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Nicolas Hugot[1,2,3*], Alexandre Imperiale[1], and Martin Vohralík[2,3]

[1]Université Paris-Saclay, CEA, List, 91120 Palaiseau, France
[2]Inria, 48 rue Barrault, 75647 Paris, France
[3]CERMICS, Ecole nationale des ponts et chaussées, IP Paris, 77455 Marne-la-Vallée, France

*Corresponding author: nicolas.hugot@cea.fr
Contributing authors: alexandre.imperiale@cea.fr, martin.vohralik@inria.fr

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Abstract

We consider the transient acoustic wave equation and we are interested in discretising it using the spectral finite element method in space and the explicit leapfrog scheme in time. We reconstruct a $\mathcal{C}^1$-in-time approximation from the leapfrog snapshots which satisfies a suitable Galerkin orthogonality relation. Therefrom, we develop *a posteriori* error estimators and prove their global reliability and local space-time efficiency, with constants independent of the final time. This includes residual- and flux-based (averaged and equilibrated) estimators. Numerical experiments confirm the theoretical results and show a tight upper bound together with an excellent localisation of the error in space and in time. These results are an application of a larger general framework that we develop, based on the inf-sup stable weak formulation from [J. Math. Anal. Appl. 505 (2022), 125457]. The proof of local space-time efficiency uses appropriately scaled space-time bubble functions and norms on possibly anisotropic space-time meshes following [SIAM J. Numer. Anal. 51 (2013), 773-793].

Keywords: Wave equation, a posteriori estimates, spectral finite element method

Contents

1 Introduction

We consider the acoustic wave equation with zero initial and boundary conditions: find $u : (0,T) \longrightarrow \mathbb{R}$ such that

$$\partial_{tt}u - \Delta u = f \qquad \text{in } (0,T)\times\Omega, \tag{1.1a}$$
$$u = 0 \qquad \text{on } (0,T)\times\partial\Omega, \tag{1.1b}$$
$$u = 0 \qquad \text{on } \{0\}\times\Omega, \tag{1.1c}$$
$$\partial_t u = 0 \qquad \text{on } \{0\}\times\Omega, \tag{1.1d}$$

where Ω is an open, connected, bounded, and polytopal domain of $\mathbb{R}^d$, $d > 1$, with a Lipschitz boundary, and $T > 0$ is the final simulation time. We denote as Q the space-time domain $\Omega \times (0,T)$ and take $f \in L^2(Q)$.

The acoustic wave equation (1.1) is a fundamental model in countless applications. In particular, it governs the pressure field propagation of an ultrasonic non-destructive testing model [20, 23]. Numerical simulation is of paramount importance for reliable defect localization and material characterization. It however, comes with constraints due to computing cost at higher frequencies (time and memory). The objective is to allow for simulations that balance sufficient precision with minimal cost. While *a priori* estimates enable to justify the order of convergence of the scheme, they cannot be used to precisely predict the numerical error of the simulation, nor its distribution in the space-time domain during the simulation. To achieve this, we derive reliable and locally space-time efficient *a posteriori* error estimates, which enable both the certification of the computed solution against required tolerances and the creation of a localised error map. This identifies precisely which space-time regions contain the biggest part of the error, thereby guiding the user towards a targeted and efficient revision of the simulation if needed.

The literature on *a posteriori* estimates for the wave equation already contains some results that can be broadly categorised into those that are reliable (upper bound of the error) and those that are also efficient (lower bound of the error). The authors in [16, 17] give reliability results in L^∞ in time norms, while [13] presents reliable and unknown-constant-free estimates in $L^\infty(L^2)$ norm. [29] proposes reliable estimates using reconstructed solutions and [18, 19] use similar results to implement space-time mesh adaptivity. These works, however, do not show any theoretical efficiency result. In [3], the authors work with the acoustic wave equation discretised in space by low order piecewise polynomials and by the backward Euler scheme in time. They show both reliability and local efficiency, though the norm they use to evaluate the error differs between the two results. Later, [6, 7] present both reliability and global (robust) efficiency results. The authors use a specific exponentially-damped energy norm to evaluate the error. They devise solution reconstructions to construct a global estimator (on the whole space-time domain) that is globally both reliable and efficient under some assumptions on the smoothness of the source term and up to higher order terms. These appear to be the first reliable and efficient results for (1.1), whereas such results exist for parabolic-type partial differential equations like in [12] for the non-linear advection-diffusion case and [15] for the heat equation.

Our purpose is to derive reliable (also guaranteed and constant-free) and locally space-time efficient *a posteriori* estimates for the wave equation (1.1). To achieve this, we choose the variational setting from the recent work [26] that gives a space-time $\inf - \sup$ stable weak formulation of (1.1). We focus on the spectral finite element method with an explicit leapfrog time stepping scheme [9, 22]. In our procedure, we need to reconstruct the leapfrog iterates into a space-time solution that conforms to the continuous setting. Such reconstructions are already discussed in the literature as pairs of linked reconstructions (hybrid schemes) in [17, 29], or unique ones for discretisations of the primal problem such as the one in [7]. [1, 2] also discusses such reconstructions for other pointwise-in-time schemes for parabolic problems and ordinary differential equations. To the best of our knowledge, none of the existing reconstructions fit exactly the admissibility constraint our framework comes with. We are thus lead to introduce a suitable novel reconstruction that is $\mathcal{C}^1$ and piecewise cubic in time. Therefrom, we prove the reliability using a Prager–Synge-type inequality [24]. We apply the methodologies from [12, 15, 27] to prove our local space-time efficiency results, using an appropriate anisotropic, mesh-dependent norm for the test space and well-chosen space-time bubbles as test functions.

This contribution is organised as follows. In Section 2, we introduce the spectral finite element method with a leapfrog time-stepping scheme [9, 22], simplified, for the moment, by using a uniform space-time mesh. We show, in Section 3, how to reconstruct the leapfrog iterates into an admissible discrete solution, as well as how to construct the fluxes used in our estimators. In Section 4, we state our main result, the guaranteed and locally space-time efficient *a posteriori* estimates, before numerically illustrating them in Section 5. This includes residual-based, averaged flux-based and equilibrated flux-based estimators. Then, in Section 6, we generalise both the setting and our main result into an abstract framework that allows for a broader range of numerical methods (still $H^1(Q)$-conforming) and non-uniform, possibly space-time anisotropic space-time meshes. Section 7 contains proofs of some generic reliability and efficiency results that are finally used in Section 8 to prove the results of the general framework.

2 Setting

This section introduces the setting and basic notation.

2.1 Basic notation

For any time subinterval $I \subset (0,T)$ and space subdomain $\omega \subset \Omega$, we identify $L^2(\omega \times I)$ with the Bochner space $L^2(I; L^2(\omega))$ and use the following shortened notation for the L^2 inner products and norms:

$$
\begin{aligned}
(u,v)_\omega &:= \int_\omega u(\boldsymbol{x})v(\boldsymbol{x})\mathrm{d}x, & ||u||_\omega &:= \sqrt{(u,u)_\omega}, & u,v &\in L^2(\omega),\\
(u,v)_{\omega\times I} &:= \int_I (u(t),v(t))_\omega \mathrm{d}t, & ||u||_{\omega\times I} &:= \sqrt{(u,u)_{\omega\times I}}, & u,v &\in L^2(\omega\times I).
\end{aligned}
$$

$\mathcal{P}_p(\omega)$ denotes the space containing all real-valued polynomials on ω of total degree less than or equal to $p \in \mathbb{N}$. For V any vector space, we also denote $\mathcal{P}_p(I;V)$ the set containing all V-valued polynomials on I of degree less than or equal to p. We finally define

$$\mathcal{Q}_p([0,1]^d) := \operatorname{span}\{x_1^{\alpha_1}x_2^{\alpha_2}\cdots x_d^{\alpha_d},\ \text{s.t. } \forall i \in [\![1,d]\!],\ \alpha_i \in [\![1,p]\!]\}$$

the space of polynomials of componentwise degrees at most p over the reference cube $[0,1]^d$.

2.2 Mesh and piecewise polynomial spaces

Let $\mathcal{T}_h(\Omega)$ be a mesh of Ω composed of either simplices or of affine-mapped hypercubes such that any face of an element is either the whole face of another one, or part of the boundary

$\partial\Omega$. Let $\mathcal{F}_h(\Omega)$ and $\mathcal{S}_h(\Omega)$ be the sets containing the faces and vertices of $\mathcal{T}_h(\Omega)$, respectively. We specifically denote by $\mathcal{S}_h^{\text{int}}(\Omega)$ and $\mathcal{S}_h^{\text{ext}}(\Omega)$ the sets of interior and boundary vertices and $\mathcal{F}_h^{\text{int}}(\Omega)$ and $\mathcal{F}_h^{\text{ext}}(\Omega)$ the sets of interior and boundary faces of $\mathcal{T}_h(\Omega)$. We use the notation $\hat{K}$ for the reference element: either the reference simplex $\{\boldsymbol{x} \in [0,1]^d \text{ s.t. } \sum_{k=1}^d x_k \leq 1\}$ or the unit hypercube $[0,1]^d$. For any element $K \in \mathcal{T}_h(\Omega)$, we assume that K is an affine map of $\hat{K}$, and we denote as:

- $h_K > 0$ its diameter;
- $\boldsymbol{T}_K : \hat{K} \longrightarrow K$ the affine mapping between the reference element $\hat{K}$ and K;
- $\mathbf{J}_K : \hat{K} \longrightarrow \mathbb{R}^{d\times d}$ the constant Jacobian matrix of $\boldsymbol{T}_K$ taken such that $\det \mathbf{J}_K > 0$;
- $\mathcal{F}_h(K)$ and $\mathcal{S}_h(K)$ the sets containing respectively the faces and vertices of K.

Let $N \in \mathbb{N}\setminus\{0\}$ and $\mathcal{S}_\tau(0,T) := \{0 = t^0 < t^1 < \ldots < t^{N-1} < t^N = T\}$ be a partition of the time interval $(0,T)$, and, for each $n \in [\![1,N]\!]$, let $I_n := (t^{n-1}, t^n)$ be the n-th time interval of size $\tau_n := t^n - t^{n-1}$. We denote the time mesh as $\mathcal{T}_\tau(0,T) := \{I_n,\ n \in [\![1,N]\!]\}$. Then $\mathcal{T}_{h\tau}(Q) := \mathcal{T}_h(\Omega) \times \mathcal{T}_\tau(0,T)$ stands for the space-time mesh.

In Sections 2 to 5, we assume that all elements of the mesh $\mathcal{T}_h(\Omega)$ are of similar shape and diameter $h > 0$. We also take a constant time step $\tau := c_{\text{CFL}} \times h$ with $c_{\text{CFL}} > 0$ close to 1. These assumptions cover practically relevant cases and allow to present the developed theory in a simple and accessible way. Later, starting from Section 6, we develop a more general abstract framework allowing for arbitrary shape-regular spatial meshes and temporal meshes with a non-uniform time step size.

Let $p > 0$ be the polynomial degree of the space approximation. Then, we define two piecewise polynomial, finite-dimensional, conforming approximation spaces for $L^2(\Omega)$ and $H_0^1(\Omega)$:

$$U_h^p := \left\{ v_h \in L^2(\Omega) \text{ s.t. } \forall K \in \mathcal{T}_h(\Omega),\ v_h|_K \circ \boldsymbol{T}_K \in \left| \begin{array}{l} \mathcal{P}_p(\hat{K}) \text{ if } \hat{K} \text{ is a simplex} \\ \mathcal{Q}_p(\hat{K}) \text{ if } \hat{K} \text{ is a hypercube} \end{array} \right. \right\}$$

and

$$V_h^p := U_h^p \cap H_0^1(\Omega).$$

Here, V_h^p imposes the piecewise polynomials to be continuous on Ω and zero on $\partial\Omega$.

2.3 Finite element space-discretisation with explicit leapfrog time-stepping

The leapfrog time-discretisation can be derived from the second-order weak formulation of the wave equation [21]. We approximate the solution u by a sequence of pointwise-in-time snapshots

$$(u_h^n)_{n\in[\![-1,N+1]\!]} \subset V_h^p$$

representing the discrete approximation at each discrete time (also including the additional values at t^{-1} and t^{N+1}). The first and second time derivatives in (1.1) are replaced by second order finite-difference approximations, so (1.1c) and (1.1d) are approximated by

$$u_h^0 = 0, \tag{2.1a}$$

$$\frac{1}{2\tau}(u_h^1 - u_h^{-1}) = 0. \tag{2.1b}$$

Then, the fully discrete version of (1.1a) consists, for all $n \in [\![0, N-1]\!]$, in finding $u_h^{n+1} \in V_h^p$ such that

$$\frac{1}{\tau^2}(u_h^{n+1} - 2u_h^n + u_h^{n-1}, v_h)_\Omega + (\nabla u_h^n, \nabla v_h)_\Omega = (f(t^n), v_h)_\Omega \qquad \forall v_h \in V_h^p. \tag{2.1c}$$

For this to work, we assume in Sections 2 to 5 that actually $f \in \mathcal{C}^0(0, T; L^2(\Omega))$.

2.4 Inf-sup stable weak formulation

In order to derive space-time *a posteriori* estimates, we use well-posedness results for the wave equation from [25] and the inf-sup formulation developed in [26]. We introduce the solution space Y_0 by imposing zero values on $\partial\Omega \times (0, T)$ and on $\Omega \times \{0\}$ for functions of $H^1(Q)$:

$$Y_0 := \left\{ v \in H^1(Q) \text{ s.t. } v = 0 \text{ on } \partial Q \setminus (\{T\} \times \Omega) \right\}. \tag{2.2}$$

Then, we introduce the test space Y_T similarly by imposing zero values on $\partial\Omega \times (0, T)$ and on $\Omega \times \{T\}$ for functions of $H^1(Q)$:

$$Y_T := \left\{ v \in H^1(Q) \text{ s.t. } v = 0 \text{ on } \partial Q \setminus (\{0\} \times \Omega) \right\}. \tag{2.3}$$

First, in the simplified setting of Sections 2 to 5, we equip Y_0 and Y_T with the $H^1(Q)$ semi-norm

$$|\cdot|^2_{H^1(Q)} := ||\partial_t \cdot||_Q^2 + ||\nabla \cdot||_Q^2 \tag{2.4}$$

which is equivalent to the full $H^1(Q)$ norm $||\cdot||^2_{H^1(Q)} := ||\cdot||_Q^2 + |\cdot|^2_{H^1(Q)}$. We also introduce the associated dual norm for Y_T':

$$||\cdot||_{Y_T'} := \sup_{v \in Y_T \setminus \{0\}} \frac{\langle \cdot, v \rangle_{Y_T}}{|v|_{H^1(Q)}}, \tag{2.5}$$

where $\langle \cdot, \cdot \rangle_{Y_T}$ denotes the duality bracket for $Y_T' \times Y_T$. For $f \in L^2(Q)$, [25] shows the well-posedness of the space-time weak formulation that consists in searching for $u \in Y_0$ such that:

$$-(\partial_t u, \partial_t v)_Q + (\nabla u, \nabla v)_Q = (f, v)_Q \qquad \forall v \in Y_T. \tag{2.6}$$

We introduce the associated residual $r : Y_0 \to Y_T'$ such that for any $u_{h\tau} \in Y_0$

$$\langle r(u_{h\tau}), v \rangle_{Y_T} := (f, v)_Q + (\partial_t u_{h\tau}, \partial_t v)_Q - (\nabla u_{h\tau}, \nabla v)_Q, \qquad \forall v \in Y_T. \tag{2.7}$$

Notably, the residual, when applied to the solution of (2.6), gives $r(u) = 0$. Then, [26] introduces a Hilbert space $\mathcal{Y}_0 \supset Y_0$ (see (6.1) below for the definition) with the associated norm $||\cdot||_{\mathcal{Y}_0}$ such that for $u \in Y_0$ solution of (2.6) and any $u_{h\tau} \in Y_0$,

$$||u - u_{h\tau}||_{\mathcal{Y}_0} = ||r(u_{h\tau})||_{Y_T'}. \tag{2.8}$$

We introduce the local version of both norms for I a subinterval of $(0,T)$ and ω a polytopal open subdomain of Ω:

$$||\cdot||_{Y'_T,\omega\times I} := \sup_{\substack{v\in Y_T\setminus\{0\}\\ \mathrm{supp}(v)\subset\omega\times I}} \frac{\langle\cdot,v\rangle_{Y_T}}{|v|_{H^1(Q)}} \qquad \text{and} \qquad ||u-u_{h\tau}||_{\mathcal{Y}_0,\omega\times I} := ||r(u_{h\tau})||_{Y'_T,\omega\times I}. \tag{2.9}$$

This equivalence between the norm of the error and the dual norm of the residual is the basis of the *a posteriori* estimates derived in what follows. (2.8) is equivalent to [15, equation (2.7)] for the wave equation instead of the heat equation. Furthermore, we point out that this somewhat theoretical norm of the error $||u-u_{h\tau}||_{\mathcal{Y}_0}$ can be bounded from above by

$$||u-u_{h\tau}||_{\mathcal{Y}_0} \le |u-u_{h\tau}|_{H^1(Q)}. \tag{2.10}$$

Indeed, to see this result, we use (2.4) to (2.8) with the Cauchy-Schwarz inequality as follows:

$$\begin{aligned}
||u-u_{h\tau}||_{\mathcal{Y}_0} &\overset{(2.8)}{=} ||r(u_{h\tau})||_{Y'_T}\\
&\overset{(2.5)\text{ to }(2.7)}{=} \sup_{v\in Y_T\setminus\{0\}} \frac{-(\partial_t(u-u_{h\tau}),\partial_t v)_Q + (\nabla(u-u_{h\tau}),\nabla v)_Q}{|v|_{H^1(Q)}}\\
&\le \sup_{v\in Y_T\setminus\{0\}} \frac{||\partial_t(u-u_{h\tau})||_Q||\partial_t v||_Q + ||\nabla(u-u_{h\tau})||_Q||\nabla v||_Q}{|v|_{H^1(Q)}}\\
&\overset{(2.4)}{\le} |u-u_{h\tau}|_{H^1(Q)}.
\end{aligned}$$

This gives an idea of the relation between the theoretical norm $||u-u_{h\tau}||_{\mathcal{Y}_0}$ (or equivalently the dual norm of the residual $||r(u_{h\tau})||_{Y'_T}$) and the classical and easily understandable semi-norm $|u-u_{h\tau}|_{H^1(Q)}$. In the test cases in Section 5, replacing $||u-u_{h\tau}||_{\mathcal{Y}_0}$ by $|u-u_{h\tau}|_{H^1(Q)}$ does not degrade much the effectivity indices of the estimators developed for $||u-u_{h\tau}||_{\mathcal{Y}_0}$. In other words, for the test cases, $|u-u_{h\tau}|_{H^1(Q)} \lesssim ||u-u_{h\tau}||_{\mathcal{Y}_0}$ also holds, in addition to (2.10). Details about the functional setting and the weak formulation are postponed to Section 6.1.

3 Discrete reconstructions

This section prepares the temporal and spatial reconstructions the *a posteriori* analysis relies on.

3.1 Temporal potential reconstruction

The leapfrog scheme (2.1) is based on pointwise-in-time values $(u_h^n)_{n\in[\![-1,N+1]\!]}$ of the discrete solution and does not give a representation of the discrete solution that can be used as $u_{h\tau}$ in the residual (2.7) of the weak formulation. This calls for a reconstruction $u_{h\tau}$ of $(u_h^n)_{n\in[\![-1,N+1]\!]}$ lying in Y_0.

