Error estimates for finite element approximations of effective elastic properties of periodic structures

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Abstract

Techniques for a posteriori error estimation for finite element approximations of an elliptic partial differential equation are studied. This extends previous work on localized error control in finite element methods for linear elasticity. The methods are then applied to the problem of homogenization of periodic structures. In particular, error estimates for the effective elastic properties are obtained.

The usefulness of these estimates is twofold. First, adaptive methods using mesh refinements based on the estimates can be constructed. Secondly, one of the estimates can give reasonable measure of the magnitude of the error. Numerical examples of this are given.

Feluppskattningar för finita element-approximationer av effektiva elastiska egenskaper hos periodiska strukturer

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Sammanfattning

Tekniker för a posteriori feluppskattningar för finita element-approximationer till en elliptisk partiell differentialekvation studeras. Detta utvidgar tidigare arbeten av lokaliserad felkontroll i finita element-metoder för linjär elasticitet. Metoderna tillämpas sedan på homogeniseringsproblemet för periodiska strukturer. Speciellt erhålls feluppskattningar för de effektiva elastiska egenskaperna.

Nyttan med dessa uppskattningar är tvåfaldig. För det första kan adaptiva metoder för meshförfining baserade på uppskattningarna konstrueras. För det andra kan en av uppskattningarna ge ett rimligt mått av storleken på felet. Numeriska exempel på detta ges.

Contents

1 Introduction

The practical application of differential equations to the modelling of elastic properties of periodic structures presents problems both in analysis and computational mathematics. The analytical issues arise because of the need to approximate the periodic structure in a way that makes it possible for numerical calculations to be carried out. Once this is established, there is a need to compute approximate solutions of still difficult problems. In an application it is therefore critically important to understand the introduced errors in these respective steps. We will consider the computational error in this work.

A method for approximating the behavior of periodic structures is periodic homogenization (see [9, 14, 25]). The periodic structure is typically approximated by a homogeneous structure. Quantities of interest are the elastic properties, the so-called effective elastic properties, of this auxiliary homogeneous structure. We will consider the local problems, the so-called cell problems, arising from the homogenization method when applied to some of the equations of linear elasticity (see [14, 22, 24]). The effective elastic properties are calculated from the solutions of these cell problems. The cell problems are elliptic partial differential equations which are known to give a good approximation of the periodic structure if the size of a period is sufficiently small in comparison with the size of the structure. We will assume that is the case and focus on the problem of finding approximate solutions of the cell problems.

The cell problems will be solved numerically for approximate solutions using the finite element method. Our goal is to estimate the numerical error in the effective elastic properties. This will be done using a posteriori error estimation techniques. A treatment of the scalar Dirichlet problem by standard method can, for example, be found in [18]. Other techniques have been used by Carstensen, Funken, Morin, Nochetto, Oden, Thiele, among others, for similar problems, see [7, 21, 26]. Alternatives to the finite element method for the numerical calculation exist. For example, Helsing has studied the two dimensional case using the methods of complex analysis in his papers [12, 15]. In this work we will focus on the technique studied by Carstensen et al.

Our contributions are the following. We study an elliptic equation appearing in the linear theory of elasticity and the homogenization of this theory for periodic structures. This extends the two-dimensional work of Carstensen et al in [8] to a more general problem in $\mathbf{R}^n$. Some differences in the results appears. However, these are more connected to the method used rather than the dimension n. In particular, we find local spaces similar to used by Morin et al in [21] to be best suited for our problem. This is somewhat surprising since the problem studied by Carstensen et al is a special case of our equation and this is not the case of the problem studied by Morin et al. Afterwards these our general estimates are applied to the cell problems mentioned above. Numerical results for the in-plane effective elastic properties of an effectively transverse isotropic structure are also given.

The main results of this work is the estimates presented in Proposition 1 and Theorem 4. These estimates are applied to the studied applications, giving the main applied results exposed in Corollary 2–5.

The rest of this text is organized as follows. For the sake of completeness, detailed definitions and some preliminarier are given in Section 1.1. The physical problem and the applications in mind are described in Section 1.2-3. In Section 2, we derive the a posteriori error estimates, and in Section 3 apply them to the cell problems. Finally, a numerical example is given.

1.1 Definitions and notation

A point x of the Euclidean space $\mathbf{R}^n$, will be denoted by $x = (x_1, x_2, \ldots, x_n)$. Let X be a subset of $\mathbf{R}^n$. The measure of X will be written $|X|$. The interior and closure of X are denoted by $\mathrm{Int}(X)$ and $\overline{X}$, respectively. We denote the diameter of X by $\mathrm{diam}(X)$ and the radius of the largest ball contained in $\overline{X}$ by θ_X. Let $p_i : \mathbf{R}^n \to \mathbf{R}$ denote the projection map $x \mapsto x_i$.

We will primary work over the field $\mathbf{R}$. The elements of a matrix A will be denoted by A_{ij} or $A_{i,j}$. We denote the set of real symmetric $n \times n$ matrices by $\mathbf{S}$. We denote the set of real skew-symmetric $n \times n$ matrices by $\mathbf{K}$. When we want to emphasize the dimension, we write $\mathbf{S}^n$ and $\mathbf{K}^n$ in place of $\mathbf{S}$ and $\mathbf{K}$, respectively.

