0, \\ \tau_*, & \text{if } \mathrm{mod}(n,2) = 1, \end{cases} \tag{5.6}$$

TABLE 1. Effectivity indices for the problem (5.1) with the exact solution $u = \cos(\sqrt{A}t)$, constant time step.

A	τ	$\sum_{k=0}^{N-1} \tau_k \eta_T(t_k)$	$\sum_{k=3}^{N-1} \tau_k \hat{\eta}_T(t_k)$	$e(t_N)$	$ei_T(t_N)$	$\hat{ei}_T(t_N)$
100	0.01	.21	.203	.085	2.47	2.39
100	0.001	.0021	.0021	8.34e-04	2.5	2.49
100	0.0001	2.08e-05	2.08e-05	8.35e-06	2.5	2.5
1000	0.01	20.51	19.47	8.35	2.46	2.33
1000	0.001	.209	.208	.084	2.5	2.49
1000	0.0001	.0021	.0021	8.33e-04	2.5	2.5
10000	0.01	1.68e+03	1.4e+03	200	8.38	6.98
10000	0.001	20.8	20.7	8.34	2.5	2.49
10000	0.0001	.208	.208	.083	2.5	2.5

TABLE 2. Effectivity indices for the problem (5.1) with the exact solution $u = \cos(\sqrt{A}t)$, variable time step (5.6).

A	τ_*	$\sum_{k=0}^{N-1} \tau_k \eta_T(t_k)$	$\sum_{k=3}^{N-1} \tau_k \hat{\eta}_T(t_k)$	$e(t_N)$	$ei_T(t_N)$	$\hat{ei}_T(t_N)$
100	0.01	.09	.087	.077	1.17	1.13
100	0.001	8.85e-04	8.82 e-04	7.59e-04	1.17	1.16
100	0.0001	8.83e-06	8.83e-06	7.6e-06	1.16	1.16
1000	0.01	8.91	8.52	7.6	1.17	1.13
1000	0.001	.089	.088	.076	1.17	1.16
1000	0.0001	8.84e-04	8.83e-04	7.59e-04	1.16	1.16
10000	0.01	802.84	725.1	200	4.01	3.63
10000	0.001	8.84	8.8	7.58	1.17	1.16
10000	0.0001	.088	.088	.076	1.16	1.16

where τ_* is a given fixed value, see Table 2. As in the case of constant time step we have the equivalence between the true error and both estimated errors. We have plotted on Figure 1 evolution in time of the values $\sum_{k=0}^{n-1} \tau_k \eta_T(t_k)$ and $\sum_{k=3}^{n-1} \tau_k \hat{\eta}_T(t_k)$ compared to the error $e(t_n)$.

Table 3 contains the results for even more non-uniform time step $\forall n: \; 0 \le n \le N$

$$\tau_n = \begin{cases} 0.01\tau_*, & \text{if } \mathrm{mod}(n,2) = 0, \\ \tau_*, & \text{if } \mathrm{mod}(n,2) = 1, \end{cases} \tag{5.7}$$

on otherwise the same test case. Note that in case when $A = 100$ and $\tau_* = 0.001$ the 5-points error estimator significantly over-predicts the true error, while the 3-point estimator remains very close to it. This effect is consistent with Theorem 3.2. Indeed, the constants the 5-point error estimator may depend on the meshes regularity in time.

Our conclusion is that both 3-point and 5-point *a posteriori* error estimators are reliable for the toy model (5.1), although not asymptotically exact. The effectivity indices range from 1 to around 8 so that the the estimates can be rather pessimistic with respect to the true error. Moreover, Figure 1 suggests that the effectivity of the error estimator can deteriorate in the long time simulations.