For $k,p\in\mathbb{N}\setminus\{0\}$, let's introduce the space-time finite-dimensional functional spaces:

$$\begin{aligned}
U_{h\tau}^{pk} &:= \{v_{h\tau}\in L^2(0,T;U_h^p) \text{ s.t. } \forall n\in[\![1,N]\!],\ v_{h\tau}|_{I_n}\in\mathcal{P}_k(I_n,U_h^p)\},\\
V_{h\tau}^{pk} &:= U_{h\tau}^{pk}\cap Y_0.
\end{aligned}$$

We also need a time-reconstruction of the source term. For this purpose, we first introduce its discrete pointwise-in-time and elementwise L^2 projections $(f_h^n)_{n\in[\![0,N]\!]}$ defined for all $n \in [\![0,N]\!]$ by:

$$f_h^n \in U_h^p \quad \text{with} \quad (f_h^n, v_h)_\Omega := (f(t^n), v_h)_\Omega, \qquad \forall v_h \in U_h^p. \tag{3.1}$$

From there, we employ a piecewise affine-in-time interpolation to reconstruct our discrete source term.

Definition 3.1 (Source term interpolation). *We define $f_{h\tau} \in U_{h\tau}^{p1} \cap \mathcal{C}^0(0,T;U_h^p)$ such that for $I_n \in \mathcal{T}_\tau(0,T)$ and $t \in I_n$,*

$$f_{h\tau}(t) := \frac{t-t^{n-1}}{\tau} f_h^n + \frac{t^n - t}{\tau} f_h^{n-1}.$$

To define the time-reconstruction of the discrete solution, we introduce some notation for the discrete time derivatives. For $n \in [\![0,N]\!]$, let

$$\begin{aligned} \dot{u}_h^n &:= \frac{1}{2\tau}(u_h^{n+1} - u_h^{n-1}), & \ddot{u}_h^n &:= \frac{1}{\tau^2}(u_h^{n+1} - 2u_h^n + u_h^{n-1}), \\ \dddot{u}_h^n &:= \frac{1}{2\tau}(\ddot{u}_h^{n+1} - \ddot{u}_h^{n-1}), & \ddddot{u}_h^n &:= \frac{1}{\tau^2}(\ddot{u}_h^{n+1} - 2\ddot{u}_h^n + \ddot{u}_h^{n-1}). \end{aligned} \tag{3.2}$$

Definition 3.2 (Reconstructed temporal potential). *Let $(u_h^n)_{n\in[\![-1,N+1]\!]}$ be given by the leapfrog scheme in (2.1), for $f_h^0 = 0$. We define $u_{h\tau} \in V_{h\tau}^{p3} \cap \mathcal{C}^1(0,T;V_h^p)$ such that, for all $I_n \in \mathcal{T}_\tau(0,T)$ and $t \in I_n$,*

$$\begin{aligned} u_{h\tau}(t) &:= u_h^{n-1} + \dot{u}_h^{n-1}(t-t^{n-1}) + \ddot{u}_h^{n-1}\frac{1}{2}(t-t^{n-1})^2 + \dddot{u}_h^{n-1}\frac{1}{6}(t-t^{n-1})^3 \\ &+ \frac{\tau^2}{2}\left[\frac{1}{6}\ddot{u}_h^{n-1} - \frac{\tau}{2}\left(\dddot{u}_h^{n-1} + \frac{\tau}{2}\ddddot{u}_h^{n-1}\right)\left(\frac{t-t^{n-1}}{\tau}\right)^2 + \frac{\tau}{3}\left(\dddot{u}_h^{n-1} + \tau\,\ddddot{u}_h^{n-1}\right)\left(\frac{t-t^{n-1}}{\tau}\right)^3\right]. \end{aligned} \tag{3.3}$$

Remarks:

- The reconstruction $u_{h\tau}$ is built as a $\mathcal{C}^1$-in-time function such that for $I_n \in \mathcal{T}_\tau(0,T)$,

  $$\frac{1}{\tau}\int_{I_n} u_{h\tau}(t)\mathrm{d}t = \frac{1}{2}\left(u_h^n + u_h^{n-1}\right) \quad \text{and} \quad \frac{1}{\tau}\int_{I_n} \partial_{tt}u_{h\tau}(t)\mathrm{d}t = \frac{1}{2}\left(\ddot{u}_h^n + \ddot{u}_h^{n-1}\right).$$

  Then, as a by-product of the design, we also get the following pointwise values for $t^n \in \mathcal{S}_\tau(0,T)$:

  $$u_{h\tau}(t^n) = u_h^n + \frac{\tau^2}{12}\ddot{u}_h^n \quad \text{and} \quad \partial_t u_{h\tau}(t^n) = \dot{u}_h^n. \tag{3.4}$$

- Here, we accept a second-order consistency error on the value of $u_{h\tau}(t^n)$ in exchange for keeping a reconstruction of polynomial order 3. It would be possible to also get $u_{h\tau}(t^n) = u_h^n$ by using a reconstruction of polynomial order 4 with the additional constraint

  $$\frac{1}{\tau}\int_{I_n} \partial_t u_{h\tau}(t)\mathrm{d}t = \frac{1}{\tau}\left(u_h^n - u_h^{n-1}\right) \quad \forall I_n \in \mathcal{T}_\tau(0,T).$$

Lemma 3.3 (Properties of $u_{h\tau}$ and $f_{h\tau}$). *The following properties hold for the reconstructions:*

1. *Regularity:*
$$u_{h\tau} \in \mathcal{C}^1(0,T;V_h^p) \text{ or, equivalently, } u_{h\tau} \in H^2(0,T;V_h^p).$$

2. *Initial conditions:*
$$\partial_t u_{h\tau}(0) = 0 \qquad \text{and,} \qquad \text{if } f_h^0 = 0, \text{ then } u_{h\tau}(0) = 0.$$

3. *Galerkin orthogonality:*
$$\int_{I_n} (f_{h\tau}(t) - \partial_{tt} u_{h\tau}(t), v_h)_\Omega - (\nabla u_{h\tau}(t), \nabla v_h)_\Omega \mathrm{d}t = 0 \qquad \forall I_n \in \mathcal{T}_\tau(0,T), \ \forall v_h \in V_h^p.$$

Proof. 1. Regularity: Since for $I_n \in \mathcal{T}_\tau(0,T)$, $u_{h\tau} \in \mathcal{P}_3(I_n, V_h^p)$, we only need to show the continuity of $u_{h\tau}$ and $\partial_t u_{h\tau}$ at each t^n to prove that $u_{h\tau} \in \mathcal{C}^1(0,T;V_h^p)$. Let $n \in [\![1, N-1]\!]$, then for $t \in I_n$, we derive from the definition of $u_{h\tau}$ that:

$$\begin{aligned} \partial_t u_{h\tau}(t) = \dot{u}_h^{n-1} &+ \left(\ddot{u}_h^{n-1} - \frac{\tau}{2} \dddot{u}_h^{n-1} - \frac{\tau^2}{4} \ddddot{u}_h^{n-1} \right) \times (t - t^{n-1}) \\ &+ \left(\dddot{u}_h^{n-1} + \frac{\tau}{2} \ddddot{u}_h^{n-1} \right) \times (t - t^{n-1})^2. \end{aligned} \tag{3.5}$$

By (3.3) and (3.5), we have:

$$u_{h\tau|I_{n+1}}(t^n) = u_h^n + \frac{\tau^2}{12} \ddot{u}_h^n \quad \text{and} \quad \partial_t u_{h\tau|I_{n+1}}(t^n) = \dot{u}_h^n.$$

To show the regularity result, we only need to show that $u_{h\tau}|_{I_n}(t^n)$ and $\partial_t u_{h\tau}|_{I_n}(t^n)$ bear the same values. We do this by manipulating the definitions of the finite-difference time derivative formulas from (3.2):

$$\begin{aligned} u_{h\tau}|_{I_n}(t^n) &= \left(u_h^{n-1} + \frac{\tau^2}{12} \ddot{u}_h^{n-1} \right) + \tau \dot{u}_h^{n-1} + \frac{\tau^2}{2} \left(\ddot{u}_h^{n-1} - \frac{\tau}{2} \dddot{u}_h^{n-1} - \frac{\tau^2}{4} \ddddot{u}_h^{n-1} \right) \\ &\quad + \frac{2\tau^3}{6} \left(\dddot{u}_h^{n-1} + \frac{\tau}{2} \ddddot{u}_h^{n-1} \right) \\ &= \left(u_h^{n-1} + \tau \dot{u}_h^{n-1} + \frac{\tau^2}{2} \ddot{u}_h^{n-1} \right) + \left(\frac{\tau^2}{12} \ddot{u}_h^{n-1} + \frac{\tau^3}{12} \dddot{u}_h^{n-1} + \frac{\tau^4}{24} \ddddot{u}_h^{n-1} \right) \\ &= \frac{1}{2} \left(2u_h^{n-1} + u_h^n - u_h^{n-2} + u_h^n - 2u_h^{n-1} + u_h^{n-2} \right) \\ &\quad + \frac{\tau^2}{24} \left(2\ddot{u}_h^{n-1} + \ddot{u}_h^n - \ddot{u}_h^{n-2} + \ddot{u}_h^n - 2\ddot{u}_h^{n-1} + \ddot{u}_h^{n-2} \right) \\ &= u_h^n + \frac{\tau^2}{12} \ddot{u}_h^n, \end{aligned}$$

$$
\begin{aligned}
\partial_t u_{h\tau}|_{I_n}(t^n) &= \dot{u}_h^{n-1} + \tau\left(\ddot{u}_h^{n-1} - \frac{\tau}{2}\dddot{u}_h^{n-1} - \frac{\tau^2}{4}\ddddot{u}_h^{n-1}\right) + \tau^2\left(\dddot{u}_h^{n-1} + \frac{\tau}{2}\ddddot{u}_h^{n-1}\right) \\
&= \dot{u}_h^{n-1} + \tau\ddot{u}_h^{n-1} + \frac{\tau^2}{2}\dddot{u}_h^{n-1} + \frac{\tau^3}{4}\ddddot{u}_h^{n-1} \\
&= \dot{u}_h^{n-1} + \frac{\tau}{4}\left(4\ddot{u}_h^{n-1} + \ddot{u}_h^{n} - \ddot{u}_h^{n-2} + \ddot{u}_h^{n} - 2\ddot{u}_h^{n-1} + \ddot{u}_h^{n-2}\right) \\
&= \dot{u}_h^{n-1} + \frac{\tau}{2}\ddot{u}_h^{n} + \frac{\tau}{2}\ddot{u}_h^{n-1} \\
&= \frac{1}{2\tau}\left(u_h^n - u_h^{n-2} + u_h^{n+1} - 2u_h^n + u_h^{n-1} + u_h^n - 2u_h^{n-1} + u_h^{n-2}\right) \\
&= \frac{1}{2\tau}\left(u_h^{n+1} - u_h^{n-1}\right) \\
&= \dot{u}_h^n.
\end{aligned}
$$

2. Initial conditions: These are a direct result of the scheme (2.1) and the previously computed pointwise values of the reconstruction at $t = 0$:

$$
\begin{aligned}
\partial_t u_{h\tau}(0) &= \dot{u}_h^0 = \frac{1}{\tau}\left(u_h^1 - u_h^{-1}\right) \overset{(2.1b)}{=} 0, \\
u_{h\tau}(0) &= u_h^0 + \frac{\tau^2}{12}\ddot{u}_h^0 \overset{(2.1a)}{=} \frac{\tau^2}{12}\ddot{u}_h^0 \overset{(2.1a)\text{ and }(2.1c)}{=} \frac{\tau^2}{12}f_h^0.
\end{aligned}
$$

3. Galerkin orthogonality: Let $I_n \in \mathcal{T}_\tau(0,T)$. Recall that $\int_{I_n}(t-t^{n-1})^m \mathrm{d}t = \frac{\tau^{m+1}}{m+1}$ for $m \in \mathbb{N}$. Then there holds that:

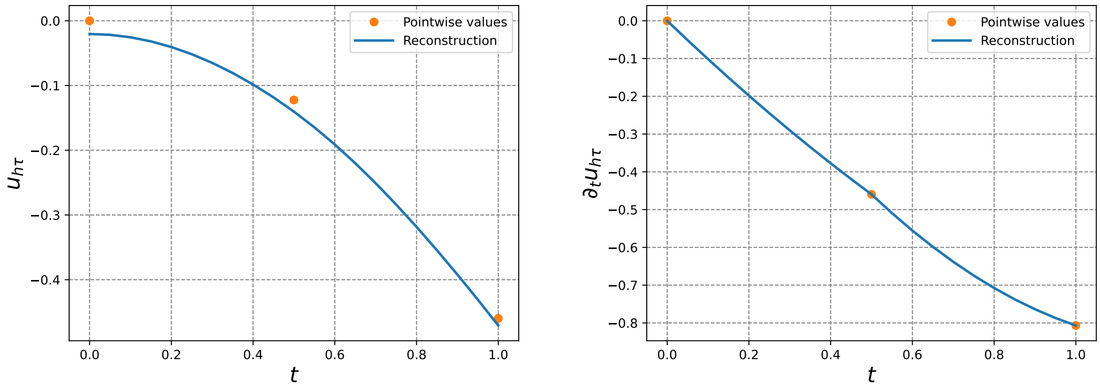
$$
\begin{aligned}
\int_{I_n} f_{h\tau}(t)\mathrm{d}t &= \frac{\tau}{2}(f_h^n + f_h^{n-1}), \\
\int_{I_n} \partial_{tt} u_{h\tau}(t)\mathrm{d}t &= \left[\partial_t u_{h\tau}\right]_{t^{n-1}}^{t^n} \overset{(3.4)}{=} \dot{u}_h^n - \dot{u}_h^{n-1} \\
&= \frac{1}{2\tau}\left(u_h^{n+1} - u_h^{n-1} - u_h^n + u_h^{n-2}\right) = \frac{\tau}{2}(\ddot{u}_h^n + \ddot{u}_h^{n-1}), \\
\int_{I_n} u_{h\tau}(t)\mathrm{d}t &= \tau\left(u_h^{n-1} + \frac{\tau^2}{12}\ddot{u}_h^{n-1}\right) + \frac{\tau^2}{2}\dot{u}_h^{n-1} \\
&\quad + \frac{\tau^3}{6}\left(\ddot{u}_h^{n-1} - \frac{\tau}{2}\dddot{u}_h^{n-1} - \frac{\tau^2}{4}\ddddot{u}_h^{n-1}\right) + \frac{2\tau^4}{24}\left(\dddot{u}_h^{n-1} + \frac{\tau}{2}\ddddot{u}_h^{n-1}\right) \\
&= \tau u_h^{n-1} + \frac{\tau^2}{2}\dot{u}_h^{n-1} + \frac{\tau^3}{4}\ddot{u}_h^{n-1} = \frac{\tau}{2}(u_h^n + u_h^{n-1}).
\end{aligned}
$$

Then for $v_h \in V_h^p$, there holds that:

$$
\int_{I_n} (f_{h\tau}(t) - \partial_{tt}u_{h\tau}(t), v_h)_\Omega - (\nabla u_{h\tau}(t), \nabla v_h)_\Omega \mathrm{d}t =
$$

$$
\frac{\tau}{2}\left(\underbrace{(f_h^{n-1} - \ddot{u}_h^{n-1}, v_h)_\Omega - (\nabla u_h^{n-1}, \nabla v_h)_\Omega}_{=0 \text{ by } (2.1c)} + \underbrace{(f_h^n - \ddot{u}_h^n, v_h)_\Omega - (\nabla u_h^n, \nabla v_h)_\Omega}_{=0 \text{ by } (2.1c)}\right)
$$

$\square$



(a) Reconstruction

(b) First derivative

Figure 1: Example of reconstruction from finite difference values of $t \mapsto \cos(t) - 1$.

Figure 1 shows an example of the reconstruction (blue lines) in time from pointwise values where $u_h^n = \cos(t^n) - 1$ (orange dots). As established, the reconstruction is $\mathcal{C}^1$-in-time, exactly takes the finite difference first derivative values (Figure 1b) on the sample points, but only approximates the function values (Figure 1a).

3.2 Vector-valued piecewise polynomial spaces and partition of unity

Recall that $p > 0$ is the polynomial order of the space discretisation and let $k > 0$ be the polynomial order in time. On the unit hypercube $\hat{K} = [0,1]^d$, we introduce, for $i \in [\![1, d]\!]$,

$$\mathcal{Q}^-_{p,i}(\hat{K}) := \operatorname{span}\left\{ \boldsymbol{x} \mapsto \prod_{j=1}^{d} x_j^{\alpha_j}, \text{ s.t. } \forall j \in [\![1,d]\!],\ \alpha_j \in \left| \begin{matrix} [\![1, p-1]\!] & \text{if } i = j \\ [\![1, p]\!] & \text{else} \end{matrix} \right. \right\}, \tag{3.6}$$

$$\mathcal{Q}^+_{p,i}(\hat{K}) := \operatorname{span}\left\{ \boldsymbol{x} \mapsto \prod_{j=1}^{d} x_j^{\alpha_j}, \text{ s.t. } \forall j \in [\![1,d]\!],\ \alpha_j \in \left| \begin{matrix} [\![1, p+1]\!] & \text{if } i = j \\ [\![1, p]\!] & \text{else} \end{matrix} \right. \right\}. \tag{3.7}$$

Then, the Raviart–Thomas space on the reference cell $\hat{K}$ is defined by [4, Remark 2.3.1, equation (2.4.1)] as

$$\boldsymbol{RT}_p(\hat{K}) := \begin{cases} \mathcal{P}_p(\hat{K})^d + \boldsymbol{x}\mathcal{P}_p(\hat{K}) & \text{if } \hat{K} \text{ is a simplex,} \\ \mathcal{Q}^+_{p,1}(\hat{K}) \times \mathcal{Q}^+_{p,2}(\hat{K}) \times \cdots \times \mathcal{Q}^+_{p,d}(\hat{K}) & \text{if } \hat{K} \text{ is a hypercube.} \end{cases}$$

It is defined on any cell $K \in \mathcal{T}_h(\Omega)$ by [4, Remark 2.3.1] as

$$\boldsymbol{RT}_p(K) := \frac{1}{\det \mathbf{J}_K} \mathbf{J}_K \boldsymbol{RT}_p(\hat{K}) \circ \boldsymbol{T}_K^{-1}.$$

The global $\boldsymbol{H}(\mathrm{div}, \Omega)$-conforming space and space-time approximation spaces are then

$$\begin{aligned} \boldsymbol{W}_h^p &:= \left\{ \boldsymbol{w}_h \in \boldsymbol{H}(\mathrm{div}, \Omega),\ \text{s.t. } \forall K \in \mathcal{T}_h(\Omega),\ \boldsymbol{w}_h|_K \in \boldsymbol{RT}_p(K) \right\}, \\ \boldsymbol{W}_{h\tau}^{pk} &:= \left\{ \boldsymbol{w}_{h\tau} \in L^2(0, T; \boldsymbol{H}(\mathrm{div}, \Omega)),\ \text{s.t. } \forall n \in [\![1, N]\!],\ \boldsymbol{w}_{h\tau}|_{I_n} \in \mathcal{P}_k(I_n; \boldsymbol{W}_h^p) \right\}. \end{aligned}$$