The scalar product that will be used on $\mathbf{S}$ is $A \cdot B := \sum_{i,j} A_{ij} B_{ij}$, $A, B \in \mathbf{S}$. In particular, we have $|A|^2 = A \cdot A = \sum_{i,j} A_{ij}^2$. A special matrix norm on $\mathbf{S}$ is

$$||A||_\infty := \max_i \sum_j |A_{ij}|,$$

where $A \in \mathbf{S}$.

Throughout the text we will not explicitly trace all constants in equations and inequalities. For example, by $C = C(\beta)$, where β is some parameter, we will mean a positive real number depending on β and which is independent of the rest of the symbols in the context. So every occurrence of such a C may represent a distinct constant. For example, with $x, y > 0$, we may write $2x + 3y \leq Cx + 3y \leq C(x + y)$. In the first place C may be 2 and in the second it must be at least 3. In either case, C is independent of x and y. Occasionally, we will not explicitly give all dependences. That will be clear from the context.

The set of integers will be denoted by $\mathbf{Z}$ and the set of natural numbers by $\mathbf{N}$, that is the set of nonnegative integers.

1.1.1 Some function spaces

By a domain, we will mean a connected open subset of $\mathbf{R}^n$, $n \geq 2$, which is bounded and Lipschitz. For more on domain regularity properties, see [2] and [23].

Let Ω be a domain. Let $C^k(\Omega)$ be the set of all k times continuously differentiable functions, where $k \in \mathbf{N} \cup \{\infty\}$. We denote by $C^k(\overline{\Omega})$ the set of functions which belongs to $C^k(\Omega)$ and together with their derivatives extend continuously to $\overline{\Omega}$. We say that a function is smooth if it is sufficiently regular in the context.

We denote by $L^2(\Omega)$ the space of square integrable functions $f : \Omega \to \mathbf{R}^d$, $d \geq 1$, with respect to the Lebesgue measure on a domain Ω. What d is will be clear from the context. For $f \in L^2(\Omega)$, we will write $f = (f_1, f_2, \dots, f_d)$. The measure space $L^2(\Omega)$ equipped with the inner product

$$(f, g) := \int_\Omega f \cdot g \, dx$$

forms a Hilbert space. More on the definitions of the usual measure spaces can be found in [10, 28].

For suitable elements of $L^2(\Omega)$, the gradient ∇f is defined as the matrix with elements

$$(\nabla f)_{ij} := \frac{\partial f_i}{\partial x_j},$$

where the partial derivatives will be understood in the sense of distributions. The gradient can be written as follows, where T denotes matrix transpose:

$$\nabla f = \frac{1}{2}(\nabla f + (\nabla f)^T) + \frac{1}{2}(\nabla f - (\nabla f)^T).$$

The first and the second term in the above sum are symmetric and skew-symmetric, respectively. These are naturally called the symmetric and skew-symmetric part of the gradient of f. The symmetric part, the so-called strain map, plays a central role in the linear theory of elasticity, and it is denoted by $e(f)$. The skew-symmetric part will be denoted by $w(f)$. That is

$$e(f) := \frac{1}{2}(\nabla f + (\nabla f)^T), \qquad w(f) := \frac{1}{2}(\nabla f - (\nabla f)^T).$$

We note that the elements of the matrices $e(f)$ and $w(f)$, which we also write $e_{ij}(f)$ and $w_{ij}(f)$, respectively, may be written

$$e_{ij}(f) = \frac{1}{2}\left(\frac{\partial f_i}{\partial x_j} + \frac{\partial f_j}{\partial x_i}\right), \qquad w_{ij}(f) = \frac{1}{2}\left(\frac{\partial f_i}{\partial x_j} - \frac{\partial f_j}{\partial x_i}\right).$$

In particular,

$$|\nabla f|^2 = \sum_{i,j} \left|\frac{\partial f_i}{\partial x_j}\right|^2, \qquad |e(f)|^2 = \frac{1}{4}\sum_{i,j} \left|\frac{\partial f_i}{\partial x_j} + \frac{\partial f_j}{\partial x_i}\right|^2.$$

The divergence of f will be written $\nabla \cdot f$ and is defined by

$$\nabla \cdot f := \sum_i \frac{\partial f_i}{\partial x_i}.$$

The Sobolev space $H^1(\Omega)$ corresponding to $L^2(\Omega)$ is the subspace of $L^2(\Omega)$ where the elements in addition have square integrable gradients in the weak sense. The space $H^1(\Omega)$ is a Hilbert space when equipped with the following inner product:

$$\langle f, g \rangle_{H^1(\Omega)} := (f, g) + (\nabla f, \nabla g). \tag{1}$$

The space $H^1(\Omega)$ is also the completion of all smooth functions with respect to the norm induced by (1). A subspace of $H^1(\Omega)$ of interest is $H^1_0(\Omega)$ which is defined by the condition of vanishing trace on $\partial\Omega$. Some other subsets of $L^2(\Omega)$ which are of interest will be defined below. Let $H^1_{\mathrm{per}}(\Omega)$ be the completion of the set of smooth periodic vector valued functions on Ω, with respect to the $H^1(\Omega)$ norm. For a more extensive exposition on Sobolev spaces, see [2].