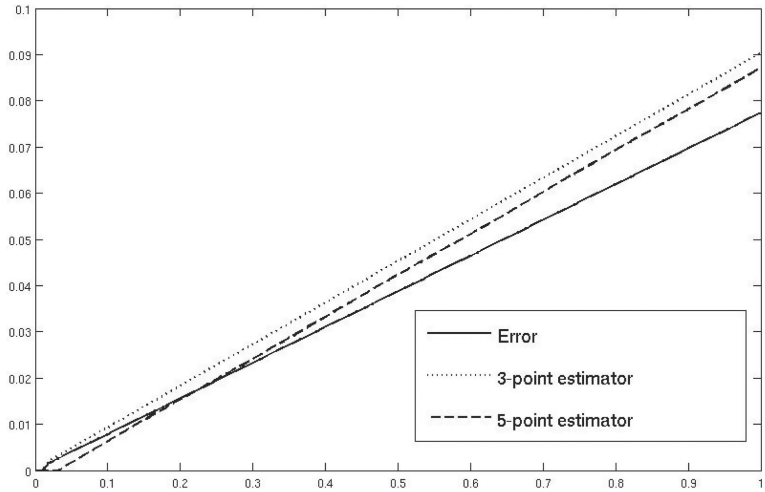

FIGURE 1. Evolution in time of 3-point and 5-point time estimators: the error at time t_n defined by (5.3) and the error estimators (5.4) and (5.5) on the y-axis *vs.* time t_n on the x-axis. The results are computed for variable time step (5.6), $A = 100$, $\tau_* = 0.01$, $T = 1$.

TABLE 3. Effectivity indices for the problem (5.1) with the exact solution $u = \cos(\sqrt{A}t)$, variable time step (5.7).

A	τ_*	$\sum_{k=0}^{N-1} \tau_k \eta_T(t_k)$	$\sum_{k=3}^{N-1} \tau_k \hat{\eta}_T(t_k)$	$e(t_N)$	$ei_T(t_N)$	$\hat{ei}_T(t_N)$
100	0.01	.086	.083	.084	1.02	0.98
100	0.001	8.39e-04	8.36 e-04	8.26e-04	1.02	1.01
100	0.0001	8.38e-06	1.82e-05	8.1e-06	1.03	2.24
1000	0.01	8.47	8.1	8.26	1.02	0.98
1000	0.001	.083	.084	.0827	1.02	1.01
1000	0.0001	8.37e-04	8.37e-04	8.26e-04	1.01	1.01
10000	0.01	764.2	691.7	200	3.82	3.46
10000	0.001	8.39	8.35	8.25	1.02	1.01
10000	0.0001	.084	.084	.083	1.01	1.01

5.2. The error estimator for the wave equation on Delaunay mesh

We now report numerical results for initial boundary-value problem for the wave equation (2.1) using piecewise linear finite elements in space) and Newmark scheme with non-uniform time steps and study the behavior of the 3-point time error estimator (3.3) and the 5-point time error estimator (4.11). All the computations are done with the help of FreeFEM++ [16]. In practice, we compute the space estimator (3.2) as follows:

$$\eta_S(t_N) = \max_{1\le n\le N-1} \left[\sum_{K\in\mathcal{T}_h} h_K^2 \left\|\partial_n v_h - I_h f^n\right\|^2_{L^2(K)} + \sum_{E\in\mathcal{E}_h} h_E \|[n\cdot\nabla u_h^n]\|^2_{L^2(E)} \right]^{1/2}$$
$$+ \sum_{n=1}^{N-1} \tau_n \left[\sum_{K\in\mathcal{T}_h} h_K^2 \left\|\partial_n^2 v_h - \partial_n I_h f\right\|^2_{L^2(K)} + \sum_{E\in\mathcal{E}_h} h_E \left\|[n\cdot\nabla\partial_n u_h]\right\|^2_{L^2(E)} \right]^{1/2} \tag{5.8}$$

TABLE 4. Effectivity inidices for the problem (2.1) with the exact solution (5.9), non-uniform time step.

h	τ_0	$ei(t_N)$	$\hat{ei}(t_N)$	$\sum_{k=0}^{N-1} \tau_k \eta_T(t_k)$	$\sum_{k=3}^{N-1} \tau_k \hat{\eta}_T(t_k)$	$\eta_S(t_N)$	τ_F	$e(t_N)$
.05	.01	4.85	4.83	.096	.088	2.55	.0063	.58
.025	.0071	5.39	5.38	.054	.051	1.39	.0045	.27
.0125	.005	5.94	5.93	.028	.026	.72	.0032	.13
.00625	.0035	5.94	5.94	.014	.013	.36	.0022	.065
.003125	.0025	5.94	5.94	.0067	.0065	.18	.0016	.032

with I_h denoting the nodal interpolator to piecewise linear functions.