Partition of unity and local subdomains

Let $a \in \mathcal{S}_h(\Omega)$ be a mesh vertex. We introduce $\psi_a \in \mathcal{C}^0(\overline{\Omega})$, the hat function around a, such that for $K \in \mathcal{T}_h(\Omega)$,

$$\psi_a|_K \circ \boldsymbol{T}_K \in \begin{cases} \mathcal{P}_1(\hat{K}) & \text{if } \hat{K} \text{ is a simplex,} \\ \mathcal{Q}_1(\hat{K}) & \text{if } \hat{K} \text{ is a hypercube,} \end{cases}$$

and that for $a' \in \mathcal{S}_h(\Omega)$,

$$\psi_a(a') := \begin{cases} 1 & \text{if } a = a', \\ 0 & \text{else.} \end{cases}$$

Remarks:

- For $a \in \mathcal{S}_h(\Omega)$, ψ_a is in $U_h^1 \cap \mathcal{C}^0(\overline{\Omega})$ and if $a \in \mathcal{S}_h^{\text{int}}(\Omega)$, ψ_a is in V_h^1.
- The family of hat functions forms a partition of unity in the sense that

$$\sum_{a \in \mathcal{S}_h(\Omega)} \psi_a = 1.$$

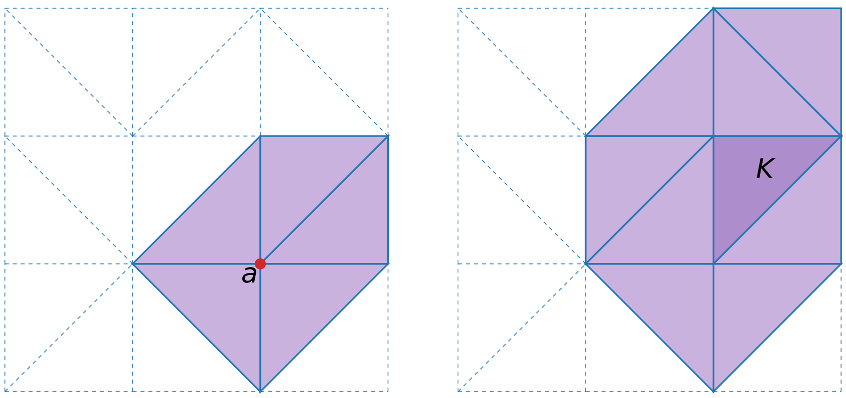
We define the local patch around a vertex $a \in \mathcal{S}_h(\Omega)$ as

$$\omega_a := \text{supp}(\psi_a) \text{ of diameter } h_{\omega_a} \text{ and } \quad \mathcal{T}_h(\omega_a) := \{K \in \mathcal{T}_h(\Omega), \text{ s.t. } K \subset \omega_a\}.$$

We define the local patch around an element $K \in \mathcal{T}_h(\Omega)$ as

$$\omega_K := \bigcup_{a \in \mathcal{S}_h(K)} \omega_a \quad \text{and} \quad \mathcal{T}_h(\omega_K) := \{K' \in \mathcal{T}_h(\Omega) \text{ s.t. } K' \subset \omega_K\}.$$

An example of such patches is given by Figure 2.



(a) Around a vertex $a \in \mathcal{S}_h(\Omega)$ (b) Around an element $K \in \mathcal{T}_h(\Omega)$

Figure 2: Examples of patches in a triangular mesh

3.3 Spatial flux reconstruction

Now that we have reconstructed a discrete approximation $u_{h\tau} \in Y_0$ of u (actually in $H^2(0,T;V_h^p)$), we want to obtain an approximation of ∇u in $L^2(0,T;\boldsymbol{H}(\mathrm{div},\Omega))$. We propose two ways to reconstruct fluxes by local procedures. The first is created with an inexpensive procedure (we just remove the non-conformity by local averaging like in [14, 28]), but does not give equilibrium. The second one, while computationally more expensive, is patchwise optimal (in a sense employed in Definition 3.5, similar to [5, 11, 15]), while also giving equilibrium.

Definition 3.4 (Averaged flux)**.** *Let $u_{h\tau} \in V_{h\tau}^{pk}$. We define the averaged flux $\boldsymbol{p}_{h\tau}^{\mathrm{avg}} \in \boldsymbol{W}_{h\tau}^{pk}$ such that for any $t \in (0,T)$ and $K \in \mathcal{T}_h(\Omega)$, there holds:*

$$\begin{cases} (\boldsymbol{p}_{h\tau}^{\mathrm{avg}}(t), \boldsymbol{z}_h)_K := -(\nabla u_{h\tau}(t), \boldsymbol{z}_h)_K & \forall \boldsymbol{z}_h \in \boldsymbol{Z}_h^p(K), \\ \boldsymbol{p}_{h\tau}^{\mathrm{avg}}(t)|_K \cdot \boldsymbol{n}_F := -\langle\!\langle \nabla u_{h\tau}(t) \cdot \boldsymbol{n}_F \rangle\!\rangle_F & \forall F \in \mathcal{F}_h(K), \end{cases}$$

with $\boldsymbol{Z}_h^p(K)$ a space that matches the local interior degrees of freedom of the Raviart–Thomas space:

$$\boldsymbol{Z}_h^p(K) := \mathbf{J}_K^{-T} \left\{ \begin{matrix} \mathcal{P}_{p-1}(\hat{K})^d & \text{if } \hat{K} \text{ is a simplex,} \\ \mathcal{Q}_{p,1}^-(\hat{K}) \times \mathcal{Q}_{p,2}^-(\hat{K}) \times \cdots \times \mathcal{Q}_{p,d}^-(\hat{K}) & \text{if } \hat{K} \text{ is a hypercube.} \end{matrix} \right\} \circ \boldsymbol{T}_K^{-1},$$

and with the interior averaging operator on any face F:

$$\langle\!\langle g_h \rangle\!\rangle_F := \begin{cases} g_h|_F & \text{if } F \in \mathcal{F}_h^{\mathrm{ext}}(\Omega), \\ \frac{1}{2}\left(g_h|_{K_1}|_F + g_h|_{K_2}|_F\right) & \text{if } F \in \mathcal{F}_h^{\mathrm{int}}(\Omega) \text{ shared by } K_1, K_2 \in \mathcal{T}_h(\Omega). \end{cases}$$

The flux reconstruction procedure in Definition 3.4 is illustrated in Figure 3. It is inspired by the one in [14, equations (5) and (6)] and [28, equation (4.1)] for simplices.

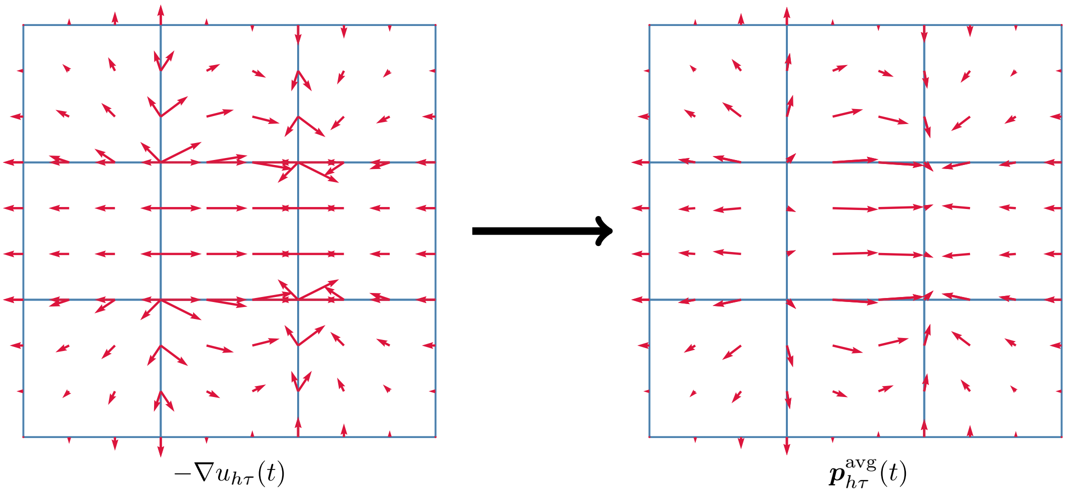


Figure 3: Construction of the averaged flux $\boldsymbol{p}_{h\tau}^{\mathrm{avg}}(t)$ from Definition 3.4

Definition 3.5 (Patchwise optimal equilibrated flux)**.** *Let $u_{h\tau} \in V_{h\tau}^{pk}$ and $f_{h\tau} \in U_{h\tau}^{pk}$ be such that:*

$$\int_{I_n} (f_{h\tau}(t) - \partial_{tt} u_{h\tau}(t), \psi_a)_\Omega - (\nabla u_{h\tau}(t), \nabla \psi_a)_\Omega \mathrm{d}t = 0 \quad \forall (a, I_n) \in \mathcal{S}_h^{\mathrm{int}}(\Omega) \times \mathcal{T}_\tau(0,T). \tag{3.8a}$$

For $(a, I_n) \in \mathcal{S}_h(\Omega) \times \mathcal{T}_\tau(0,T)$*, we define the patchwise optimal equilibrated local flux*

$$\boldsymbol{p}^{\text{equ}}_{h\tau,a}|_{I_n} := \operatorname{argmin} \Bigg\{ \sum_{K \in \mathcal{T}_h(\omega_a)} \frac{1}{h_K^2} ||\boldsymbol{q}_{h\tau} + \psi_a \nabla u_{h\tau}||^2_{K \times I_n}, \ \boldsymbol{q}_{h\tau} \in \boldsymbol{W}^{p+1,k}_{h\tau}|_{\omega_a \times I_n}$$
$$\text{with } \boldsymbol{q}_{h\tau} {\cdot} \boldsymbol{n} = 0 \text{ on } (\partial\omega_a \cap \{\psi_a = 0\}) \times I_n \text{ and}$$
$$\int_{I_n} (\operatorname{div} \boldsymbol{q}_{h\tau}(t) - \psi_a(f_{h\tau}(t) - \partial_{tt} u_{h\tau}(t)) + \nabla\psi_a \cdot \nabla u_{h\tau}(t), v_h)_{\omega_a} \, \mathrm{dt} = 0 \quad \forall v_h \in U_h^{p+1}|_{\omega_a} \Bigg\}. \tag{3.8b}$$

The global flux $\boldsymbol{p}^{\text{equ}}_{h\tau} \in \boldsymbol{W}^{p+1,k}_{h\tau}$ *is defined by*

$$\boldsymbol{p}^{\text{equ}}_{h\tau}|_{I_n} := \sum_{a \in \mathcal{S}_h(\Omega)} \boldsymbol{p}^{\text{equ}}_{h\tau,a}|_{I_n}, \quad \forall I_n \in \mathcal{T}_\tau(0,T). \tag{3.8c}$$

Remarks:

- Figure 4 shows an example of the local equilibration procedure of Definition 3.5. It consists in approximating the gradient in the best possible way in $\boldsymbol{H}(\text{div}, \omega_a)$ while keeping its divergence constrained to fit (1.1a). This is reflected by the equilibration property which follows from (3.8b):

$$\int_{I_n} (f_{h\tau}(t) - \partial_{tt} u_{h\tau}(t) - \operatorname{div} \boldsymbol{p}^{\text{equ}}_{h\tau}(t), v_h)_\Omega \, \mathrm{dt} = 0 \qquad \forall I_n \in \mathcal{T}_\tau(0,T), \ \forall v_h \in U_h^{p+1}. \tag{3.9}$$

- The flux reconstruction procedure in Definition 3.5 is inspired by the one in [15, Definition 4.1]. The main difference is that while [15, Definition 4.1] equilibrates the flux in a strong space-time manner, (3.8b) only does it strongly in space and in average in time due to the weaker assumption on the discrete solution $u_{h\tau}$ in (3.8a).

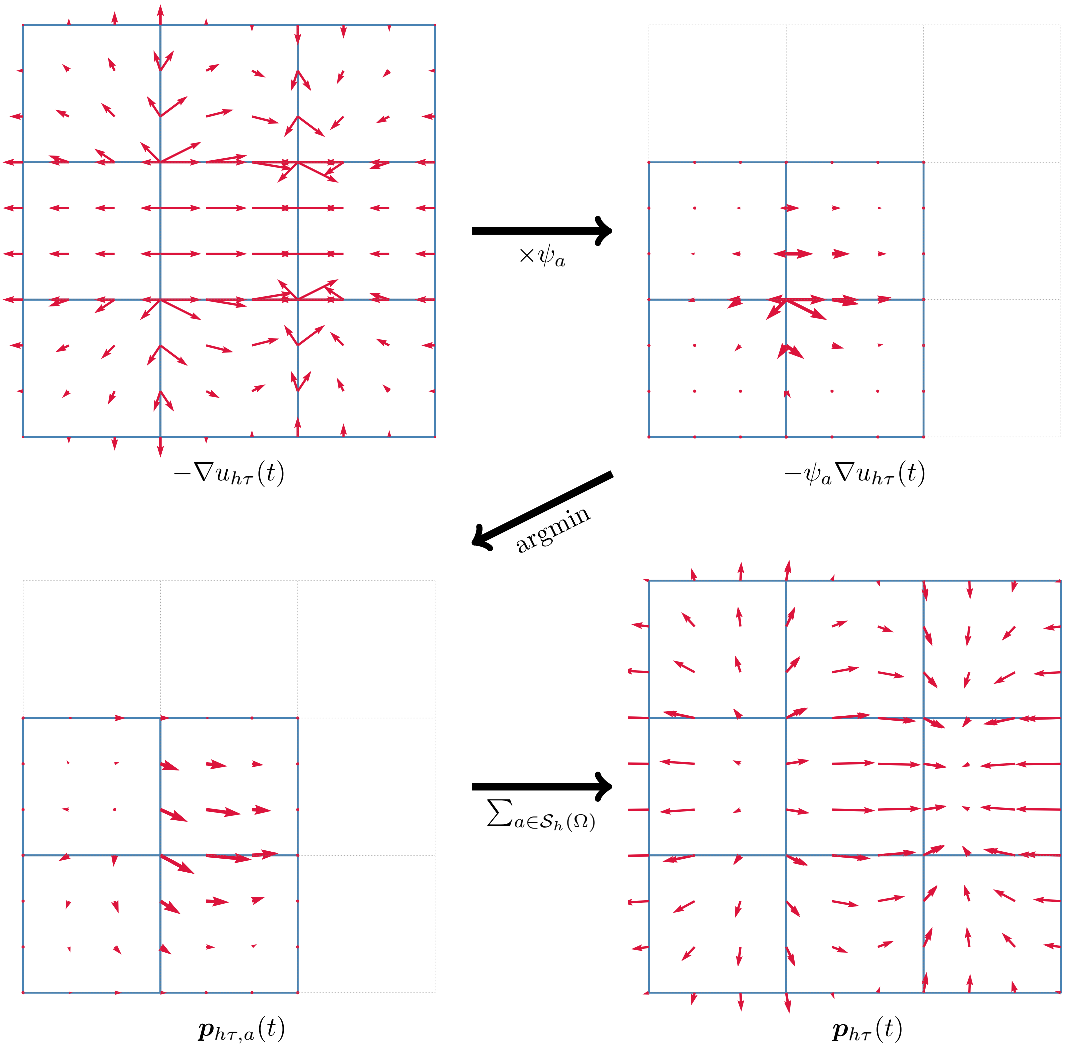


Figure 4: Construction of the patchwise optimal equilibrated flux $\boldsymbol{p}_{h\tau}^{\mathrm{equ}}(t)$ from Definition 3.5

4 Guaranteed and locally space-time efficient *a posteriori* estimates

In this section, we present our *a posteriori* error estimates.

Definition 4.1 (Estimators)**.** *Let $(u_h^n)_{n\in[\![-1,N+1]\!]}$ be the discrete solution given by the leapfrog scheme (2.1), for $f_h^0 = 0$. Let $u_{h\tau}$ be the reconstructed discrete solution from Definition 3.2, $f_{h\tau}$ the approximate source term from Definition 3.1, and $(K, I_n) \in \mathcal{T}_{h\tau}(Q)$ a space-time mesh* *element. We define the local residual-based estimator as*

$$\begin{aligned}\eta^{\mathrm{R,res}}_{K\times I_n} &:= c^{\mathrm{R,res}} h_K \|f_{h\tau} - \partial_{tt} u_{h\tau} + \Delta u_{h\tau}\|_{K\times I_n},\\ (\eta^{\mathrm{J,res}}_{K\times I_n})^2 &:= (c^{\mathrm{J,res}})^2 \sum_{F\in\mathcal{F}_h(K)\cap\mathcal{F}_h^{\mathrm{int}}(\Omega)} h_K \|[\![\nabla u_{h\tau}\cdot \boldsymbol{n}_F]\!]\|^2_{F\times I_n}.\end{aligned} \tag{4.1}$$

For $\star \in \{\mathrm{avg}, \mathrm{equ}\}$, we define the local estimator based on $\boldsymbol{p}^\star_{h\tau}$ respectively from Definitions 3.4 and 3.5 as

$$\begin{aligned}\eta^{\mathrm{R},\star}_{K\times I_n} &:= c^{\mathrm{R},\star}_K h_K \|f_{h\tau} - \partial_{tt} u_{h\tau} - \operatorname{div} \boldsymbol{p}^\star_{h\tau}\|_{K\times I_n},\\ \eta^{\mathrm{J},\star}_{K\times I_n} &:= \|\boldsymbol{p}^\star_{h\tau} + \nabla u_{h\tau}\|_{K\times I_n}.\end{aligned} \tag{4.2}$$

Here $c^{\mathrm{R,equ}}_K = \frac{1}{\pi}$ whereas the constants $c^{\mathrm{R,avg}}_K$, $c^{\mathrm{R,res}}$, and $c^{\mathrm{J,res}}$ can only depend on the space dimension d and the shape-regularity of the space mesh $\mathcal{T}_h(\Omega)$. $c^{\mathrm{R,res}}$ and $c^{\mathrm{J,res}}$ can possibly also depend on the polynomial orders p and k.

For $\star \in \{\mathrm{res}, \mathrm{avg}, \mathrm{equ}\}$, we also denote the global estimators as:

$$(\eta^{\mathrm{R},\star}_Q)^2 := \sum_{(K,I_n)\in\mathcal{T}_{h\tau}(Q)} (\eta^{\mathrm{R},\star}_{K\times I_n})^2 \quad \text{and} \quad (\eta^{\mathrm{J},\star}_Q)^2 := \sum_{(K,I_n)\in\mathcal{T}_{h\tau}(Q)} (\eta^{\mathrm{J},\star}_{K\times I_n})^2, \tag{4.3}$$

and the local and global aggregate estimators as:

$$\eta^\star_{K\times I_n} := \eta^{\mathrm{R},\star}_{K\times I_n} + \eta^{\mathrm{J},\star}_{K\times I_n} \quad \text{and} \quad \eta^\star_Q := \eta^{\mathrm{R},\star}_Q + \eta^{\mathrm{J},\star}_Q. \tag{4.4}$$

Theorem 4.2 (Reliable and locally space-time efficient *a posteriori* estimates)**.** *Let u be the weak solution of (2.6) and let the hypotheses of Definition 4.1 be satisfied. Then for $\star \in \{\mathrm{res}, \mathrm{avg}, \mathrm{equ}\}$, the estimators from above $\eta^\star$ verify the following properties:*

- ***Global space-time reliability**:*

$$\|u - u_{h\tau}\|_{\mathcal{Y}_0} \le \|f - f_{h\tau}\|_{Y'_T} + \eta^\star_Q. \tag{4.5a}$$

- ***Local space-time efficiency**: For $(K, I_n) \in \mathcal{T}_{h\tau}(Q)$,*

$$\eta^\star_{K\times I_n} \lesssim \|u - u_{h\tau}\|_{\mathcal{Y}_0,\omega_K\times I_n} + \|f - f_{h\tau}\|_{Y'_T,\omega_K\times I_n}. \tag{4.5b}$$

- ***Global space-time efficiency**:*

$$\eta^\star_Q \lesssim \|u - u_{h\tau}\|_{\mathcal{Y}_0} + \|f - f_{h\tau}\|_{Y'_T}. \tag{4.5c}$$

Here $\lesssim$ means up to a constant that only depends on the space dimension d, the polynomial orders p and k, the shape-regularity of the space mesh $\mathcal{T}_h(\Omega)$, and the CFL constant $\frac{\tau}{h}$.