The strain map e and its properties will be frequently used in the present text. Let e be defined on $H^1(\Omega)$. The set $\mathcal{R}$ of all elements for which e vanish, its kernel (null space), is an important subspace of $H^1(\Omega)$. The elements of $\mathcal{R}$ are called the rigid body displacements. We have the following characterization:

$$\begin{aligned} \mathcal{R} := \ker(e) &:= \left\{ f \in H^1(\Omega) : e(f) = 0 \right\} \\ &= \left\{ f \in H^1(\Omega) : f = bx + c, b \in \mathbf{K}, c \in \mathbf{R}^n \right\}. \end{aligned} \tag{2}$$

This follows from the Cesaro formula (see [14]). We write $\mathcal{R}^n$ when we want to emphasize the dimension n, where $\Omega \subset \mathbf{R}^n$.

We will follow Kufner's approach to define weighted Sobolev spaces (see [16]). Here we will be using slightly more general weight functions than in [16]. However, we will not need the full machinery of Kufner's exposition. Specifically, we only consider the square integrable functions.

Let $n \geq 2$ and let Ω be a bounded Lipschitz domain in $\mathbf{R}^n$. Let ρ be a nonnegative (positive almost everywhere) measurable function on Ω. Let $k \in \mathbf{N}$. Let α be a multi-index: $\alpha \in \mathbf{R}^n$, $\alpha = (\alpha_1, \ldots, \alpha_n) \in \mathbf{N}^n$. We write $|\alpha| = \sum_i \alpha_i$. The weighted Sobolev space $W^{k,2}(\Omega;\, \rho)$ is defined as the set of all functions u which are defined almost everywhere on Ω and whose derivatives in the sense of distributions $D^\alpha u$ for orders $|\alpha| \leq k$ satisfy

$$\int_\Omega |D^\alpha u|^2 \rho \, dx < \infty.$$

We equip $W^{k,2}(\Omega;\, \rho)$ with the norm defined by

$$||u||_{\Omega,k,\rho} = \sum_{|\alpha| \leq k} \int_\Omega |D^\alpha u|^2 \rho \, dx. \tag{3}$$

For the case $k = 0$, we write $W^{0,2}(\Omega;\, \rho) = L^2(\Omega;\, \rho)$. The space $L^2(\Omega;\, \rho)$ can be regarded as a special case of the space $L^2(S, \Sigma, \mu)$, where (S, Σ, μ) is a measure space. These spaces are separable Banach spaces when equipped with the norm (3). See [11, 30].

The space $W^{k,2}(\Omega;\, \rho)$ can be identified with a closed subspace of the Cartesian product

$$\prod_{|\alpha|\le k} L^2(\Omega;\, \rho),$$

associating an element $u \in W^{k,2}(\Omega;\, \rho)$ with a vector $v \in \Pi_{|\alpha|\le k} L^2(\Omega;\, \rho)$ with u and its derivatives as components belonging to $L^2(\Omega;\, \rho)$. Therefore, the spaces $W^{k,2}(\Omega;\, \rho)$ are separable Banach spaces. The space $W^{1,2}(\Omega;\, \rho)$ will be denoted by $H^1(\Omega;\, \rho)$.

Actually, the space $W^{k,2}(\Omega;\, \rho)$ is a Hilbert space when equipped with the inner product

$$\langle u, v\rangle_{k,\rho,\Omega} = \int_\Omega \Big(\sum_{|\alpha|\le k} D^\alpha u \cdot D^\alpha v \Big) \rho \, dx,$$

which induces the norm (3). The reader may compare with [16].

We collect the various norm of some function u that will be used in suitable function spaces, where ρ is some weight function and A is a suitable function:

$$\begin{aligned}
||u||_{L^2(\Omega)} &:= ||u||_{0,0,\Omega} = (u, u)^{\frac{1}{2}}, \\
||u||_{H^1(\Omega)} &:= ||u||_{0,1,\Omega} = \langle u, u\rangle^{\frac{1}{2}}_{H^1(\Omega)}, \\
||u||_{L^2(\Omega;\, \rho)} &:= ||u||_{0,\rho,\Omega} = \left|\left|\rho^{\frac{1}{2}} u\right|\right|_{L^2(\Omega)} = \langle u, u\rangle^{\frac{1}{2}}_{0,\rho,\Omega}, && (4) \\
||u||_{H^1(\Omega;\, \rho)} &:= ||u||_{1,\rho,\Omega} = \langle u, u\rangle^{\frac{1}{2}}_{1,\rho,\Omega}, && (5) \\
||u||_{E,\rho,\Omega} &:= \left(\int_\Omega e(u) \cdot Ae(u) \rho \, dx \right)^{\frac{1}{2}}. && (6)
\end{aligned}$$

Among the subscripts, the domain will be dropped if it is clear from in context and the weight dropped if it is 1. For example $||u||_{E,1,\Omega} = ||u||_{E,\Omega} = ||u||_E$.

For a normed space V, the set of continuous linear functionals on V will be denoted by V^* and is called the dual space of V. The dual space will be equipped with the norm

$$||q||_{V^*} = \sup \{ |q(v)| : v \in V, ||v||_V = 1 \},$$

which makes it a Banach space.