The quality of our error estimators in space and time is determined by the effectivity indices

$$ei(t_N) = \frac{\sum_{k=0}^{N-1} \tau_k \eta_T(t_k) + \eta_S(t_N)}{e(t_N)}, \quad \hat{ei}(t_N) = \frac{\sum_{k=3}^{N-1} \tau_k \hat{\eta}_T(t_k) + \eta_S(t_N)}{e(t_N)},$$

for, respectively, the 3-point and the 5-point time error estimators combined with the space error estimator. The true error is

$$e(t_N) = \max_{0\leqslant n\leqslant N} \left(\left\| v_h^n - \frac{\partial u}{\partial t}(t_n) \right\|^2_{L^2(\Omega)} + |u_h^n - u(t_n)|^2_{H^1(\Omega)} \right)^{1/2}.$$

Consider the problem (2.1) with $\Omega = (0,1)\times(0,1),\ T = 1$ and the exact solution u given by

$$u(x,y,t) = \mathrm{e}^{-100 r^2(x,y,t)}, \tag{5.9}$$

where

$$r^2(x,y,t) = (x - 0.3 - 0.4t^2)^2 + (y - 0.3 - 0.4t^2)^2. \tag{5.10}$$

Thus, u is a Gaussian function, whose center moves from point $(0.3, 0.3)$ at $t = 0$ to point $(0.7, 0.7)$ at $t = 1$. The transport velocity $0.8t(1,1)^T$ is peaking at $t = 1$. We choose non-uniform time step for $n = 1, \ldots, N-1$ as

$$\tau_n = \frac{\tau_0}{\sqrt{t_n}}.$$

The initial conditions are computed with the orthogonal projections as in (3.7), *cf.* Remarks 3.4 and 4.7. Unstructured Delaunay meshes in space are used in all the experiments. Numerical results are reported in Table 4. Note that this case is chosen so that the non-uniform time step is required, see Figure 2.

Referring to Table 4, we observe that when setting initial time step as $\tau^2 \sim O(h)$ the error is divided by 2 each time h is divided by 2, consistent with $e \sim O(\tau^2 + h)$. The space error estimator and the two time error estimators behave similarly and thus provide a good representation of the true error. Both effectivity indices tend to a constant value.

We therefore conclude that our space and time error estimators are reliable in the regime of non-uniform time steps and Delaunay space meshes. They separate well the two sources of the error and can be thus used for the mesh adaptation in space and time. In particularly, 3-point and 5-point time estimators become more and more close to each other when h and τ tend to 0.

Finally, we report in Table 5 the computational times of our simulations using either 3-point or 5-point error estimators for the Newmark scheme on uniform meshes in time (with time step τ) and unstructured