Proof. This theorem is a direct application of the general Theorem 6.3 below, the hypotheses of which are verified by Lemma 3.3. Here, we use the simplified assumptions of Sections 2 to 5 where for all elements (K, I_n) of the space-time mesh $\mathcal{T}_{h\tau}(Q)$, there holds that $(h_K, \tau_n) = (h, \tau)$ with $\tau = c_{\mathrm{CFL}} h$. To get to Theorem 4.2, one only needs to multiply the result from Theorem 6.3 by h. ☐

5 Numerical illustration

In this section, we illustrate the reliability and local space-time efficiency results from Theorem 4.2 using numerical experiments. We anticipate that the equilibrated flux-based estimator should provide a better estimate of the error compared to the averaged flux-based estimator, though we find that both deliver very close results. In turn, the residual-based estimator (not implemented) would feature multiplicative factors the exact values of which are unknown.

5.1 Configuration

Let $\Omega = [0,1] \times [0,2]$, $T = 5$, a source term $f = (t, \boldsymbol{x}) \mapsto f_T(t) f_X(\boldsymbol{x})$ with:

$$f_T(t) = -\sin(4\pi(t-1)) \times e^{-\left(\frac{t-1}{0.1}\right)^2} \quad \text{and} \quad f_X(\boldsymbol{x}) = \exp\left(-\frac{(x_1-0.5)^2 + (x_2-1.5)^2}{0.1^2}\right).$$

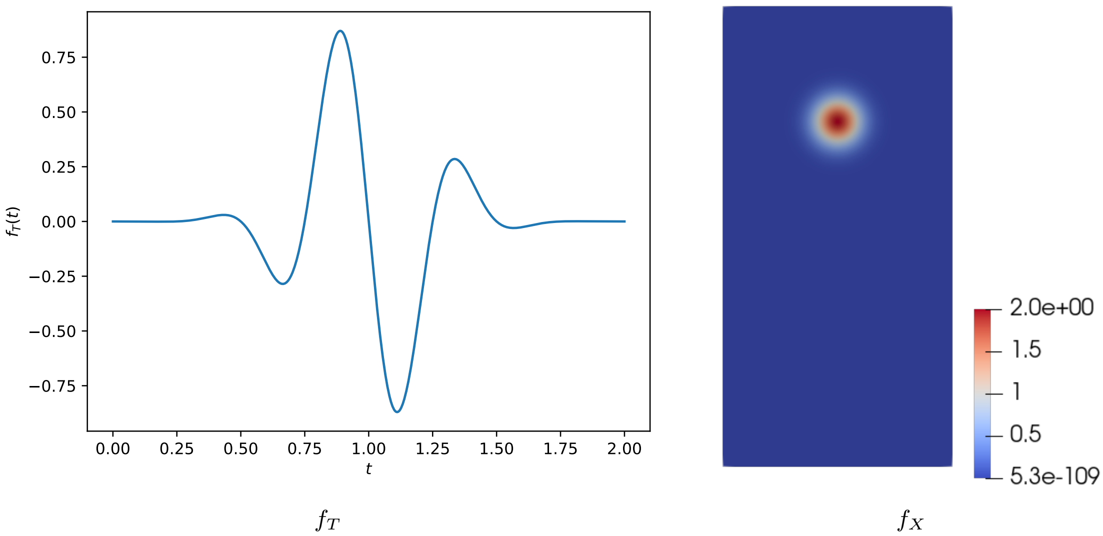
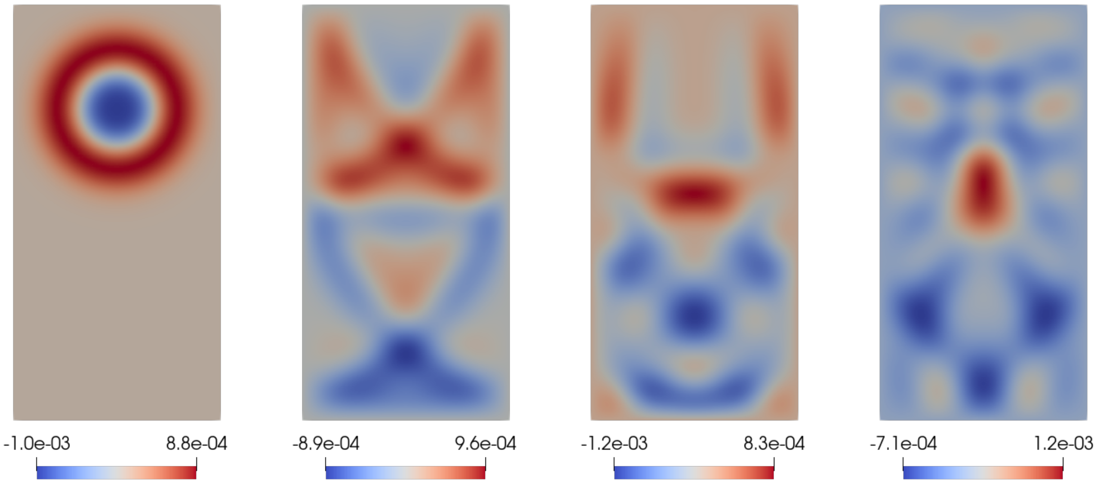


Figure 5: Time and space components of the source term f for the numerical experiments

The numerical approximation is computed using fourth-order spectral finite elements ($p = 4$ on quadrangles) with the leapfrog time stepping scheme (2.1). We use the finite element kernel of the `CIVA` platform [8] for the simulations. The inner products $(\cdot,\cdot)_\Omega$ and $(\nabla\cdot,\nabla\cdot)_\Omega$ are represented by the discrete operators $\mathbb{M}_h$ and $\mathbb{K}_h$. Here, the time stepping also includes mass lumping (the influence of which is ignored here), which means that $\mathbb{M}_h$ and $\mathbb{K}_h$ are approximated using well-chosen quadrature formulae [9, 22] to ensure that $\mathbb{M}_h$ is diagonal. Whenever a time step is not specified, an approximation of the following CFL time step is used, ensuring numerical stability of the leapfrog scheme:

$$\tau_{\mathrm{CFL}} = \frac{2}{\sqrt{\rho(\mathbb{M}_h^{-1}\mathbb{K}_h)}},$$

where ρ is the spectral radius (numerically evaluated using the power iteration algorithm). [21, Equation (51) and remarks below] shows that $\tau_{\mathrm{CFL}} = O(h)$. Figure 6 shows a few snapshots of the numerical approximation.



$t \approx 1.2$ $t \approx 2.4$ $t \approx 3.6$ $t \approx 4.8$

Figure 6: Discrete solution of the test case for different times t

We compare our estimators to an approximation of the error built by comparing $u_{h\tau}$ to a refined discrete solution $u_{h'\tau'}$ computed on a fine mesh $\mathcal{T}_{h'\tau'}(Q)$ with at least $\tau' \leq \frac{1}{10}\tau$ and $h' \leq \frac{1}{2}h$. Moreover, we do not compute the $\mathcal{Y}_0$ dual norm which is difficult to evaluate. Instead, we use the $H^1(Q)$ semi-norm as in [12]. By (2.10) we in particular have

$$||u - u_{h\tau}||_{\mathcal{Y}_0} \leq |u - u_{h\tau}|_{H^1(Q)} \approx |u_{h'\tau'} - u_{h\tau}|_{H^1(Q)}.$$

For any $(K, I_n) \in \mathcal{T}_{h\tau}(Q)$, the elementwise error is then approximated by

$$e_{K\times I_n} := |u_{h'\tau'} - u_{h\tau}|_{H^1(K\times I_n)} = \sqrt{||\partial_t(u_{h'\tau'} - u_{h\tau})||^2_{K\times I_n} + ||\nabla(u_{h'\tau'} - u_{h\tau})||^2_{K\times I_n}}. \quad (5.1)$$

5.2 Results

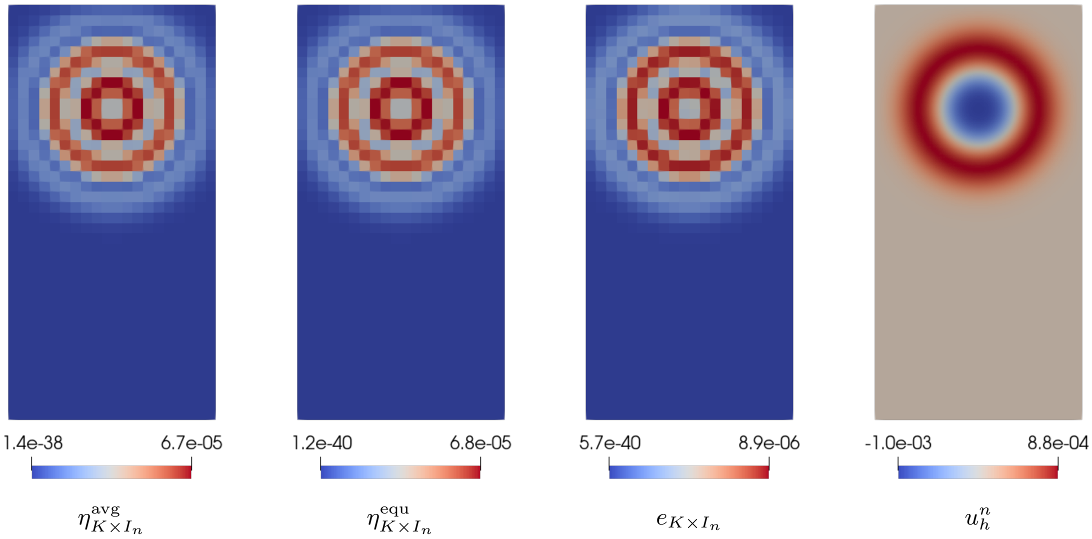


Figure 7: Elementwise error, and approximate solution for $h = 0.05$ and $\tau = \tau_{\text{CFL}}$ at $t \approx 1.2$.

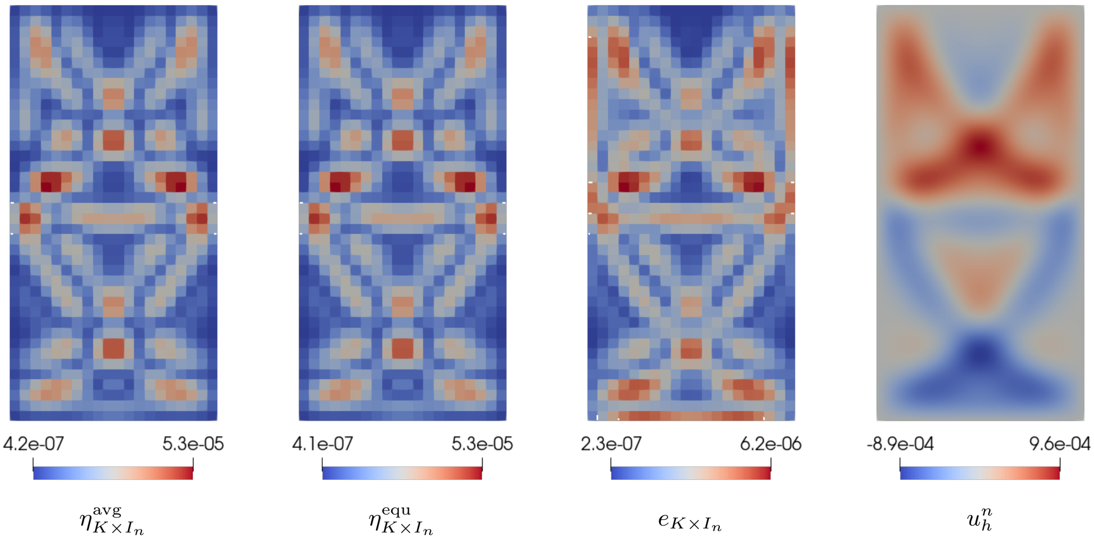
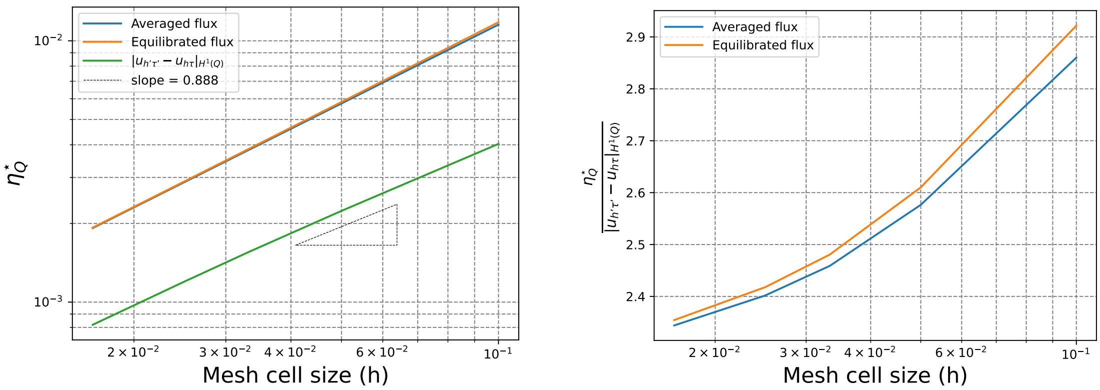


Figure 8: Elementwise error, and approximate solution for $h = 0.05$ and $\tau = \tau_{\text{CFL}}$ at $t \approx 2.4$.

Figures 7 and 8 show snapshots of elementwise values of the flux estimators from Definition 4.1, the approximate error (5.1), and the discrete solution. The error maps show the space-time local estimators from (4.4). In particular, both flux estimators yield similar results in terms of value and distribution. The theoretical result of local space-time efficiency (4.5b) implies that where the estimators predict the existence of discretisation error, it effectively is present. The result still holds despite the error not being computed for u and in the theoretically applied dual norm.

In what follows, we show figures presenting the global values of the estimators. To evaluate their sharpness, we also present the effectivity indices, *i.e.*, the estimators divided by the approximate error. The closer the effectivity index is to 1, the closer the estimator is to the error.

Figure 9 shows both the values and the effectivity indices of the global estimates over the space-time domain Q, as a function of the space mesh cell size h (recall that τ is $O(h)$, allowing to use h as the unique parameter). Figure 9a shows that the estimators have the same convergence as the error. Figure 9b confirms this by showing that the effectivity indices stay bounded when h decreases. In this particular example, the effectivity indices are in the range $[2.3, 3]$, which we find particularly precise.

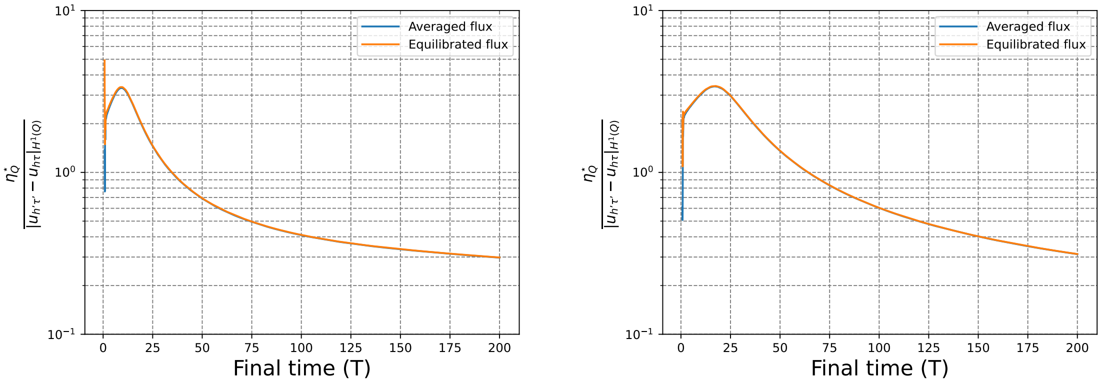


(a) Global estimator value

(b) Global estimator effectivity index

Figure 9: Global estimators and their effectivity indices depending on the mesh step size h ($\tau = \tau_{\mathrm{CFL}}$, $T = 5$)

Figure 10 shows the effectivity index when changing the final time T for a given discretisation step h. This illustrates the fact that the effectivity indices do not vary much when the final time increases, as implied by the theory (the constant hidden in (4.5c) does not depend on T). We observe effectivity indices lower than 1, but this is not in contradiction with the theory. Indeed, Theorem 4.2 states the reliability and efficiency results while quantifying the error using $||u - u_{h\tau}||_{\mathcal{Y}_0}$ and not $|u_{h'\tau'} - u_{h\tau}|_{H^1(Q)}$ like here. Despite that, the effectivity indices stay around 1 even for time windows longer by orders of magnitude.



(a) Global estimator effectivity for $h = 0.1$

(b) Global estimator effectivity for $h = 0.05$

Figure 10: Effectivity indices of the global estimators depending on the final time T ($\tau = \tau_{\text{CFL}}$)

Performance was not prioritised in our testing implementation, so a rigorous comparison of estimator evaluation times cannot be conducted. Nevertheless, the equilibrated flux-based estimator incurs a significant computational cost overhead when compared to the industrial-grade spectral finite-element solver with explicit time stepping employed here. The averaged flux-based estimator gives numerical results of similar quality with a milder overhead, on par with the simulation time itself.

6 Abstract framework for guaranteed and locally space-time efficient *a posteriori* estimates

In this section, we present an abstract framework which in particular covers the results of the simplified setting in Sections 2 to 5.