1.1.2 Setting of the finite elements

Now we fix the setting of the finite elements. Let $\mathcal{T}$ be a simplicial subdivision of Ω. Denote the diameter of a simplex K by

$$h_K := \operatorname{diam}(K).$$

This means that $\mathcal{T}$ is a partition of Ω into n-simplexes and we denote the set of points defining these simplexes by $\mathcal{N}$. The elements of $\mathcal{N}$ will be called the nodes of the so-called mesh $\mathcal{T}$. We assume that the mesh is nondegenerate, that is there exists a positive constant γ such that

$$\max_{K\in\mathcal{T}} \frac{h_K}{\theta_K} \leq \gamma.$$

Let P_m^d be the set of polynomials over $\mathbf{R}$ in d variables of degree less then or equal to m. Let the finite element space V_h on the mesh $\mathcal{T}$ be defined by

$$V_h = \left\{ v \in C^0(\overline{\Omega}) : \forall K \in \mathcal{T}, v_{|K} \in P_m^n \right\}.$$

For further details about the terminology of such meshes see [13, 29].

For $v \in H^1(\Omega)$ and any n-simplex $K \in \mathcal{T}$, we have the following trace inequality (see [13, 18]): There is a nonnegative constant $D = D(\Omega)$ such that

$$||v||_{L^2(\partial K)} \leq D(h_K^{-1/2} ||v||_{L^2(K)} + h_K^{1/2} ||\nabla v||_{L^2(K)}). \tag{7}$$

For finite element interpolation of nonsmooth functions satisfying boundary conditions we will use the Scott-Zhang interpolation operator

$$\pi : H^1(\Omega) \to V_h$$

(see [29] equation (2.13) for the definition). From approximation theory we have the following estimates (see inequality (4.6) in [29]): There are nonnegative constants $C = C(\Omega, \gamma)$ such that

$$\sum_{K\in\mathcal{T}} h_K^{-2} ||u - \pi(u)||_{L^2(K)}^2 \leq C ||u||_{H^1(\Omega)}^2, \tag{8}$$

$$\sum_{K\in\mathcal{T}} ||u - \pi(u)||_{H^1(K)}^2 \leq C ||u||_{H^1(\Omega)}^2, \tag{9}$$

The estimates given above also cover cases when the finite element spaces are of the form $\left\{ v \in V_h : v_{|\Gamma} = 0 \right\}$ for some $\Gamma \subset \partial\Omega$, provided that $\mathcal{T}$ matches Γ appropriately.

For any mesh node $z \in \mathcal{N}$, let ω_z be defined by

$$\omega_z := \operatorname{Int} \bigcup_{\substack{K\in\mathcal{T},\\ z\in\overline{K}}} \overline{K}.$$

The patches ω_z will be called stars of the mesh. Let ϕ_z denote the piecewise affine function $\omega_z \to \mathbf{R}$ satisfying $\phi_z(z) = 1$ and $\phi_{|\partial\omega_z} = 0$. Note that ϕ_z is continuous.

With $K \in \mathcal{T}$, let f be a function with values in $\mathbf{R}^n$ which is defined on the patch

$$\bigcup_{\substack{R\in\mathcal{T},\\ |\partial K\cap\partial R|>0}} \overline{R}.$$

We define the jump function $J_K : \partial K \to \mathbf{R}^n$ by $J_K(f) := f_{|K} - f_{|R}$ on edges for which there exists a neighbouring simplex $R \in \mathcal{T}$ such that $|\partial K \cap \partial R| > 0$, and $J_K(f) := 2f$ otherwise.

1.2 The physical problem

In the theory of elasticity, the deformation of a body, as a result of external forces, is determined by the material properties of the body. Suppose that the body occupies a domain Ω and x is some point in Ω. After a deformation this point is located at $x + u(x)$, where $u = u(x)$ is called the displacement vector. In general, if the deformation is caused by some external forces, internal surface forces arise. Such forces are called stresses and are denoted by σ.

We want to study deformations of the body and the corresponding stresses. Since rigid body displacements (any combination of a translation and a rotation) do not cause any internal forces we want to quantify how much the displacement field u differs from being a rigid body displacement. One possibility is to use the (linearized) strain $e = e(u)$, defined above, which is a function of the displacement field u. As noted above, the null space of e is precisely the set of rigid body displacements.

Material properties are prescribed at the points of the domain Ω. Finally, we assume the internal surface forces σ to be linearly related to the strain e via the Hooke's law:

$$\sigma(u) = Ae(u), \tag{10}$$

where A describes the elastic properties of the material in the body. In this way we have a relation between internal forces on the one hand and the deformation of the structure on the second. Now the equilibrium of forces can be written

$$\nabla \cdot \sigma(u) = f, \tag{11}$$

where f is some force density function. For the existence and uniqueness of a solution u of the equation (11), appropriate conditions on u, Ω, and f are needed. In summary, the state of an elastic body is described by the displacement, the stress, and the strain. Given a displacement u, the elastic energy $W = W(u)$ due to this deformation can be written

$$W(u) := \frac{1}{2} \int_\Omega e(u) \cdot \sigma(u)\, dx. \tag{12}$$

In the usual setting, the quantities above are of the following nature. The domain Ω is some subset of $\mathbf{R}^3$. The displacement vector u is a 3-vector with elements in $H^1(\Omega)$. The linear operator A is a fourth order Cartesian tensor field with Lebesgue measurable components a_{ijkl}. These components satisfy, in addition, the symmetry properties

$$a_{ijkl} = a_{klij} = a_{jikl},$$

for all indices. The stress $\sigma(u)$ and the strain $e(u)$ are both second order Cartesian tensors with components in $L^2(\Omega)$. The derivatives are understood in the sense of distributions. The force density function f lives naturally in $L^2(\Omega)$.