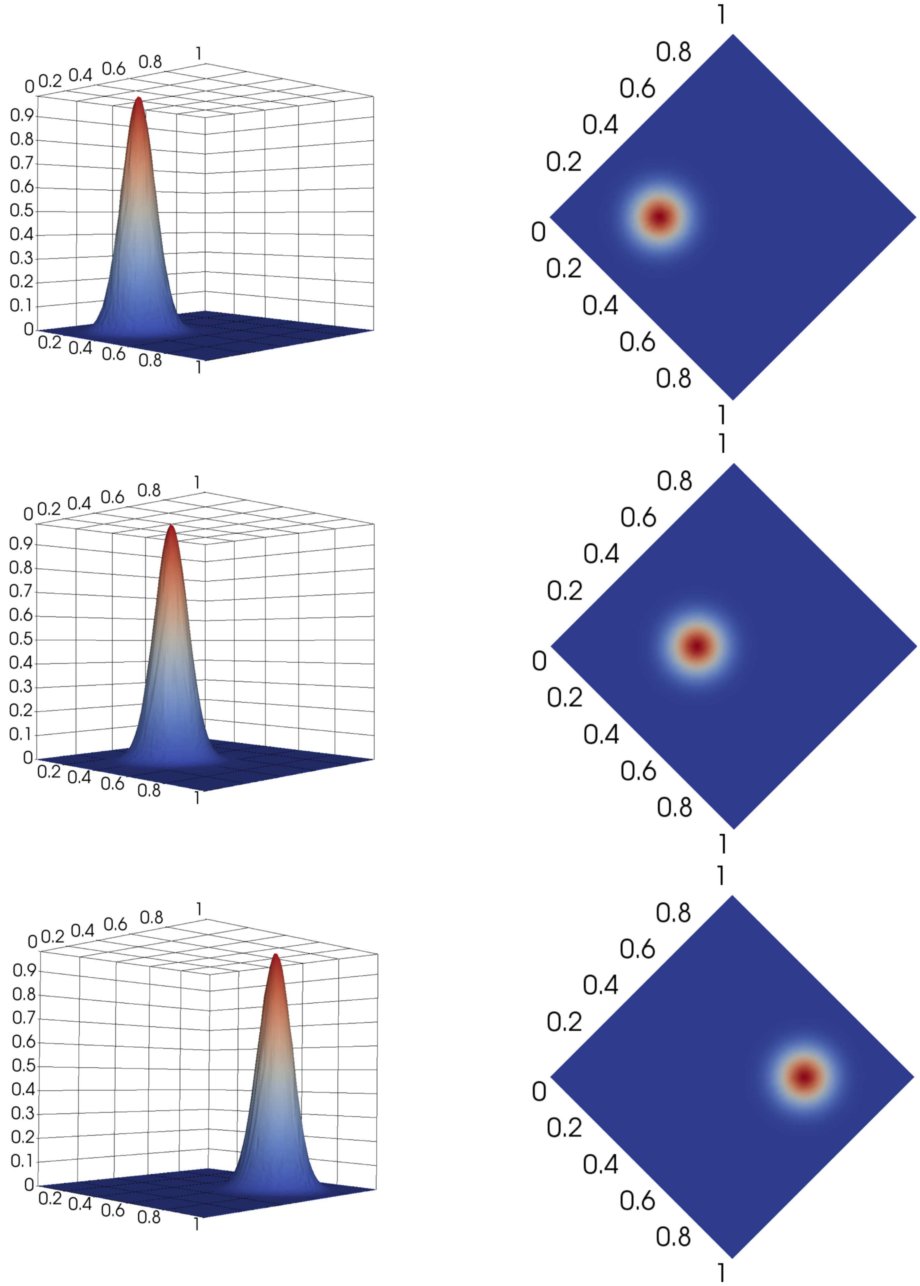

FIGURE 2. Solution (5.9) at $t = 0,\ 0.5,\ 1$ from *top* to *bottom*.

quasi-uniform Delaunay meshes in space with maximum mesh size h. We have used FreeFEM++ to implement the algorithm and run it on a modern laptop computer with Intel Core I7 processor and 16GB of memory. The reported CPU times correspond to the whole computation, including the construction of the mesh, setting up the initial conditions, and factorizing the matrices, which is done only once before entering into the time marching loop (we have used the default UMFPACK direct sparse solver). We observe that the advantage of the 5-point estimator over the 3-point one which grows with refining the mesh and is up to 20% in our experiments.

TABLE 5. Numerical experiments for the test case (5.9) with constant time step τ, CPU3 – computational time in seconds for program using the 3-point estimator, CPU5 – the same for the 5-point estimator.

h	τ	CPU3	CPU5
$1/128$	$1/100$	18.5	16.6
$1/256$	$1/100$	75.8	65.5
$1/512$	$1/100$	351	292
$1/128$	$1/200$	33.1	28.2
$1/256$	$1/200$	133	113
$1/512$	$1/200$	594	490

Some preliminary results for a fully adaptive algorithm showing the behavior of the estimators from [15] and from this article in more realistic settings are available in the Ph.D. thesis of the first author [14].

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