6.1 Generalised space-time setting of Steinbach and Zank

We keep the functional setting from [26], where the authors derive an inf − sup stable formulation of the acoustic wave equation (1.1). Let $Q_- := (-T, T) \times \Omega$ be the extended space-time domain and $\Box : L^2(Q) \longrightarrow \mathcal{C}_0^\infty(Q_-)'$ the extended d'Alembert operator defined such that for $u \in L^2(Q)$ and $\phi \in \mathcal{C}_0^\infty(Q_-)$,

$$\langle \Box u, \phi \rangle := (u, \partial_{tt}\phi - \Delta\phi)_Q \,.$$

The authors in [26] introduce the Banach space

$$\mathcal{H}(Q) = \left\{ v \in L^2(Q), \text{ s.t. } \Box v \in H_0^1(Q_-)' \right\} \quad \text{with} \quad ||\cdot||^2_{\mathcal{H}(Q)} := ||\cdot||^2_Q + ||\Box \cdot||^2_{H_0^1(Q_-)'}.$$

Then by completion, they define

$$\mathcal{Y}_0 := \left\{ v \in \mathcal{H}(Q), \text{ s.t. } \exists (v_i)_{i\in\mathbb{N}} \subset Y_0, \ ||v - v_i||_{\mathcal{H}(Q)} \underset{i\to\infty}{\longrightarrow} 0 \right\}. \tag{6.1}$$

The previous simplified weak formulation (2.6) is generalised for any source term $f \in Y_T'$ as:

$$\text{find } u \in \mathcal{Y}_0 \text{ such that } \langle \Box u, \mathcal{E}v \rangle_{H_0^1(Q_-)} = \langle f, v \rangle_{Y_T} \quad \forall \in Y_T \tag{6.2}$$

where $\mathcal{E} : Y_T \longrightarrow H_0^1(Q_-)$ is any continuous and injective extension operator. [26, equation (3.11)] also shows that for $f \in L^2(Q)$, there holds that $u \in Y_0$ and

$$\langle \Box u, \mathcal{E}v \rangle_{H_0^1(Q_-)} = -(\partial_t u, \partial_t v)_Q + (\nabla u, \nabla v)_Q = (f, v)_Q \qquad \forall v \in Y_T.$$

Therefore, if we assume that $f \in L^2(Q)$, the weak formulation and the residual stay the same as before, in (2.6) and (2.7). In this case, the well-posedness of (2.6) in this new setting comes from [26, Theorem 3.9] which in turn is possible because [26, Lemma 3.4] shows that the generalised bilinear form defines a norm for $\mathcal{Y}_0$ (inf − sup stability) [26, Equation (3.10)]:

$$||\cdot||_{\mathcal{Y}_0} := ||\Box \cdot||_{H_0^1(Q_-)'} = \sup_{v \in Y_T \setminus \{0\}} \frac{\langle \Box \cdot, \mathcal{E}v \rangle_{H_0^1(Q_-)}}{|v|_{H^1(Q)}}.$$

6.2 Space-time anisotropic meshes and norms

Now that that the variationnal setting is set, we still need to address the issue that $|\cdot|_{H^1(Q)}$, as a norm over Y_T, does not have a coherent scaling of the time and space derivatives (there are in different physical units). This lack of appropriate scaling would also cause problems later when showing the efficiency (constants that depend on the anisotropy of the space-time mesh would arise). We follow the methodology of [12] and we introduce the following equivalent norm on Y_T:

$$|||\cdot|||_{Y_T}^2 := \sum_{(K,I_n) \in \mathcal{T}_{h\tau}(Q)} |||\cdot|||_{Y_T,K\times I_n}^2 \tag{6.3a}$$

with

$$|||\cdot|||_{Y_T,K\times I_n}^2 := \tau_n^2 ||\partial_t \cdot||_{K\times I_n}^2 + h_K^2 ||\nabla \cdot||_{K\times I_n}^2, \quad \forall (K, I_n) \in \mathcal{T}_{h\tau}(Q). \tag{6.3b}$$

We also update the dual norms for Y_T' and $\mathcal{Y}_0$ (in both local and global forms) such that for any interval $I \subset (0, T)$ and subdomain $\omega \subset \Omega$ either a mesh cell or a patch of mesh cells,

$$|||\cdot|||_{Y_T',\omega\times I} := \sup_{\substack{v \in Y_T \setminus \{0\} \\ \mathrm{supp}(v) \subset \omega \times I}} \frac{\langle \cdot, v \rangle_{Y_T}}{|||v|||_{Y_T}} \qquad \text{and} \qquad |||\cdot|||_{Y_T'} := |||\cdot|||_{Y_T',Q}. \tag{6.3c}$$

Then, the local and global norms of the error become

$$|||u - u_{h\tau}|||_{\mathcal{Y}_0,\omega\times I} := |||r(u_{h\tau})|||_{Y_T',\omega\times I} \qquad \text{and} \qquad |||u - u_{h\tau}|||_{\mathcal{Y}_0} := |||r(u_{h\tau})|||_{Y_T'}. \tag{6.3d}$$

6.3 Estimators

The residual-based *a posteriori* error estimator stays similar to (4.1), up to the scaling implied by the one in (6.3).

Definition 6.1 (Residual-based *a posteriori* estimator)**.** *Let $f_{h\tau} \in U_{h\tau}^{pk}$ and $u_{h\tau} \in V_{h\tau}^{pk}$. The local residual-based estimators for $(K, I_n) \in \mathcal{T}_{h\tau}(Q)$ are defined as*

$$\begin{aligned} \eta_{K\times I_n}^{\mathrm{R,res}} &:= c^{\mathrm{R,res}} ||f_{h\tau} - \partial_{tt} u_{h\tau} + \Delta u_{h\tau}||_{K\times I_n}, \\ (\eta_{K\times I_n}^{\mathrm{J,res}})^2 &:= \frac{(c^{\mathrm{J,res}})^2}{h_K} \sum_{F \in \mathcal{F}_h(K) \cap \mathcal{F}_h^{\mathrm{int}}(\Omega)} |||[\![\nabla u_{h\tau} \cdot \boldsymbol{n}_F]\!]|||_{F\times I_n}^2, \end{aligned} \tag{6.4}$$

with $c^{\mathrm{R,res}}$ and $c^{\mathrm{J,res}}$ two positive constants that can only depend on the space dimension d, the polynomial orders p and k, and the shape-regularity of $\mathcal{T}_h(\Omega)$.

Let the averaged and equilibrated fluxes be respectively given by Definitions 3.4 and 3.5. We again rescale (4.2) appropriately.

Definition 6.2 (Flux-based *a posteriori* estimators)**.** *Let $f_{h\tau} \in U_{h\tau}^{pk}$, $u_{h\tau} \in V_{h\tau}^{pk}$, $\star \in \{\mathrm{avg}, \mathrm{equ}\}$, and $\boldsymbol{p}_{h\tau}^\star$ from Definitions 3.4 and 3.5. Then the local estimators based on $\boldsymbol{p}_{h\tau}^\star$ for $(K, I_n) \in \mathcal{T}_{h\tau}(Q)$ are defined as*

$$\eta_{K\times I_n}^{\mathrm{R},\star} := c_K^{\mathrm{R},\star} ||f_{h\tau} - \partial_{tt} u_{h\tau} - \operatorname{div} \boldsymbol{p}_{h\tau}^\star||_{K\times I_n} \quad \text{and} \quad \eta_{K\times I_n}^{\mathrm{J},\star} := \frac{1}{h_K} ||\boldsymbol{p}_{h\tau}^\star + \nabla u_{h\tau}||_{K\times I_n}. \tag{6.5}$$

Here, for a mesh vertex $a \in \mathcal{S}_h(\Omega)$, $c_{\mathrm{P},a}$ is the Poincaré constant on ω_a such that for all $v \in H_0^1(\Omega)$,

$$||v - \bar{v}_a||_{\omega_a} \leq c_{\mathrm{P},a} h_{\omega_a} ||\nabla v||_{\omega_a} \quad \text{with } \bar{v}_a = \begin{cases} \frac{1}{|\omega_a|}(v, 1)_{\omega_a} & \text{if } a \in \mathcal{S}^{\mathrm{int}}(\Omega), \\ 0 & \text{if } a \in \mathcal{S}^{\mathrm{ext}}(\Omega), \end{cases} \tag{6.6}$$

and

$$c_K^{\mathrm{R,avg}} := \sqrt{\max_{K\in\mathcal{T}_h(\Omega)} \sum_{a\in\mathcal{S}_h(K)} \frac{c_{\mathrm{P},a}^2 h_{\omega_a}^2}{h_K^2}} \quad \text{and} \quad c_K^{\mathrm{R,equ}} := \frac{1}{\pi}.$$

6.4 Reliability and space-time local efficiency

Theorem 6.3 (Reliable and locally space-time efficient a posteriori estimates)**.** *Let the assumptions from Definitions 6.1 and 6.2 be satisfied and let u be the weak solution of (1.1) in the sense of (2.6). Let additionally $u_{h\tau}$ be in $H^2(0, T; V_h^p)$ such that $\partial_t u_{h\tau}(0) = 0$ and that for all $(a, I_n) \in \mathcal{S}_h^{\mathrm{int}}(\Omega) \times \mathcal{T}_\tau(0, T)$,*

$$\int_{I_n} (f_{h\tau}(t) - \partial_{tt} u_{h\tau}(t), \psi_a)_\Omega - (\nabla u_{h\tau}(t), \nabla \psi_a)_\Omega \mathrm{d}t = 0, \tag{6.7}$$

such as $u_{h\tau}$ from Definition 3.2. Then, for $\star \in \{\mathrm{res}, \mathrm{avg}, \mathrm{equ}\}$, $\eta^\star$ given from (6.4) and (6.5) by (4.3) and (4.4), verify the following properties:

- ***Global space-time reliability**:*

$$|||u - u_{h\tau}|||_{\mathcal{Y}_0} \leq |||f - f_{h\tau}|||_{Y_T'} + \eta_Q^\star. \tag{6.8a}$$

- ***Local space-time efficiency**: For $(K, I_n) \in \mathcal{T}_{h\tau}(Q)$,*

$$\eta_{K\times I_n}^\star \lesssim |||u - u_{h\tau}|||_{\mathcal{Y}_0, \omega_K\times I_n} + |||f - f_{h\tau}|||_{Y_T', \omega_K\times I_n}. \tag{6.8b}$$

- ***Global space-time efficiency**:*

$$\eta_Q^\star \lesssim |||u - u_{h\tau}|||_{\mathcal{Y}_0} + |||f - f_{h\tau}|||_{Y_T'}. \tag{6.8c}$$

Here, $\lesssim$ means up to a constant that only depends on the space dimension d, the polynomial orders p and k, and the shape-regularity of $\mathcal{T}_h(\Omega)$.

Proof. This theorem is proven in Section 8. □

7 Reliability and efficiency results

The goal of this section is to establish the building blocks for the proof of Theorem 6.3 in Section 8. We first show reliability when using $\boldsymbol{H}(\mathrm{div})$ fluxes in Section 7.1, using Parger–Synge-type inequalities. Then, we prove the space-time efficiency of residual-based terms in Sections 7.2 and 7.3, using well-chosen finite-dimensional bubble functions following the methodology in [12, 27]. To be able to show both the reliability of the residual-based estimator and the efficiency of the flux-based estimators, we prove that the flux-based estimators are locally bounded from above by the residual-based ones. We show in Section 7.4 that this is a direct application of existing results (from [12]) for the averaged flux. For the patchwise optimal equilibrated flux, we first introduce a space-time decoupling (similar to [15]) in Section 7.5 before recalling existing results to show the boundedness of the estimator by residual terms in Section 7.6.

7.1 Reliability using $\boldsymbol{H}(\mathrm{div})$ fluxes

A key tool we use to show the reliability of flux-based estimators is the scaled local space-time Poincaré inequality found in [12, Lemma 2.2]. We recall it here in the two specific cases we use in this section.

Lemma 7.1 (Scaled local space-time Poincaré inequality)**.**

- ***On elements****: Let $(K, I_n) \in \mathcal{T}_{h\tau}(Q)$ and $v \in H^1(K \times I_n)$. Let $\bar{v}_{K\times I_n}$ be the average of v on $K \times I_n$. Then, there holds*

$$||v - \bar{v}_{K\times I_n}||^2_{K\times I_n} \leq \frac{1}{\pi^2}|||v|||^2_{Y_T,K\times I_n}. \tag{7.1}$$

- ***On patches****: Let $I_n \in \mathcal{T}_\tau(0,T)$ and $a \in \mathcal{S}_h(\Omega)$. Let $v \in Y_T$ and let $c_{\mathrm{P},a}$ be defined in (6.6). Then, with*

$$\bar{v}_{\omega_a\times I_n} := \begin{cases} \frac{1}{|\omega_a\times I_n|}(v,1)_{\omega_a\times I_n} & \text{if } a \in \mathcal{S}^{\mathrm{int}}(\Omega) \\ 0 & \text{if } a \in \mathcal{S}^{\mathrm{ext}}(\Omega) \end{cases},$$

there holds

$$||v - \bar{v}_{\omega_a\times I_n}||^2_{\omega_a\times I_n} \leq c^2_{\mathrm{P},a}\left(\tau_n^2||\partial_t v||^2_{\omega_a\times I_n} + h^2_{\omega_a}||\nabla v||^2_{\omega_a\times I_n}\right). \tag{7.2}$$

Lemma 7.2 (Guaranteed upper bound for elementwise equilibration in space)**.** *Let $f \in L^2(Q)$, $f_{h\tau} \in L^2(Q)$, $u_{h\tau} \in Y_0 \cap H^2(0,T;L^2(\Omega))$ such that $\partial_t u_{h\tau}(0) = 0$, and a flux $\boldsymbol{p}_{h\tau} \in L^2(0,T;\boldsymbol{H}(\mathrm{div},\Omega))$ such that*

$$\int_{I_n}(f_{h\tau}(t) - \partial_{tt}u_{h\tau}(t) - \mathrm{div}\,\boldsymbol{p}_{h\tau}(t), 1)_K \mathrm{d}t = 0 \quad \forall (K, I_n) \in \mathcal{T}_{h\tau}(Q) \tag{7.3}$$

be given. Then

$$|||u - u_{h\tau}|||_{\mathcal{Y}_0} \leq |||f - f_{h\tau}|||_{Y_T'} + \sqrt{\sum_{(K,I_n)\in\mathcal{T}_{h\tau}(Q)} \frac{1}{h_K^2}||\boldsymbol{p}_{h\tau} + \nabla u_{h\tau}||^2_{K\times I_n}}$$
$$+ \frac{1}{\pi}\sqrt{\sum_{(K,I_n)\in\mathcal{T}_{h\tau}(Q)} ||f_{h\tau} - \partial_{tt}u_{h\tau} - \mathrm{div}\,\boldsymbol{p}_{h\tau}||^2_{K\times I_n}}.$$

Proof. Denote $\xi_{\mathrm{R}} := f_{h\tau} - \partial_{tt} u_{h\tau} - \operatorname{div} \boldsymbol{p}_{h\tau} \in L^2(Q)$ and $\boldsymbol{\xi}_{\mathrm{J}} := \boldsymbol{p}_{h\tau} + \nabla u_{h\tau} \in L^2(Q)^d$ and let $v \in Y_T$. Recall from (6.3d) that $|||u - u_{h\tau}|||_{\mathcal{Y}_0} = |||r(u_{h\tau})|||_{Y_0'}$. Then we only need to bound $|||r(u_{h\tau})|||_{Y_0'}$. Since $\partial_t u_{h\tau} \in H^1(0,T;L^2(\Omega))$ with $\partial_t u_{h\tau}(0) = 0$ and $\boldsymbol{p}_{h\tau} \in L^2(0,T;\boldsymbol{H}(\operatorname{div},\Omega))$, by integration by parts, there holds

$$\begin{aligned}\langle r(u_{h\tau}), v\rangle_{Y_T} &\overset{(2.7)}{=} (f,v)_Q + (\partial_t u_{h\tau}, \partial_t v)_Q - (\nabla u_{h\tau}, \nabla v)_Q \\ &= (f - f_{h\tau}, v)_Q + (\underbrace{f_{h\tau} - \partial_{tt} u_{h\tau} - \operatorname{div} \boldsymbol{p}_{h\tau}}_{\xi_{\mathrm{R}}}, v)_Q - (\underbrace{\boldsymbol{p}_{h\tau} + \nabla u_{h\tau}}_{\boldsymbol{\xi}_{\mathrm{J}}}, \nabla v)_Q.\end{aligned}$$

Using (6.3c), the first term is bounded by $(f - f_{h\tau}, v)_Q \leq |||f - f_{h\tau}|||_{Y_T'} |||v|||_{Y_T}$. For $(K, I_n) \in \mathcal{T}_{h\tau}(Q)$, let $\bar{v}_{K\times I_n}$ be the average of v on $K \times I_n$. We decompose the term containing ξ_{R} on the space-time mesh and since for all $(K, I_n) \in \mathcal{T}_{h\tau}(Q)$, we assume $(\xi_{\mathrm{R}}, 1)_{K\times I_n} = 0$, there holds that

$$(\xi_{\mathrm{R}}, v)_Q = \sum_{(K,I_n)\in\mathcal{T}_{h\tau}(Q)} (\xi_{\mathrm{R}}, v)_{K\times I_n} = \sum_{(K,I_n)\in\mathcal{T}_{h\tau}(Q)} (\xi_{\mathrm{R}}, v - \bar{v}_{K\times I_n})_{K\times I_n}.$$

We first apply the Cauchy–Schwarz inequality on the local inner product and then bound it by applying the scaled Poincaré inequality (7.1) on the space-time cell,

$$\begin{aligned}(\xi_{\mathrm{R}}, v)_Q &\leq \sum_{(K,I_n)\in\mathcal{T}_{h\tau}(Q)} ||\xi_{\mathrm{R}}||_{K\times I_n} ||v - \bar{v}_{K\times I_n}||_{K\times I_n} \\ &\leq \sum_{(K,I_n)\in\mathcal{T}_{h\tau}(Q)} ||\xi_{\mathrm{R}}||_{K\times I_n} \times \frac{1}{\pi} |||v|||_{Y_T, K\times I_n}.\end{aligned}$$

The term with $\boldsymbol{\xi}_{\mathrm{J}}$ is also decomposed on the space-time mesh and bounded using the Cauchy–Schwarz inequality:

$$\begin{aligned}(\boldsymbol{\xi}_{\mathrm{J}}, \nabla v)_Q &\leq \sum_{(K,I_n)\in\mathcal{T}_{h\tau}(Q)} \frac{1}{h_K} ||\boldsymbol{\xi}_{\mathrm{J}}||_{K\times I_n} \times h_K ||\nabla v||_{K\times I_n} \\ &\leq \sum_{(K,I_n)\in\mathcal{T}_{h\tau}(Q)} \frac{1}{h_K} ||\boldsymbol{\xi}_{\mathrm{J}}||_{K\times I_n} |||v|||_{Y_T, K\times I_n}.\end{aligned}$$

Then, we conclude by applying the Cauchy–Schwarz inequality on both sums. □

Lemma 7.2 is be used to show the reliability of the patchwise optimal equilibrated flux from Definition 3.5, which exhibits the required elementwise equilibration property (7.3). The averaged flux from Definition 3.4 verifies a weaker property, for which the following lemma shows the reliability.