We will exclusively work with the equation (11) written on variational form. For example, when u is required to be zero on the boundary of Ω, we have the Dirichlet problem

$$u \in H_0^1(\Omega), \qquad \int_\Omega e(u) \cdot \sigma(v)\, dx = \int_\Omega f \cdot v\, dx, \quad \forall v \in H_0^1(\Omega). \tag{13}$$

The problem (13) above is usually written as "Find $u \in H_0^1(\Omega)$ such that [...]". However, we will use this more compact notation. Of course, u and v are here zero on $\partial\Omega$ in the sense of traces which imposes restrictions of the domain.

In the present text, we will study a particular application of the above model to periodic structures. The equations appearing are similar to problem (13).

Some classical texts on the linear theory of elasticity are [17, 22].

1.3 Homogenization of periodic structures

Here we will describe a problem of the form of (13) which appears in the study of periodic structures. In physical applications the domain lives in two- or three-space. For our concerns, there is technically no difference, so we will consider perforated periodic structures in $\mathbf{R}^n$, $n \geq 2$. The domain is constructed as follows: Let

$$Y = \prod_{i=1}^{n} \Big(-\frac{l_i}{2}, \frac{l_i}{2} \Big),$$

where $0 < l_i \in \mathbf{R}$, represent one period of the structure. That is Y is a box in $\mathbf{R}^n$, centered at the origin, with side lengths l_i. The domain Y is called the cell of the problem. Let Υ be a finite collection of domains in $\mathbf{R}^n$ such that all elements of Υ intersect Y and are mutually disjoint. Now we define the material domain (the cell) Ω of Y by

$$\Omega = Y \setminus \bigcup_{X \in \Upsilon} \overline{X}.$$

Moreover, we assume that the subset of $\mathbf{R}^n$ occupied by the material,

$$\mathrm{Cl} \bigcup_{\lambda \in \mathbf{Z}^n} (\Omega + (\lambda_1 l_1, \ldots, \lambda_n l_n)),$$

is connected. Note that Ω is the cell which is a bounded domain. The imposed restrictions are of technical nature and will not be used explicitly in what follows. They are however needed for the referred results. An example of such a domain is given below in Figure 1(b) and a part of the resulting structure in Figure 1(a).

The effective elastic properties of a periodic structure is described by the constant tensor A^* defined by

$$\xi \cdot A^* \xi = \frac{1}{|Y|} \min_{u \in H^1_{\mathrm{per}}(\Omega)} \int_\Omega (\xi + e(u)) \cdot A(\xi + e(u))\, dx, \tag{14}$$

where ξ varies over $\mathbf{S}$. This is the cell problem for the cell Y. This is justified by the methods of homogenization where it is known that $A(x/\varepsilon) \to A^*$ as $\varepsilon \to 0$, in the sense of G-convergens (see [14, 24]). When such a minimizer u is found, A^* can be calculated using the relation

$$A^* \xi = \frac{1}{|Y|} \int_\Omega A(\xi + e(u))\, dx \tag{15}$$

and the fact that a minimizer u in (14) also solves the following Euler equation (see [14]):

$$u \in H^1_{\mathrm{per}}(\Omega), \qquad \int_\Omega (\xi + e(u)) \cdot \sigma(v)\, dx = 0, \quad \forall v \in H^1_{\mathrm{per}}(\Omega). \tag{16}$$

For extensive studies of the homogenization problems of linear elasticity, see [3, 19, 24] and the references therein.

Clearly, the minimizer in (14) is unique only up to some element in $\mathcal{R}$. We will single out and work with the unique solution which belongs to the subspace $\widehat{H}^1_{\mathrm{per}}(\Omega)$ of $H^1_{\mathrm{per}}(\Omega)$ defined by

$$\widehat{H}^1_{\mathrm{per}}(\Omega) = \left\{ v \in H^1_{\mathrm{per}}(\Omega) : \int_\Omega v\, dx = 0 \right\}.$$

The reason why it is enough to fix the translation in the definition of $\widehat{H}^1_{\mathrm{per}}(\Omega)$ is that the rotation is fixed by the condition of periodicity (compare Lemma

8 and Lemma 9 below). With $D \in \mathbf{R}^n$ and $\xi \in \mathbf{S}$, let $\Phi_\xi = \xi x + D$. Observe that $e(\Phi_\xi) = \xi$. Now we can write equation (16) as

$$u - \Phi_\xi \in \widehat{H}^1_{\text{per}}(\Omega), \quad \int_\Omega e(u) \cdot \sigma(v)\, dx = 0, \qquad \forall v \in \widehat{H}^1_{\text{per}}(\Omega). \tag{17}$$

We will use the affine function Φ_ξ because then we can write the problem on the form which enables a direct application of Lax-Milgram's lemma.