Lemma 7.3 (Guaranteed upper bound for patchwise equilibration in space)**.** *Let $f \in L^2(Q)$, $f_{h\tau} \in L^2(Q)$, $u_{h\tau} \in Y_0 \cap H^2(0,T;L^2(\Omega))$ such that $\partial_t u_{h\tau}(0) = 0$, and a flux $\boldsymbol{p}_{h\tau} \in L^2(0,T;\boldsymbol{H}(\operatorname{div},\Omega))$ such that*

$$\int_{I_n} (f_{h\tau}(t) - \partial_{tt} u_{h\tau}(t) - \operatorname{div} \boldsymbol{p}_{h\tau}(t), \psi_a)_{\omega_a} \mathrm{d}t = 0 \quad \forall I_n \in \mathcal{T}_\tau(0,T),\ \forall a \in \mathcal{S}_h^{\mathrm{int}}(\Omega)$$

be given. Then

$$|||u - u_{h\tau}|||_{\mathcal{Y}_0} \leq |||f - f_{h\tau}|||_{Y_T'} + \sqrt{\sum_{(K,I_n)\in\mathcal{T}_{h\tau}(Q)} \frac{1}{h_K^2}||\boldsymbol{p}_{h\tau} + \nabla u_{h\tau}||^2_{K\times I_n}}$$

$$+ \sqrt{\max_{K\in\mathcal{T}_h(\Omega)} \sum_{a\in\mathcal{S}_h(K)} \frac{c_{\mathrm{P},a}^2 h_{\omega_a}^2}{h_K^2}} \times \sqrt{\sum_{(K,I_n)\in\mathcal{T}_{h\tau}(Q)} ||f_{h\tau} - \partial_{tt}u_{h\tau} - \operatorname{div}\boldsymbol{p}_{h\tau}||^2_{K\times I_n}}.$$

Proof. The beginning of the proof is the same as the one for Lemma 7.2. We only need to adapt the part that deals with $\xi_{\mathrm{R}} := f_{h\tau} - \partial_{tt}u_{h\tau} - \operatorname{div}\boldsymbol{p}_{h\tau} \in L^2(Q)$. Let $n \in [\![1, N]\!]$. We decompose $(\xi_{\mathrm{R}}, v)_{\Omega\times I_n}$ using the family of hat functions as a partition of unity. Recall that for $a \in \mathcal{S}_h^{\mathrm{int}}(\Omega)$, $\bar{v}_{\omega_a\times I_n}$ is the average of v on $\omega_a \times I_n$ and that we assume that $\int_{I_n}(\xi_{\mathrm{R}}(t), \psi_a)_{\omega_a} dt = 0$. Then

$$\begin{aligned}(\xi_{\mathrm{R}}, v)_{\Omega\times I_n} &= \sum_{a\in\mathcal{S}_h(\Omega)} (\xi_{\mathrm{R}}, \psi_a v)_{\Omega\times I_n}\\ &= \sum_{a\in\mathcal{S}_h^{\mathrm{int}}(\Omega)} (\xi_{\mathrm{R}}, \psi_a(v - \bar{v}_{\omega_a\times I_n}))_{\omega_a\times I_n} + \sum_{a\in\mathcal{S}_h^{\mathrm{ext}}(\Omega)} (\xi_{\mathrm{R}}, \psi_a v)_{\omega_a\times I_n}.\end{aligned}$$

By applying the Cauchy–Schwarz inequality, we obtain

$$(\xi_{\mathrm{R}}, v)_{\Omega\times I_n} \leq \sum_{a\in\mathcal{S}_h^{\mathrm{int}}(\Omega)} ||\psi_a\xi_{\mathrm{R}}||_{\omega_a\times I_n}||v - \bar{v}_{\omega_a\times I_n}||_{\omega_a\times I_n} + \sum_{a\in\mathcal{S}_h^{\mathrm{ext}}(\Omega)} ||\psi_a\xi_{\mathrm{R}}||_{\omega_a\times I_n}||v||_{\omega_a\times I_n}.$$

To proceed, we use the scaled Poincaré inequality on patches from (7.2), which gives

$$(\xi_{\mathrm{R}}, v)_{\Omega\times I_n} \leq \sum_{a\in\mathcal{S}_h(\Omega)} ||\psi_a\xi_{\mathrm{R}}||_{\omega_a\times I_n} \times c_{\mathrm{P},a}\sqrt{\tau_n^2||\partial_t v||^2_{\omega_a\times I_n} + h_{\omega_a}^2||\nabla v||^2_{\omega_a\times I_n}}.$$

We reapply the Cauchy–Schwarz inequality to get

$$(\xi_{\mathrm{R}}, v)_{\Omega\times I_n} \leq \sqrt{\sum_{a\in\mathcal{S}_h(\Omega)} ||\psi_a\xi_{\mathrm{R}}||^2_{\omega_a\times I_n}} \times \sqrt{\sum_{a\in\mathcal{S}_h(\Omega)} c_{\mathrm{P},a}^2\left(\tau_n^2||\partial_t v||^2_{\omega_a\times I_n} + h_{\omega_a}^2||\nabla v||^2_{\omega_a\times I_n}\right)}.$$

We finally estimate both terms by decomposing and reordering the sums:

$$\begin{aligned}\sum_{a\in\mathcal{S}_h(\Omega)} ||\psi_a\xi_{\mathrm{R}}||^2_{\omega_a\times I_n} &= \sum_{a\in\mathcal{S}_h(\Omega)}\sum_{K\in\mathcal{T}_h(\omega_a)} ||\psi_a\xi_{\mathrm{R}}||^2_{K\times I_n} = \sum_{K\in\mathcal{T}_h(\Omega)}\sum_{a\in\mathcal{S}_h(K)} ||\psi_a\xi_{\mathrm{R}}||^2_{K\times I_n}\\ &= \int_{I_n}\sum_{K\in\mathcal{T}_h(\Omega)}\int_K \underbrace{\left(\sum_{a\in\mathcal{S}_h(K)}\psi_a^2\right)}_{\leq 1} |\xi_{\mathrm{R}}(t)|^2 \mathrm{d}\boldsymbol{x}\mathrm{d}t \leq \sum_{K\in\mathcal{T}_h(\Omega)} ||\xi_{\mathrm{R}}||^2_{K\times I_n};\end{aligned}$$

$$\begin{aligned}\sum_{a\in\mathcal{S}_h(\Omega)} c_{\mathrm{P},a}^2 h_{\omega_a}^2||\nabla v||^2_{\omega_a\times I_n} &= \sum_{a\in\mathcal{S}_h(\Omega)}\sum_{K\in\mathcal{T}_h(\omega_a)} c_{\mathrm{P},a}^2 h_{\omega_a}^2||\nabla v||^2_{K\times I_n}\\ &= \sum_{K\in\mathcal{T}_h(\Omega)}\left(\sum_{a\in\mathcal{S}_h(K)} c_{\mathrm{P},a}^2 h_{\omega_a}^2\right)||\nabla v||^2_{K\times I_n}\\ &\leq \left(\max_{K\in\mathcal{T}_h(\Omega)}\sum_{a\in\mathcal{S}_h(K)}\frac{c_{\mathrm{P},a}^2 h_{\omega_a}^2}{h_K^2}\right) \times \sum_{K\in\mathcal{T}_h(\Omega)} h_K^2||\nabla v||^2_{K\times I_n}.\end{aligned}$$

We conclude by summing on all time steps. $\square$

7.2 Volume residual efficiency using cell bubble functions

In this and the next section we use the methodology from [12, 27] to show the space-time local efficiency of the residual-based estimator. We first work on the discrete volume residual $f_{h\tau} - \partial_{tt} u_{h\tau} - \Delta u_{h\tau}$ and use finite-dimensional cell bubble functions to localise it and then bound it. This methodology allows us to show local and global efficiencies, but it uses finite-dimensional arguments (inverse inequalities, equivalence of norms in finite dimension) that depend on the dimension of the discrete approximation space, which in turn depends on the polynomial orders. Therefore, our efficiency results are not robust with respect to the polynomial orders p and k.

Definition 7.4 (Time hat function). *For $t^n \in \mathcal{S}_\tau(0,T)$ we define the time hat function $\psi^n \in \mathcal{C}^0(0,T)$ such that*

$$\begin{cases} \psi^n|_{I_m} \in \mathcal{P}_1(I_m;\mathbb{R}) & \forall I_m \in \mathcal{T}_\tau(0,T), \\ \psi^n(t^m) = 0 & \forall t^m \in \mathcal{S}_\tau(0,T) \setminus \{t^n\}, \\ \psi^n(t^n) = 1. \end{cases} \tag{7.4}$$

Definition 7.5 (Space-time cell bubble function). *For $(K, I_n) \in \mathcal{T}_{h\tau}(Q)$, let ψ_K^n be the bubble function such that for $(\boldsymbol{x}, t) \in Q$,*

$$\psi_K^n(\boldsymbol{x}, t) := c_K^n \times \prod_{k\in\{n-1,n\}} \psi^k(t) \times \prod_{a\in\mathcal{S}_h(K)} \psi_a(\boldsymbol{x}), \tag{7.5}$$

with c_K^n a scaling constant to ensure that

$$\max_{(x,t)\in K\times I_n} \psi_K^n(\boldsymbol{x}, t) = 1.$$

Properties: Let $(K, I_n) \in \mathcal{T}_{h\tau}(Q)$ and $\phi \in U_{h\tau}^{pk}$. Then, there holds:

1. **Positivity and local support**:

$$0 < \psi_K^n \leq 1 \text{ on the interior of } K \times I_n \text{ and } \psi_K^n = 0 \text{ elsewhere.} \tag{7.6}$$

2. **Space-time inverse inequality**: (see [12, Equation (6.3)])

$$|||\psi_K^n \phi|||_{Y_T, K\times I_n} \lesssim ||\psi_K^n \phi||_{K\times I_n}. \tag{7.7}$$

3. **Equivalence of norms in finite dimension**: (see [12, Equation (6.2)])

$$(\psi_K^n \phi, \phi)_{K\times I_n} \leq ||\phi||^2_{K\times I_n} \lesssim (\psi_K^n \phi, \phi)_{K\times I_n}. \tag{7.8}$$

Lemma 7.6 (Volume residual efficiency). *Let $f \in L^2(Q)$, $f_{h\tau} \in U_{h\tau}^{pk}$, and $u_{h\tau} \in V_{h\tau}^{pk}$. Then, there holds:*

- ***Local efficiency**: For $(K, I_n) \in \mathcal{T}_{h\tau}(Q)$,*

$$||f_{h\tau} - \partial_{tt} u_{h\tau} + \Delta u_{h\tau}||_{K\times I_n} \lesssim |||f - f_{h\tau}|||_{Y_T', K\times I_n} + |||u - u_{h\tau}|||_{\mathcal{Y}_0, K\times I_n}.$$

- ***Global efficiency:***

$$\sqrt{\sum_{(K,I_n)\in\mathcal{T}_{h\tau}(Q)} ||f_{h\tau} - \partial_{tt} u_{h\tau} + \Delta u_{h\tau}||^2_{K\times I_n}} \lesssim |||f - f_{h\tau}|||_{Y_T'} + |||u - u_{h\tau}|||_{\mathcal{Y}_0}.$$

Proof. In this proof, let ∂_{tt} and Δ, be the broken elementwise versions of the second time-derivative and the Laplace operator in space. Let $\xi_{\mathrm{R}} := f_{h\tau} - \partial_{tt} u_{h\tau} + \Delta u_{h\tau} \in U^{pk}_{h\tau}$. Then, for $(K, I_n) \in \mathcal{T}_{h\tau}(Q)$, (7.8) gives:

$$||\xi_{\mathrm{R}}||^2_{K\times I_n} \lesssim (\psi^n_K \xi_{\mathrm{R}}, \xi_{\mathrm{R}})_{K\times I_n} = -(f - f_{h\tau}, \psi^n_K \xi_{\mathrm{R}})_{K\times I_n} + (f - \partial_{tt} u_{h\tau} + \Delta u_{h\tau}, \psi^n_K \xi_{\mathrm{R}})_{K\times I_n}.$$

Using (7.6) and the fact that $\xi_{\mathrm{R}}|_{K\times I_n}$ is both polynomial on $K \times I_n$ and in $H^1(K \times I_n)$, we get that $(\psi^n_K \xi_{\mathrm{R}})|_{K\times I_n} \in H^1_0(K \times I_n)$ thus having $\psi^n_K \xi_{\mathrm{R}} \in Y_T$ with $\mathrm{supp}(\psi^n_K \xi_{\mathrm{R}}) \subset K \times I_n$. Then, we can extend the integrals from $K \times I_n$ to Q and then integrate by parts to get

$$||\xi_{\mathrm{R}}||^2_{K\times I_n} \lesssim -(f - f_{h\tau}, \psi^n_K \xi_{\mathrm{R}})_Q + (f, \psi^n_K \xi_{\mathrm{R}})_Q + (\partial_t u_{h\tau}, \partial_t(\psi^n_K \xi_{\mathrm{R}}))_Q - (\nabla u_{h\tau}, \nabla(\psi^n_K \xi_{\mathrm{R}}))_Q.$$

We recognise the residual from (2.7) and obtain

$$||\xi_{\mathrm{R}}||^2_{K\times I_n} \lesssim -(f - f_{h\tau}, \psi^n_K \xi_{\mathrm{R}})_Q + \langle r(u_{h\tau}), \psi^n_K \xi_{\mathrm{R}}\rangle_{Y_T}. \tag{7.9}$$

Since $\mathrm{supp}(\psi^n_K \xi_{\mathrm{R}}) \subset K \times I_n$, by definition of the localised dual norm in (6.3c), there holds that

$$\begin{aligned} &-(f - f_{h\tau}, \psi^n_K \xi_{\mathrm{R}})_Q + \langle r(u_{h\tau}), \psi^n_K \xi_{\mathrm{R}}\rangle_{Y_T} \\ &\qquad\qquad \leq \left(|||f - f_{h\tau}|||_{Y_T', K\times I_n} + |||r(u_{h\tau})|||_{Y_T', K\times I_n}\right) |||\psi^n_K \xi_{\mathrm{R}}|||_{Y_T, K\times I_n}, \end{aligned}$$

which is simplified to get the local efficiency result using

$$|||\psi^n_K \xi_{\mathrm{R}}|||^2_{Y_T, K\times I_n} \overset{(7.7)}{\lesssim} ||\psi^n_K \xi_{\mathrm{R}}||^2_{K\times I_n} \overset{(7.6)}{\leq} ||\xi_{\mathrm{R}}||^2_{K\times I_n}. \tag{7.10}$$

Let $\tilde{v}_{\mathrm{R}} := \sum_{(K,I_n)\in\mathcal{T}_{h\tau}(Q)} \psi^n_K \xi_{\mathrm{R}} \in Y_T$. To prove the global efficiency, we sum (7.9) over $\mathcal{T}_{h\tau}(Q)$:

$$\begin{aligned} \sum_{(K,I_n)\in\mathcal{T}_{h\tau}(Q)} ||\xi_{\mathrm{R}}||^2_{K\times I_n} &\lesssim -(f - f_{h\tau}, \tilde{v}_{\mathrm{R}})_Q + \langle r(u_{h\tau}), \tilde{v}_{\mathrm{R}}\rangle_{Y_T} \\ &\overset{(6.3c)}{\leq} \left(|||f - f_{h\tau}|||_{Y_T'} + |||r(u_{h\tau})|||_{Y_T'}\right) |||\tilde{v}_{\mathrm{R}}|||_{Y_T}. \end{aligned}$$

We conclude the proof of the global efficiency using the fact that all the $\psi^n_K \xi_{\mathrm{R}}$ are separately supported and by applying (6.3a) and (7.10). □

7.3 Face residual efficiency using face bubble functions

Now that we derived the efficiency result for the volume discrete residual, we do the same for the jump residual on the internal faces of the mesh. This time, we use a discrete bubble function defined on the patch around each internal face, with similar arguments as in Section 7.2. We define $\mathcal{T}_h(\omega_F) := \{K \in \mathcal{T}_h(\Omega)$, s.t. $F \in \mathcal{F}_h(K)\}$ the local mesh around any internal face $F \in \mathcal{F}^{\mathrm{int}}_h(\Omega)$ and $\omega_F \subset \Omega$, the corresponding open subdomain of diameter h_{ω_F}.

Definition 7.7 (Space-time face bubble function)**.** *For $I_n \in \mathcal{T}_\tau(0,T)$ and $F \in \mathcal{F}_h^{\text{int}}(\Omega)$, we define ψ_F^n, the bubble function around $F \times I_n$, such that for $(\boldsymbol{x},t) \in Q$,*

$$\psi_F^n(\boldsymbol{x},t) := c_F^n \times \prod_{k\in\{n-1,n\}} \psi^k(t) \times \prod_{a\in\mathcal{S}_h(F)} \psi_a(\boldsymbol{x}), \tag{7.11}$$

with c_F^n a scaling constant to ensure that

$$\max_{(\boldsymbol{x},t)\in\omega_F\times I_n} \psi_F^n(\boldsymbol{x},t) = 1.$$

Properties: Let $(F, I_n) \in \mathcal{F}_h^{\text{int}}(\Omega) \times \mathcal{T}_\tau(0,T)$, and $\phi \in U_{h\tau}^{pk}$. There holds:

- **Positivity and local support**:
$$0 < \psi_F^n \le 1 \text{ on the interior of } \omega_F \times I_n \text{ and } \psi_F^n = 0 \text{ elsewhere.} \tag{7.12}$$

- **Space-time inverse inequality**: (see [12, Equation (6.3)])
$$|||\psi_F^n\phi|||_{Y_T,\omega_F\times I_n} \lesssim ||\psi_F^n\phi||_{\omega_F\times I_n}. \tag{7.13}$$

- **Equivalence of norms in finite dimension**: (see [12, Equation (6.2)])
$$(\psi_F^n\phi,\phi)_{F\times I_n} \le ||\phi||^2_{F\times I_n} \lesssim (\psi_F^n\phi,\phi)_{F\times I_n}. \tag{7.14}$$

Following the methodology in [12, 27] (referred to as extension by constants in [12]), we also introduce for $u_{h\tau} \in V_{h\tau}^{pk}$, $F \in \mathcal{F}_h^{\text{int}}(\Omega)$, and $I_n \in \mathcal{T}_\tau(0,T)$ a function $v_F^n \in U_{h\tau}^{pk} \cap H^1(\omega_F \times I_n)$ such that

$$(v_F^n)|_{F\times I_n} = [\![\nabla u_{h\tau}\cdot\boldsymbol{n}_F]\!]_F|_{I_n} \quad \text{and} \quad ||v_F^n||^2_{\omega_F\times I_n} \le h_{\omega_F}||[\![\nabla u_{h\tau}\cdot\boldsymbol{n}_F]\!]||^2_{F\times I_n}. \tag{7.15}$$

Lemma 7.8 (Face residual efficiency)**.** *Let $f \in L^2(Q)$, $f_{h\tau} \in U_{h\tau}^{pk}$, and $u_{h\tau} \in V_{h\tau}^{pk}$. Then, there holds:*

- ***Local efficiency:*** *For $(F, I_n) \in \mathcal{F}_h^{\text{int}}(\Omega) \times \mathcal{T}_\tau(0,T)$,*
$$\frac{1}{\sqrt{h_{\omega_F}}}||[\![\nabla u_{h\tau}\cdot\boldsymbol{n}_F]\!]||_{F\times I_n} \lesssim |||f - f_{h\tau}|||_{Y_T',\omega_F\times I_n} + |||u - u_{h\tau}|||_{\mathcal{Y}_0,\omega_F\times I_n}.$$

- ***Global efficiency:***
$$\sqrt{\sum_{(F,I_n)\in\mathcal{F}_h^{\text{int}}(\Omega)\times\mathcal{T}_\tau(0,T)} \frac{1}{h_{\omega_F}}||[\![\nabla u_{h\tau}\cdot\boldsymbol{n}_F]\!]||^2_{F\times I_n}} \lesssim |||f - f_{h\tau}|||_{Y_T'} + |||u - u_{h\tau}|||_{\mathcal{Y}_0}.$$

Proof. Let $F \in \mathcal{F}_h^{\text{int}}(\Omega)$, $I_n \in \mathcal{T}_\tau(0,T)$, and let v_F^n verify (7.15). We know that there are exactly two elements in $\mathcal{T}_h(\omega_F)$ and (7.12) ensures that for $K \in \mathcal{T}_h(\omega_F)$, $\psi_F^n = 0$ on $\partial K \setminus F$. Then there holds:

$$||v_F^n||^2_{F\times I_n} \overset{(7.14)\text{ and }(7.15)}{\lesssim} (\underbrace{[\![\nabla u_{h\tau}\cdot\boldsymbol{n}_F]\!]}_{v_F^n}, \psi_F^n v_F^n)_{F\times I_n} = \sum_{K\in\mathcal{T}_h(\omega_F)} (\nabla u_{h\tau}\cdot\boldsymbol{n}_{\partial K}, \psi_F^n v_F^n)_{F\times I_n}. \tag{7.16}$$

For $K \in \mathcal{T}_h(\omega_F)$, we integrate by parts using that $\psi_F^n v_F^n \in H^1(K \times I_n)$ with $\psi_F^n v_F^n = 0$ on $\partial(K \times I_n) \setminus F \times I_n$. Furthermore, $u_{h\tau}$ is polynomial on $K \times I_n$ (thus at least in $H^2(K \times I_n)$). There holds

- $(\nabla u_{h\tau}, \nabla(\psi_F^n v_F^n))_{K\times I_n} + (\Delta u_{h\tau}, \psi_F^n v_F^n)_{K\times I_n} = (\nabla u_{h\tau}\cdot\boldsymbol{n}_{\partial K}, \psi_F^n v_F^n)_{F\times I_n}$;
- $(\partial_t u_{h\tau}, \partial_t(\psi_F^n v_F^n))_{K\times I_n} + (\partial_{tt} u_{h\tau}, \psi_F^n v_F^n)_{K\times I_n} = 0$.

Then, by adding these equalities together, we obtain:

$$\sum_{K\in\mathcal{T}_h(\omega_F)} (\nabla u_{h\tau}\cdot\boldsymbol{n}_{\partial K}, \psi_F^n v_F^n)_{F\times I_n} = \sum_{K\in\mathcal{T}_h(\omega_F)} (f - \partial_{tt}u_{h\tau} + \Delta u_{h\tau}, \psi_F^n v_F^n)_{K\times I_n}$$
$$- (f, \psi_F^n v_F^n)_{\omega_F\times I_n} - (\partial_t u_{h\tau}, \partial_t(\psi_F^n v_F^n))_{\omega_F\times I_n} + (\nabla u_{h\tau}, \nabla(\psi_F^n v_F^n))_{\omega_F\times I_n}$$

Using (2.7) and (7.16), we get

$$||v_F^n||^2_{F\times I_n} \lesssim \sum_{K\in\mathcal{T}_h(\omega_F)} (f - \partial_{tt}u_{h\tau} + \Delta u_{h\tau}, \psi_F^n v_F^n)_{K\times I_n} - \langle r(u_{h\tau}), \psi_F^n v_F^n\rangle_{\omega_F\times I_n}. \tag{7.17}$$

The Cauchy–Schwarz inequality and Lemma 7.6 ensure that

$$\sum_{K\in\mathcal{T}_h(\omega_F)} (f - \partial_{tt}u_{h\tau} + \Delta u_{h\tau}, \psi_F^n v_F^n)_{K\times I_n}$$
$$\lesssim \left(|||f - f_{h\tau}|||_{Y_T',\omega_F\times I_n} + |||u - u_{h\tau}|||_{\mathcal{Y}_0,\omega_F\times I_n}\right) ||\psi_F^n v_F^n||_{\omega_F\times I_n}, \tag{7.18}$$

while (6.3d) and (7.12) yield

$$\langle r(u_{h\tau}), \psi_F^n v_F^n\rangle_{\omega_F\times I_n} \lesssim |||u - u_{h\tau}|||_{\mathcal{Y}_0,\omega_F\times I_n} |||\psi_F^n v_F^n|||_{Y_T,\omega_F\times I_n}. \tag{7.19}$$

We also bound $|||\psi_F^n v_F^n|||_{\omega_F\times I_n}$ as follows:

$$|||\psi_F^n v_F^n|||^2_{Y_T,\omega_F\times I_n} \overset{(7.13)}{\lesssim} ||\psi_F^n v_F^n||^2_{\omega_F\times I_n} \overset{(7.12)}{\leq} ||v_F^n||^2_{\omega_F\times I_n} \overset{(7.15)}{\leq} h_{\omega_F} ||[\![\nabla u_{h\tau}\cdot\boldsymbol{n}_F]\!]||^2_{F\times I_n}. \tag{7.20}$$

We conclude the proof for the local efficiency bound by using (7.17) to (7.20).

To show the global bound, we introduce

$$\tilde{v} := \sum_{(F,I_n)\in\mathcal{F}_h^{\text{int}}(\omega_K)\times\mathcal{T}_\tau(0,T)} \frac{1}{h_{\omega_F}} \psi_F^n v_F^n \in H_0^1(Q)$$

and sum (7.17) over $\mathcal{F}_h^{\text{int}}(\Omega)\times\mathcal{T}_\tau(0,T)$. We apply the Cauchy–Schwarz inequality and (6.3d), to get

$$\sum_{(F,I_n)\in\mathcal{F}_h^{\text{int}}(\Omega)\times\mathcal{T}_\tau(0,T)} \frac{1}{h_{\omega_F}} ||[\![\nabla u_{h\tau}\cdot\boldsymbol{n}_F]\!]||^2_{F\times I_n}$$
$$\lesssim -\langle r(u_{h\tau}), \tilde{v}\rangle_{Y_T} + \sum_{(K,I_n)\in\mathcal{T}_{h\tau}(Q)} (f - \partial_{tt}u_{h\tau} + \Delta u_{h\tau}, \tilde{v})_{K\times I_n},$$
$$\leq |||u - u_{h\tau}|||_{\mathcal{Y}_0} |||\tilde{v}|||_{Y_T} + \sum_{(K,I_n)\in\mathcal{T}_{h\tau}(Q)} ||f - \partial_{tt}u_{h\tau} + \Delta u_{h\tau}||_{K\times I_n} ||\tilde{v}||_{K\times I_n},$$
$$\leq |||u - u_{h\tau}|||_{\mathcal{Y}_0} |||\tilde{v}|||_{Y_T} + ||\tilde{v}||_Q \sqrt{\sum_{(K,I_n)\in\mathcal{T}_{h\tau}(Q)} ||f - \partial_{tt}u_{h\tau} + \Delta u_{h\tau}||^2_{K\times I_n}}.$$

By applying the elementwise space-time inverse inequality [12, Equation (6.3)] we show that $|||\tilde{v}|||_{Y_T} \lesssim ||\tilde{v}||_Q$. We also use the global efficiency result from Lemma 7.6 to obtain

$$\sum_{(F,I_n)\in\mathcal{F}_h^{\rm int}(\Omega)\times\mathcal{T}_\tau(0,T)} \frac{1}{h_{\omega_F}}||[\![\nabla u_{h\tau}\cdot\boldsymbol{n}_F]\!]||^2_{F\times I_n} \lesssim \left(|||f-f_{h\tau}|||_{Y_T'} + |||r(u_{h\tau}|||_{\mathcal{Y}_0}\right)||\tilde{v}||_Q.$$

We conclude by decomposing and bounding $||\tilde{v}||_Q^2$ as follows:

$$\begin{aligned}
||\tilde{v}||_Q^2 &= \sum_{(K,I_n)\in\mathcal{T}_{h\tau}(Q)} \Bigg|\Bigg| \sum_{F\in\mathcal{F}_h^{\rm int}(\Omega)\cap\mathcal{F}_h(K)} \frac{1}{h_{\omega_F}}\psi_F^n v_F^n\Bigg|\Bigg|^2_{K\times I_n} \\
&\lesssim \sum_{(K,I_n)\in\mathcal{T}_{h\tau}(Q)} \sum_{F\in\mathcal{F}_h^{\rm int}(\Omega)\cap\mathcal{F}_h(K)} \frac{1}{h^2_{\omega_F}}||\psi_F^n v_F^n||^2_{K\times I_n} \\
&\lesssim \sum_{(F,I_n)\in\mathcal{F}_h^{\rm int}(\Omega)\times\mathcal{T}_\tau(0,T)} \frac{1}{h^2_{\omega_F}}||\psi_F^n v_F^n||^2_{\omega_F\times I_n} \\
&\overset{(7.20)}{\lesssim} \sum_{(F,I_n)\in\mathcal{F}_h^{\rm int}(\Omega)\times\mathcal{T}_\tau(0,T)} \frac{1}{h_{\omega_F}}||[\![\nabla u_{h\tau}\cdot\boldsymbol{n}_F]\!]||^2_{F\times I_n}.
\end{aligned}$$

□

7.4 Bounding the averaged flux by the residual-based estimator

Now that we have shown the efficiency of the different residual-based terms, we need to do the same for the flux-based estimators. This result is useful in Section 8 for us to show both the efficiency of the flux-based estimators and the reliability of the residual-based one. To achieve this, we notice that for any flux $\boldsymbol{p}_{h\tau} \in L^2(0,T;\boldsymbol{H}(\mathrm{div},\Omega))$, by applying the triangle inequality, there holds

$$\begin{aligned}
&||f_{h\tau} - \partial_{tt}u_{h\tau} - \mathrm{div}\,\boldsymbol{p}_{h\tau}||_{K\times I_n} + \frac{1}{h_K}||\boldsymbol{p}_{h\tau} + \nabla u_{h\tau}||_{K\times I_n} \leq \\
&\qquad ||f_{h\tau} - \partial_{tt}u_{h\tau} + \Delta u_{h\tau}||_{K\times I_n} + ||\,\mathrm{div}(\boldsymbol{p}_{h\tau} + \nabla u_{h\tau})||_{K\times I_n} + \frac{1}{h_K}||\boldsymbol{p}_{h\tau} + \nabla u_{h\tau}||_{K\times I_n}.
\end{aligned}$$

Then, if the flux is finite-dimensional, we can apply an elementwise inverse inequality in space to $||\,\mathrm{div}(\boldsymbol{p}_{h\tau} + \nabla u_{h\tau})||_{K\times I_n}$. Then, for $\star \in \{\mathrm{avg}, \mathrm{equ}\}$, there holds

$$\eta^\star_{K\times I_n} \lesssim ||f_{h\tau} - \partial_{tt}u_{h\tau} + \Delta u_{h\tau}||_{K\times I_n} + \frac{1}{h_K}||\boldsymbol{p}^\star_{h\tau} + \nabla u_{h\tau}||_{K\times I_n}. \tag{7.21}$$

Therefore, to show the efficiency of the flux-based estimators, we only need to show that $\frac{1}{h_K}||\boldsymbol{p}^\star_{h\tau} + \nabla u_{h\tau}||_{K\times I_n}$ can be locally bounded by the different residual-based terms. To achieve this, we use pre-existing results from the time-independent case. We start by recalling the boundedness result for the time-independent averaged flux from [12, Lemma 7.5]. It specifically derives from the characterisation of the Raviart–Thomas degrees of freedom that can be found for both simplices and hypercubes in [4, Propositions 2.3.4 and 2.4.1].

Lemma 7.9 (Bound on the time-independent averaged flux)**.** *Let $\boldsymbol{g}_h \in L^2(\Omega)^d$ such that for all $K \in \mathcal{T}_h(\Omega)$, $\boldsymbol{g}_h|_K \in \boldsymbol{RT}_h^p(K)$. Let $\boldsymbol{p}_h \in \boldsymbol{W}_h^p$ be the averaged flux such that for $K \in \mathcal{T}_h(\Omega)$*

$$\begin{cases} (\boldsymbol{p}_h, \boldsymbol{z}_h)_K = -(\boldsymbol{g}_h, \boldsymbol{z}_h)_K & \forall \boldsymbol{z}_h \in \boldsymbol{Z}_h^p(K), \\ \quad \boldsymbol{p}_h\cdot\boldsymbol{n}_F = -\langle\!\langle \boldsymbol{g}_h\cdot\boldsymbol{n}_F\rangle\!\rangle_F & \forall F \in \mathcal{F}_h(K). \end{cases}$$

Then, for all $K \in \mathcal{T}_h(\Omega)$, there holds

$$||\boldsymbol{p}_h + \boldsymbol{g}_h||_K \lesssim \sum_{F \in \mathcal{F}_h(K)} \sqrt{h_F} ||[\![\boldsymbol{g}_h \cdot \boldsymbol{n}_F]\!]||_F.$$

Then, by directly applying this time-independent result and integrating over time steps, we easily prove the following space-time bound.

Lemma 7.10 (Bound on the space-time averaged flux)**.** *Let $u_{h\tau} \in V_{h\tau}^{pk}$ and $\boldsymbol{p}_{h\tau}^{\mathrm{avg}}$ be the space-time averaged flux from Definition 3.4. Then, for all $(K, I_n) \in \mathcal{T}_{h\tau}(Q)$, there holds:*

$$||\boldsymbol{p}_{h\tau}^{\mathrm{avg}} + \nabla u_{h\tau}||_{K \times I_n} \lesssim \sum_{F \in \mathcal{F}_h(K)} \sqrt{h_F} ||[\![\nabla u_{h\tau} \cdot \boldsymbol{n}_F]\!]||_{F \times I_n}.$$

7.5 Decoupling time and space components of the locally optimal equilibrated flux

We now want to reproduce a result similar to Lemma 7.10 but for the locally optimal equilibrated flux. The definition of $\boldsymbol{p}_{h\tau}^{\mathrm{avg}}$ is pointwise in time, which allows to directly use the time-independent boundedness to prove the space-time one. In contrast, $\boldsymbol{p}_{h\tau}^{\mathrm{equ}}$ is locally built from the solutions of coupled space-time minimisation problems that we first need to decouple into sets of time-independent problems before applying known bounds. To achieve this, we decouple each local space-time problem into a set of independent space-only problems using a methodology similar to [15, Lemma 4.3].

Let $\Phi^n := (\phi^{n,l})_{l \in [\![0,k]\!]}$ be an orthogonal basis of $\mathcal{P}_k(I_n, \mathbb{R})$ based on the Legendre polynomials as described in [15]. Let $I_n \in \mathcal{T}_\tau(0,T)$ and $a \in \mathcal{S}_h(\Omega)$. In Sections 7.5 and 7.6, we use the following notations:

$$u_{h\tau}|_{I_n} = (x,t) \longmapsto \sum_{l=0}^{k} u_h^{n,l}(x)\phi^{n,l}(t), \qquad \partial_{tt} u_{h\tau}|_{I_n} = (x,t) \longmapsto \sum_{l=0}^{k} \ddot{u}_h^{n,l}(x)\phi^{n,l}(t),$$

$$f_{h\tau}|_{I_n} = (x,t) \longmapsto \sum_{l=0}^{k} f_h^{n,l}(x)\phi^{n,l}(t), \qquad \boldsymbol{p}_{h\tau,a}^{\mathrm{equ}}|_{I_n} = (x,t) \longmapsto \sum_{l=0}^{k} \boldsymbol{p}_{h,a}^{n,l}(x)\phi^{n,l}(t),$$

with

$$(u_h^{n,l})_{l \in [\![0,k]\!]} \subset V_h^p, \qquad (\ddot{u}_h^{n,l})_{l \in [\![0,k]\!]} \subset V_h^p,$$
$$(f_h^{n,l})_{l \in [\![0,k]\!]} \subset U_h^p, \qquad (\boldsymbol{p}_{h,a}^{n,l})_{l \in [\![0,k]\!]} \subset \boldsymbol{W}_h^{p+1}|_{\omega_a}.$$

To simplify notations, we introduce the same decomposition of $\partial_{tt} u_{h\tau}|_{I_n}$ up to degree k even if it is only of degree $k-2$ in time. Recall that we define $\boldsymbol{p}_{h\tau,a}^{\mathrm{equ}}|_{I_n}$ in (3.8b) as

$$\begin{aligned} \boldsymbol{p}_{h\tau,a}^{\mathrm{equ}}|_{I_n} := \operatorname{argmin} \Bigg\{ & \sum_{K \in \mathcal{T}_h(\omega_a)} \frac{1}{h_K^2} ||\boldsymbol{q}_{h\tau} + \psi_a \nabla u_{h\tau}||_{K \times I_n}^2, \ \boldsymbol{q}_{h\tau} \in \boldsymbol{W}_{h\tau}^{p+1,k}|_{\omega_a \times I_n} \\ & \text{with } \boldsymbol{q}_{h\tau} \cdot \boldsymbol{n} = 0 \text{ on } (\partial\omega_a \cap \{\psi_a = 0\}) \times I_n \text{ and} \\ & \int_{I_n} (\operatorname{div} \boldsymbol{q}_{h\tau}(t) - \psi_a(f_{h\tau}(t) - \partial_{tt} u_{h\tau}(t)) + \nabla\psi_a \cdot \nabla u_{h\tau}(t), v_h)_{\omega_a} \, \mathrm{d}t = 0, \ \forall v_h \in U_h^{p+1}|_{\omega_a} \Bigg\}. \end{aligned}$$

Let $(\boldsymbol{q}_h^{n,l})_{l\in[\![0,k]\!]} \subset \boldsymbol{W}_h^{p+1}|_{\omega_a}$ be the same decomposition as above but for any $\boldsymbol{q}_{h\tau} \in \boldsymbol{W}_{h\tau}^{p+1,k}|_{\omega_a \times I_n}$. Then, the minimised functional can be easily decoupled into a sum of independent terms:

$$\sum_{K\in\mathcal{T}_h(\omega_a)} \frac{1}{h_K^2} ||\boldsymbol{q}_{h\tau} + \psi_a \nabla u_{h\tau}||^2_{K\times I_n} = \sum_{l=0}^{k} \left(||\phi^{n,l}||^2_{I_n} \sum_{K\in\mathcal{T}_h(\omega_a)} \frac{1}{h_K^2} ||\boldsymbol{q}_h^{n,l} + \psi_a \nabla u_h^{n,l}||^2_K \right).$$

Using the unicity of decomposition in an orthogonal basis, the boundary condition becomes:

$$\boldsymbol{q}_h^{n,l} \cdot \boldsymbol{n} = 0 \text{ on } \partial\omega_a \cap \{\psi_a = 0\} \qquad \forall l \in [\![0,k]\!].$$

Since Φ^n is based on the Legendre polynomials, we remind that $\int_{I_n} \phi^{n,l}(t)\mathrm{d}t \neq 0$ if and only if $l = 0$. Therefore, the equilibration constraint can also be reformulated equivalently as

$$\left(\operatorname{div} \boldsymbol{q}_h^{n,0} - \psi_a(f_h^{n,0} - \ddot{u}_h^{n,0}) + \nabla\psi_a \cdot \nabla u_h^{n,0}, v_h\right)_{\omega_a} = 0 \quad \forall v_h \in U_h^{p+1}|_{\omega_a}$$

Consequently, when decomposed in the basis Φ^n, there is no coupling between components of $\boldsymbol{q}_{h\tau}$ in both the minimised functional and constraints. Therefore we can reformulate it equivalently as patchwise space-only problems the solutions of which are the components of $\boldsymbol{p}_{h\tau,a}^{\mathrm{equ}}|_{I_n}$:

$$\begin{aligned}\boldsymbol{p}_{h,a}^{n,0} := \operatorname{argmin} \Bigg\{ &\sum_{K\in\mathcal{T}_h(\omega_a)} \frac{1}{h_K^2} ||\boldsymbol{q}_h^{n,0} + \psi_a \nabla u_h^{n,0}||^2_{K\times I_n}, \ \boldsymbol{q}_h^{n,0} \in \boldsymbol{W}_h^{p+1}|_{\omega_a} \\ &\text{with } \boldsymbol{q}_h^{n,0} \cdot \boldsymbol{n} = 0 \text{ on } \partial\omega_a \cap \{\psi_a = 0\} \text{ and} \\ &\left(\operatorname{div} \boldsymbol{q}_h^{n,0} - \psi_a(f_h^{n,0} - \ddot{u}_h^{n,0}) + \nabla\psi_a \cdot \nabla u_h^{n,0}, v_h\right)_{\omega_a} = 0 \quad \forall v_h \in U_h^{p+1}|_{\omega_a} \Bigg\},\end{aligned} \tag{7.22a}$$

and, for $l \in [\![1,k]\!]$,

$$\begin{aligned}\boldsymbol{p}_{h,a}^{n,l} := \operatorname{argmin} \Bigg\{ &\sum_{K\in\mathcal{T}_h(\omega_a)} \frac{1}{h_K^2} ||\boldsymbol{q}_h^{n,l} + \psi_a \nabla u_h^{n,l}||^2_{K\times I_n}, \ \boldsymbol{q}_h^{n,l} \in \boldsymbol{W}_h^{p+1}|_{\omega_a} \\ &\text{with } \boldsymbol{q}_h^{n,l} \cdot \boldsymbol{n} = 0 \text{ on } \partial\omega_a \cap \{\psi_a = 0\} \Bigg\}.\end{aligned} \tag{7.22b}$$

For $I_n \in \mathcal{T}_\tau(0,T)$, we introduce the components of the global flux $\boldsymbol{p}_{h\tau}^{\mathrm{equ}}|_{I_n}$ in Φ^n:

$$\boldsymbol{p}_h^{n,l} := \sum_{a\in\mathcal{S}_h(\Omega)} \boldsymbol{p}_{h,a}^{n,l} \qquad l \in [\![0,k]\!]. \tag{7.22c}$$

7.6 Bounding the patchwise optimal equilibrated flux by the residual-based estimator

Now that we have characterised the components of $\boldsymbol{p}_{h\tau,a}^{\mathrm{equ}}|_{I_n}$ in Φ^n, we are able to use the pre-existing stationary bounds. We first recall the following one for the space-only patchwise optimal equilibrated flux from [10, Proof of Proposition 5.2].