An application of the finite element method to problem (17) yields the corresponding discrete problem. With $V_h' = \pi(\widehat{H}^1_{\text{per}}(\Omega))$, the discrete equation is

$$u_h - \Phi_\xi \in V_h', \quad \int_\Omega e(u_h) \cdot \sigma(v)\, dx = 0, \qquad \forall v \in V_h'. \tag{18}$$

2 A posteriori error estimates

Here we aim to establish tools for a posteriori error estimation of the error $u_h - u$ appearing when solving the equations (17) and (18). With applications in mind, we are specifically interested in the error in the components of the effective elastic tensor A^* defined by (14), when they are approximated using the discrete solutions. The measuring of this error, as well as other important quantities in applications, can be achieved by the following approach. Suppose that u_h and u live in a subspace V of $H^1(\Omega)$. Let q be a bounded linear functional on V. Then we consider the error

$$\mathcal{E}_q := q(u_h) - q(u). \tag{19}$$

This motivates the exposition of this section.

2.1 A weighted variational problem

In this section we introduce the variational problem that will be considered. We will focus on a slightly more general problem than (17). This is because we want to be able to add weight functions within the integral in (17) in order to estimate the finite element error. A suitable setting for this turns out to be a weighted Sobolev space. Specifically, the space $H^1(\Omega;\, \rho)$ defined above.

After the problem has been presented we establish the existence and uniqueness of a solution. The main tool for this, since $H^1(\Omega;\, \rho)$ is a Hilbert space, is a Korn inequality.

Let Ω be a domain in $\mathbf{R}^n$, $n \geq 2$, and let $A : \Omega \to \mathbf{R}$ be a fourth order Cartesian tensor field. We write the components of A as a_{ijkl}, the indices ranging from 1 to n. We assume that each component of A satisfies

(i) a_{ijkl} is Lebesgue measurable, and

(ii) $a_{ijkl} = a_{klij} = a_{jikl}$, for all indices.

Moreover, we assume that there exist positive constants ν_1, ν_2 such that

$$\nu_1|\xi|^2 \leq \xi \cdot A\xi \leq \nu_2|\xi|^2, \tag{20}$$

for all $\xi \in \mathbf{S}$ and almost every $x \in \Omega$.

Let $\rho \in C^0(\overline{\Omega})$ be a nonnegative function which is positive in Ω. Let V be a closed subspace of $H^1(\Omega;\,\rho)$ equipped with the norm (5). We note that

$$\left\{u \in H^1(\Omega;\,\rho) : e(u) = 0\right\} = \mathcal{R},$$

and is therefore a subset of $H^1(\Omega)$. In particular, this enables the representation (2). Assume that $V \cap \mathcal{R} = \{0\}$. Suppose that $l(v)$ is a bounded linear functional on V. Let $u \in H^1(\Omega;\,\rho)$ be defined by

$$u - \Phi_\xi \in V, \qquad \int_\Omega e(u) \cdot \sigma(v)\rho\, dx = l(v), \quad \forall v \in V, \tag{21}$$

where $D \in \mathbf{R}^n$, $\xi \in \mathbf{S}^n$, and $\Phi_\xi = \xi x + D$.

The following theorem is a version of the classical (second) Korn inequality. A proof can be found in [24] (see Theorem 2.5 on page 19 in [24]). It is slightly rewritten just to match our notation. Recall that the elements of $H^1(\Omega)$, where $\Omega \in \mathbf{R}^n$, take values in $\mathbf{R}^n$.

Theorem 1. *Let Ω be a bounded Lipschitz domain in $\mathbf{R}^n$, $n \geq 2$, and let V be a closed linear subspace of $H^1(\Omega)$, such that $V \cap \mathcal{R} = \{0\}$. Then there exists a positive constant C such that for every $v \in V$,*

$$||v||_{H^1(\Omega)} \leq C\, ||e(v)||_{L^2(\Omega)}\,.$$

By applying some standard arguments (used for example by Carstensen et al in [8]), we can prove the weighted version (Theorem 2) of the Korn inequality.

Denote by Λ^ρ the volume in $\mathbf{R}^{n+1}$ in between the hyperplane defined by $x_{n+1} = 0$ and the graph of ρ:

$$\Lambda^\rho = \left\{(x, y) \in \mathbf{R}^{n+1} : x \in \Omega,\ 0 < y < \rho(x)\right\}.$$

Theorem 2 (A Korn inequality)**.** *Let Ω be a bounded Lipschitz domain in $\mathbf{R}^n$ and let V be a closed subspace of $H^1(\Omega;\,\rho)$, such that $V \cap \mathcal{R} = \{0\}$. Let $\rho \in C^0(\overline{\Omega})$ be a nonnegative function which is positive on Ω. Then there exists a positive constant $C = C(\Omega, \rho)$ such that for every $v \in V$,*

$$||v||_{H^1(\Omega;\,\rho)} \leq C\, ||e(v)||_{L^2(\Omega;\,\rho)}\,.$$

Proof. Let $\Lambda = \Lambda^\rho$. Let W be the space of all functions $(v, 0)$ where $v \in V$ and consider Λ as their domain. We show that W is a closed subspace of $H^1(\Lambda)$ satisfying $W \cap \mathcal{R}^{n+1} = \{0\}$.

We first observe that for $u \in W$, we have $u = (v, 0)$ for some $v \in V$ and u is independent of x_{n+1}. In particular, the gradient of u is of the form

$$\nabla u = \nabla(v, 0) = \begin{pmatrix} \frac{\partial v_1}{\partial x_1} & \frac{\partial v_1}{\partial x_2} & \cdots & \frac{\partial v_1}{\partial x_n} & 0 \\ \frac{\partial v_2}{\partial x_1} & \frac{\partial v_2}{\partial x_2} & \cdots & \frac{\partial v_2}{\partial x_n} & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ \frac{\partial v_n}{\partial x_1} & \frac{\partial v_n}{\partial x_2} & \cdots & \frac{\partial v_n}{\partial x_n} & 0 \\ 0 & 0 & \cdots & 0 & 0 \end{pmatrix}, \tag{22}$$

and $|u| = |v|$, $|\nabla u| = |\nabla v|$.

To show that $W \subset H^1(\Lambda)$, we want to show that

$$\int_\Lambda (|u|^2 + |\nabla u|^2)\, dx < \infty$$

for all $u = (v, 0) \in W$, $v \in V$. The function $|u|^2 + |\nabla u|^2$ is independent of x_{n+1}. Therefore, for almost every $x \in \Omega$ we have

$$\int_0^{\rho(x)} (|u|^2 + |\nabla u|^2)(x, y)\, dy = (|v|^2 + |\nabla v|^2)(x)\rho(x).$$

An integration over Ω yields

$$\begin{aligned} &\int_\Omega \Big(\int_0^{\rho(x)} (|u|^2 + |\nabla u|^2)(x, y)\, dy \Big)\, dx \\ &\quad = \int_\Omega (|v|^2 + |\nabla v|^2)(x)\rho(x)\, dx < \infty, \end{aligned} \tag{23}$$

since $v \in V \subset H^1(\Omega; \rho)$. From Fubini's theorem it follows that

$$\int_\Lambda (|u|^2 + |\nabla u|^2)\, dx = \int_\Omega \Big(\int_0^{\rho(x)} (|u|^2 + |\nabla u|^2)(x, y)\, dy \Big)\, dx < \infty. \tag{24}$$

Thus $u \in H^1(\Lambda)$.

Since V is a closed subspace of $H^1(\Omega; \rho)$, we have that W is a closed subspace of $H^1(\Lambda)$. We will see that $W \cap \mathcal{R}^{n+1} = \{0\}$. Indeed, by letting $v \in W \cap \mathcal{R}^{n+1}$ we can argue as follows. On the one hand, since $v \in W$, there exists a $v' \in V$ such that

$$v = (v', 0). \tag{25}$$

On the other hand, since $v \in \mathcal{R}^{n+1}$, there exist a vector $a \in \mathbf{R}^{n+1}$ and a skew-symmetric matrix $b \in \mathbf{K}^{n+1}$, such that

$$v = a + bx. \tag{26}$$

So the gradient of v must be of the form

$$\nabla v = \nabla(a + bx) = b. \tag{27}$$

By combining (22) and (27), we find that in particular $b_{i,n+1} = 0$ for all $i \in \{1, 2, \ldots, n+1\}$. Let c be the $n \times n$ matrix defined by $c_{i,j} = b_{i,j}$, for $i, j = \{1, 2, \ldots, n\}$. Then $c \in \mathbf{K}^n$. By combining (25) and (26), and making use of the fact that $b_{i,n+1} = 0$, we have

$$v' = cx + a',$$

where $a' = (a_1, a_2, \ldots, a_n)$. Since $c \in \mathbf{K}^n$ and $a' \in \mathbf{R}^n$, we have by (2) that $v' \in \mathcal{R}^n$. But by hypothesis $V \cap \mathcal{R}^n = \{0\}$. Therefore we must have $v = 0$. That proves that $W \cap \mathcal{R}^{n+1} = \{0\}$.

Note that $n+1 \geq 1$ since $n \geq 1$ by hypothesis. The domain Λ is bounded and Lipschitz in $\mathbf{R}^{n+1}$ since ρ is continuously differentiable on Ω. Thus the the Korn inequality (Theorem 1) applies to W. So there exists a positive constant $C = C(\Omega, \rho)$ such that for all $w \in W$ we have

$$||w||_{H^1(\Lambda)} \leq C\, ||e(w)||_{L^2(\Lambda)}\,. \tag{28}$$

Now let $v' \in V$ and let $v = (v', 0)$ be defined on Λ. By (23) and (24), we have that

$$||v||_{H^1(\Lambda)} = \left|\left|v'\right|\right|_{H^1(\Omega;\,\rho)}\,.$$

Similarly, by making use of Fubini's theorem, we find

$$||e(v)||_{L^2(\Lambda)} = \left|\left|e(v')\right|\right|_{L^2(\Omega;\,\rho)}\,.$$

It follows from (28) that

$$\left|\left|v'\right|\right|_{1,\rho} \leq C\, \left|\left|e(v')\right|\right|_{0,\rho}\,. \tag{29}$$

Since v' was an arbitrary element in V, the proof is complete. □

We observe that the norms $||.||_{1,\rho,\Omega}$ and $||.||_{E,\rho,\Omega}$ are equivalent on V.