Lemma 7.11 (Stationary patchwise optimal equilibrated flux)**.** *Let $u_h \in V_h^p$ and $f_h \in U_h^p$ such that for $a \in \mathcal{S}_h(\Omega)$, $(\nabla u_h, \nabla \psi_a)_\Omega = (f_h, \psi_a)_\Omega$. Then, for $a \in \mathcal{S}_h(\Omega)$, there exists a unique*

$$\boldsymbol{p}_{h,a} := \operatorname{argmin}\Bigg\{ \sum_{K\in\mathcal{T}_h(\omega_a)} \frac{1}{h_K^2}||\boldsymbol{q}_h + \psi_a \nabla u_h||_K^2,\ \boldsymbol{q}_h \in \boldsymbol{W}_h^{p+1}|_{\omega_a} \\ \text{with } \boldsymbol{q}_h\cdot\boldsymbol{n} = 0 \text{ on } \partial\omega_a \cap \{\psi_a = 0\} \text{ and} \\ (\operatorname{div}\boldsymbol{q}_h - \psi_a f_h + \nabla\psi_a\cdot\nabla u_h, v_h)_{\omega_a} = 0 \quad \forall v_h \in U_h^{p+1}|_{\omega_a}\Bigg\}.$$

The global flux $\boldsymbol{p}_h := \sum_{a\in\mathcal{S}_h(\Omega)} \boldsymbol{p}_{h,a}$ verifies, for all $K \in \mathcal{T}_h(\Omega)$,

$$\frac{1}{h_K^2}||\boldsymbol{p}_h + \nabla u_h||_K^2 \lesssim \sum_{K'\in\mathcal{T}_h(\omega_K)} ||f_h + \Delta u_h||_{K'}^2 + \sum_{F\in\mathcal{F}_h^{\text{int}}(\omega_K)} \frac{1}{h_F}||[\![\nabla u_h\cdot\boldsymbol{n}_F]\!]||_F^2.$$

Lemma 7.11 gives a bound the first component of $\boldsymbol{p}_{h\tau}^{\text{equ}}|_{I_n}$, previously denoted $\boldsymbol{p}_h^{n,0}$ in (7.22a). We also show a similar result for the stationary patchwise optimal flux without equilibration, to deal with the other components ($p_h^{n,l}$ for $l \in [\![1,k]\!]$) from (7.22b).

Lemma 7.12 (Stationary patchwise optimal flux without constraint on the divergence)**.** *Let $\boldsymbol{g}_h \in L^2(\Omega)^d$ such that for all $K \in \mathcal{T}_h(\Omega)$, $\boldsymbol{g}_h|_{I_n} \in \boldsymbol{RT}_h^p(K)$. Then, for each $a \in \mathcal{S}_h(\Omega)$, there exists a unique*

$$\boldsymbol{p}_{h,a} := \operatorname{argmin}\Bigg\{ \sum_{K\in\mathcal{T}_h(\omega_a)} \frac{1}{h_K^2}||\boldsymbol{q}_h + \psi_a \boldsymbol{g}_h||_K^2,\ \boldsymbol{q}_h \in \boldsymbol{W}^{p+1}|_{\omega_a} \\ \text{with } \boldsymbol{q}_h\cdot\boldsymbol{n} = 0 \text{ on } \partial\omega_a \cap \{\psi_a = 0\}\Bigg\}.$$

The global flux $\boldsymbol{p}_h := \sum_{a\in\mathcal{S}_h(\Omega)} \boldsymbol{p}_{h,a}$ verifies for $K \in \mathcal{T}_h(\Omega)$

$$\frac{1}{h_K^2}||\boldsymbol{p}_h + \boldsymbol{g}_h||_K^2 \lesssim \sum_{F\in\mathcal{F}_h^{\text{int}}(\omega_K)} \frac{1}{h_F}||[\![\boldsymbol{g}_h\cdot\boldsymbol{n}_F]\!]||_F^2.$$

Proof. Existence and unicity of the solution of the minimisation problem come from the strict convexity of the quadratic form minimised on a non-empty vector space. Let $K \in \mathcal{T}_h(\Omega)$. There holds:

$$\frac{1}{h_K^2}||\boldsymbol{p}_h + \boldsymbol{g}_h||_K^2 = \frac{1}{h_K^2}\Big|\Big|\sum_{a\in\mathcal{S}_h(K)} (\boldsymbol{p}_{h,a} + \psi_a\boldsymbol{g}_h)\Big|\Big|_K^2 \lesssim \sum_{a\in\mathcal{S}_h(K)} \frac{1}{h_K^2}||\boldsymbol{p}_{h,a} + \psi_a\boldsymbol{g}_h||_K^2.$$

Let $a \in \mathcal{S}_h(K)$ and let $\mathfrak{p}_{h,a} \in \boldsymbol{W}_h^{p+1}$ be the averaged flux built from $\psi_a\boldsymbol{g}_h$ as defined in Lemma 7.9. Then, by definition, $\mathfrak{p}_{h,a}$ is zero outside of ω_a, and since $\psi_a = 0$ on $\partial\omega_a$, $\mathfrak{p}_{h,a}\cdot\boldsymbol{n}_{\partial\omega_a}$ is zero on $\partial\omega_a$. We first use the local optimality of $\boldsymbol{p}_{h,a}$ to obtain:

$$\frac{1}{h_K^2}||\boldsymbol{p}_{h,a} + \psi_a\boldsymbol{g}_h||_K^2 \le \sum_{K'\in\mathcal{T}_h(\omega_a)} h_{K'}^{-2}||\boldsymbol{p}_{h,a} + \psi_a\boldsymbol{g}_h||_{K'}^2 \le \sum_{K'\in\mathcal{T}_h(\omega_a)} h_{K'}^{-2}||\mathfrak{p}_{h,a} + \psi_a\boldsymbol{g}_h||_{K'}^2.$$

Then, Lemma 7.9 ensures that:

$$\sum_{K'\in\mathcal{T}_h(\omega_a)} h_{K'}^{-2}||\mathbf{p}_{h,a}+\psi_a\boldsymbol{g}_h||_{K'}^2 \lesssim \sum_{K'\in\mathcal{T}_h(\omega_a)}\sum_{F\in\mathcal{F}_h(K')}\frac{1}{h_F}||\psi_a[\![\boldsymbol{g}_h\cdot\boldsymbol{n}_F]\!]||_F^2.$$

We conclude by gathering the contributions by faces, removing the terms on the exterior faces of ω_a where ψ_a is zero and by using $0\le\psi_a\le 1$:

$$\begin{aligned}\sum_{K'\in\mathcal{T}_h(\omega_a)} h_{K'}^{-2}||\boldsymbol{p}_{h,a}+\psi_a\boldsymbol{g}_h||_{K'}^2 &\lesssim \sum_{F\in\mathcal{F}_h^{\mathrm{int}}(\omega_a)}\frac{1}{h_F}||\psi_a[\![\boldsymbol{g}_h\cdot\boldsymbol{n}_F]\!]||_F^2\\ &\lesssim \sum_{F\in\mathcal{F}_h^{\mathrm{int}}(\omega_a)}\frac{1}{h_F}||[\![\boldsymbol{g}_h\cdot\boldsymbol{n}_F]\!]||_F^2.\end{aligned}$$

□

Lemmas 7.11 and 7.12 allow us bound the locally optimal equilibrated flux by residual-based terms.

Lemma 7.13. *Let $f_{h\tau}\in U_{h\tau}$ and $u_{h\tau}\in V_{h\tau}$ be such that for $I_n\in\mathcal{T}_\tau(0,T)$ and $a\in\mathcal{S}_h^{\mathrm{int}}(\Omega)$,*

$$\int_{I_n}(f_{h\tau}(t)-\partial_{tt}u_{h\tau}(t),\psi_a)_{\omega_a}-(\nabla u_{h\tau}(t),\nabla\psi_a)_{\omega_a}\,\mathrm{d}t=0. \tag{7.23}$$

Then, the patchwise optimal equilibrated flux $\boldsymbol{p}_{h\tau}^{\mathrm{equ}}$ from Definition 3.5 uniquely exists and for $(K\times I_n)\in\mathcal{T}_{h\tau}(Q)$, there holds

$$\begin{aligned}&\frac{1}{h_K^2}||\boldsymbol{p}_{h\tau}^{\mathrm{equ}}+\nabla u_{h\tau}||_{K\times I_n}^2\\ &\qquad\lesssim \sum_{K'\in\mathcal{T}_h(\omega_K)}||f_{h\tau}-\partial_{tt}u_{h\tau}+\Delta u_{h\tau}||_{K'\times I_n}^2+\sum_{F\in\mathcal{F}_h^{\mathrm{int}}(\omega_K)}\frac{1}{h_F}||[\![\nabla u_{h\tau}\cdot\boldsymbol{n}_F]\!]||_{F\times I_n}^2.\end{aligned}$$

Proof. With the decomposition of the patchwise optimal equilibrated flux from Definition 3.5 in (7.22), to prove existence and unicity of $\boldsymbol{p}_{h\tau}^{\mathrm{equ}}$, we only need to prove it for the components of $\boldsymbol{p}_{h\tau}^{\mathrm{equ}}|_{I_n}$ in Φ^n, for $I_n\in\mathcal{T}_\tau(0,T)$.

Let $I_n\in\mathcal{T}_\tau(0,T)$. Given the notation introduced in Section 7.5, the constraint (7.23) can be reformulated as:

$$(f_h^{n,0}-\ddot{u}_h^{n,0},\psi_a)_{\omega_a}-(\nabla u_h^{n,0},\nabla\psi_a)_{\omega_a}=0.$$

This, ensures that we can apply Lemma 7.11 with $u_h=u_h^{n,0}$ and $f_h=f_h^{n,0}-\ddot{u}_h^{n,0}$ to $\boldsymbol{p}_h^{n,0}$ (obtained from (7.22a) by (7.22c)). For $l\in[\![1,k]\!]$, we also apply Lemma 7.12 with $\boldsymbol{g}_h=\nabla u_h^{n,l}$ onto $\boldsymbol{p}_h^{n,l}$ (obtained from (7.22b) by (7.22c)).

Lemmas 7.11 and 7.12 ensure the existence and unicity of all components of $\boldsymbol{p}_{h\tau}^{\mathrm{equ}}|_{I_n}$ in Φ^n which in turn ensure the existence and unicity of $\boldsymbol{p}_{h\tau}^{\mathrm{equ}}|_{I_n}$. There also holds that

$$\frac{1}{h_K^2}||\boldsymbol{p}_{h\tau}^{\mathrm{equ}}+\nabla u_{h\tau}||_{K\times I_n}^2=\sum_{l=0}^{k}\frac{1}{h_K^2}||\phi^{n,l}||_{I_n}^2||\boldsymbol{p}_h^{n,l}+\nabla u_h^{n,l}||_K^2. \tag{7.24}$$

Lemma 7.11 ensures that

$$\frac{1}{h_K^2}||\boldsymbol{p}_h^{n,0}+\nabla u_h^{n,0}||_K^2 \lesssim \sum_{K'\in\mathcal{T}_h(\omega_K)} ||f_h^{n,0}-\ddot{u}_h^{n,0}+\Delta u_h^{n,0}||_{K'}^2 + \sum_{F\in\mathcal{F}_h^{\mathrm{int}}(\omega_K)} \frac{1}{h_F}||[\![\nabla u_h^{n,0}\cdot\boldsymbol{n}_F]\!]||_F^2. \tag{7.25}$$

Lemma 7.12 ensures that for $l \in [\![1,k]\!]$,

$$\frac{1}{h_K^2}||\boldsymbol{p}_h^{n,l}+\nabla u_h^{n,l}||_K^2 \lesssim \sum_{F\in\mathcal{F}_h^{\mathrm{int}}(\omega_K)} \frac{1}{h_F}||[\![\nabla u_h^{n,l}\cdot\boldsymbol{n}_F]\!]||_F^2. \tag{7.26}$$

We conclude by injecting (7.25) and (7.26) into (7.24). $\square$

8 Proof of reliability and local space-time efficiency

We now finally apply the developments of the previous section to prove Theorem 6.3.

8.1 Proof of Theorem 6.3 for the averaged flux-based estimator

Efficiency: Let $(K, I_n) \in \mathcal{T}_{h\tau}(Q)$. Then there holds

$$\eta_{K\times I_n}^{\mathrm{avg}} \overset{(7.21)}{\lesssim} ||f_{h\tau}-\partial_{tt}u_{h\tau}+\Delta u_{h\tau}||_{K\times I_n} + \frac{1}{h_K}||\boldsymbol{p}_{h\tau}^{\mathrm{avg}}+\nabla u_{h\tau}||_{K\times I_n} \overset{\text{Lemma 7.10}}{\lesssim} \eta_{K\times I_n}^{\mathrm{res}}. \tag{8.1}$$

This shows the local and global efficiencies using Lemmas 7.6 and 7.8.

Reliability: Let $a \in \mathcal{S}_h^{\mathrm{int}}(\Omega)$. Since ψ_a is in V_h^p, $\nabla\psi_a$ itself is in $\boldsymbol{Z}_h^p$ elementwise. Then, by Definition 3.4, we know that:

$$\int_{I_n}(\nabla u_{h\tau}(t)+\boldsymbol{p}_{h\tau}^{\mathrm{avg}}(t),\nabla\psi_a)_{\omega_a}\,\mathrm{d}t = 0.$$

Then, using (6.7), we show that

$$\int_{I_n}(f_{h\tau}(t)-\partial_{tt}u_{h\tau}(t)-\operatorname{div}\boldsymbol{p}_{h\tau}^{\mathrm{avg}}(t),\psi_a)_{\omega_a}\,\mathrm{d}t = 0.$$

This verifies the hypothesis of Lemma 7.3 that we use to show the reliability result.

8.2 Proof of Theorem 6.3 for the residual-based estimator

Efficiency: Lemmas 7.6 and 7.8 immediately show both local and global efficiencies.

Reliability: We use (8.1) to show that $\eta_Q^{\mathrm{avg}} \lesssim \eta_Q^{\mathrm{res}}$. The reliability then follows from that of η_Q^{avg}.

8.3 Proof of Theorem 6.3 for the patchwise optimal equilibrated flux-based estimator

Efficiency: Let $(K, I_n) \in \mathcal{T}_{h\tau}(Q)$. Then (7.21) ensures that:

$$\eta_{K\times I_n}^{\mathrm{equ}} \lesssim ||f_{h\tau}-\partial_{tt}u_{h\tau}+\Delta u_{h\tau}||_{K\times I_n} + \frac{1}{h_K}||\boldsymbol{p}_{h\tau}^{\mathrm{equ}}+\nabla u_{h\tau}||_{K\times I_n},$$

and by applying Lemma 7.13, we obtain that:

$$(\eta^{\mathrm{equ}}_{K\times I_n})^2 \lesssim \sum_{K'\in\mathcal{T}_h(\omega_K)} ||f_{h\tau} - \partial_{tt}u_{h\tau} + \Delta u_{h\tau}||^2_{K'\times I_n} + \sum_{F\in\mathcal{F}^{\mathrm{int}}_h(\omega_K)} \frac{1}{h_F}||[\![\nabla u_{h\tau}\cdot\boldsymbol{n}_F]\!]||^2_{F\times I_n}.$$

We conclude using Lemmas 7.6 and 7.8 for both local and global efficiencies.

Reliability: Let $I_n \in \mathcal{T}_\tau(0,T)$. (3.8c) defines $\boldsymbol{p}^{\mathrm{equ}}_{h\tau}|_{I_n}$ as $\sum_{a\in\mathcal{S}_h(\Omega)} \boldsymbol{p}^{\mathrm{equ}}_{h\tau,a}|_{I_n}$ with $\boldsymbol{p}^{\mathrm{equ}}_{h\tau,a}|_{I_n}$ the solution of (3.8b) for each $a\in\mathcal{S}_h(\Omega)$. (3.8b) ensures that for each $a \in \mathcal{S}_h(\Omega)$,

$$\int_{I_n} \Big(\operatorname{div}\boldsymbol{p}^{\mathrm{equ}}_{h\tau,a}(t) - \psi_a(f_{h\tau}(t) - \partial_{tt}u_{h\tau}(t)) + \nabla\psi_a\cdot\nabla u_{h\tau}(t), v_h\Big)_{\omega_a} \mathrm{d}t = 0 \quad \forall v_h \in U^{p+1}_h|_{\omega_a}.$$

By summing this equality on $\mathcal{S}_h(\Omega)$, since $\sum_{a\in\mathcal{S}_h(\Omega)}\psi_a = 1$, we obtain

$$\int_{I_n} (\operatorname{div}\boldsymbol{p}^{\mathrm{equ}}_{h\tau}(t) - f_{h\tau}(t) + \partial_{tt}u_{h\tau}(t), v_h)_\Omega \,\mathrm{d}t = 0 \quad \forall v_h \in U^{p+1}_h.$$

This verifies the hypothesis of Lemma 7.2 that shows the reliability of η^{equ}_Q.

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