Lemma 1. *There exist positive constants $C_1 = C_1(\nu_2)$ and $C_2 = C_2(\rho, \Omega, \nu_1)$ such that*

$$C_1\, ||v||_{E,\rho,\Omega} \leq ||v||_{1,\rho,\Omega} \leq C_2\, ||v||_{E,\rho,\Omega}\,, \quad \forall v \in V.$$

Proof. Let $v \in V$. Then by the weighted Korn inequality (Theorem 2) and the first inequality in (20),

$$\begin{aligned} ||v||^2_{H^1(\Omega;\,\rho)} &\leq C(\rho, \Omega)\, ||e(v)||^2_{0,\rho} = C(\rho, \Omega) \int_\Omega |e(v)|^2 \rho\, dx \\ &\leq C(\rho, \Omega, \nu_1) \int_\Omega e(v) \cdot \sigma(v) \rho\, dx = C(\rho, \Omega, \nu_1)\, ||v||^2_{E,\rho}\,. \end{aligned}$$

On the other hand, by the second inequality in (20),

$$
\begin{aligned}
||v||_{E,\rho}^2 &= \int_\Omega e(v)\cdot\sigma(v)\rho\,dx \le C(\nu_2)\int_\Omega |e(v)|^2\rho\,dx \le C(\nu_2)\int_\Omega |\nabla v|^2\rho\,dx \\
&\le C(\nu_2)\int_\Omega (|v|^2+|\nabla v|^2)\rho\,dx = C(\nu_2)\,||v||_{H^1(\Omega;\,\rho)}^2 .
\end{aligned}
$$

Lemma 1 is proved. □

Under the above assumptions, we have

Lemma 2. *There exists a unique element $u \in H^1(\Omega;\,\rho)$ satisfying (21).*

Proof. Let $w \in V$ be defined by

$$\int_\Omega e(w)\cdot\sigma(v)\rho\,dx = l(v) - \int_\Omega \xi\cdot\sigma(v)\rho\,dx, \tag{30}$$

The left hand side of the equality in (30) is obviously bilinear on $V\times V$, and the right hand side linear on V. Let $v_1, v_2 \in V$. Since $\rho \in C^0(\overline{\Omega})$, the fact that A satisfies (20), the left hand side of the equality in (30) can be seen to be bounded on $V\times V$ by making use of the Cauchy-Schwarz inequality and Lemma 1:

$$
\begin{aligned}
\left|\int_\Omega e(v_1)\cdot\sigma(v_2)\rho\,dx\right| &\le \nu_2\int_\Omega |\rho^{\frac12}e(v_1)||\rho^{\frac12}e(v_2)|\,dx \\
&\le \nu_2\,||e(v_1)||_{0,\rho}\,||e(v_2)||_{0,\rho} \\
&\le \nu_2\,||v_1||_V\,||v_2||_V .
\end{aligned}
$$

By the weighted Korn inequality (Theorem 2), Lemma 1, and the first inequality in (20), we have

$$\int_\Omega \rho e(v_1)\cdot\sigma(v_1)\,dx \ge C\int_\Omega \rho|e(v_1)|^2\,dx = C\left|\left|\rho^{\frac12}e(v_1)\right|\right|_{L^2(\Omega)}^2 \ge C\,||v_1||_V^2 .$$

That shows that the left hand side in (30) is coercive on V. By the following estimation, the right hand side can be seen to be a bounded linear functional on V:

$$
\begin{aligned}
\left|l(v_1) - \int_\Omega \xi\cdot\sigma(v_1)\rho\,dx\right| &\le C\,||v_1||_V + \nu_2\int_\Omega |\xi||e(v_1)|\rho\,dx \\
&\le C\,||v_1||_V + \nu_2\,||\xi||_\infty\int_\Omega |e(v_1)|\rho\,dx \\
&\le C\,||v_1||_V + \nu_2\,||\xi||_\infty\left|\left|\rho^{\frac12}\right|\right|_{L^2(\Omega)}||e(v_1)||_{0,\rho} \\
&\le C\,||v_1||_V + \nu_2\,||\xi||_\infty\left|\left|\rho^{\frac12}\right|\right|_{L^2(\Omega)}||v_1||_V \\
&\le C\,||v_1||_V ,
\end{aligned}
$$

where (20), the assumptions on $l(v)$, Lemma 1, and the assumptions on ρ were used. By the Lax-Milgram lemma, that there exists a unique element $w \in V$ that satisfies (30). Now let $u = w + \varphi_\xi$. Then clearly $u \in H^1(\Omega;\rho)$, $u - \varphi_\xi \in V$ and

$$\begin{aligned}\int_\Omega e(u)\cdot\sigma(v)\rho\,dx &= \int_\Omega e(w+\varphi_\xi)\cdot\sigma(v)\rho\,dx\\ &= \int_\Omega e(w)\cdot\sigma(v)\rho\,dx + \int_\Omega e(\varphi_\xi)\cdot\sigma(v)\rho\,dx\\ &= \int_\Omega e(w)\cdot\sigma(v)\rho\,dx + \int_\Omega \xi\cdot\sigma(v)\rho\,dx\\ &= l(v) - \int_\Omega \xi\cdot\sigma(v)\rho\,dx + \int_\Omega \xi\cdot\sigma(v)\rho\,dx = l(v).\end{aligned}$$

So (21) is satisfied and that completes the proof. □

We turn to the discrete problem corresponding to (21). Let $V_h' = \pi(V) \subset V$ be the discrete version of V. Let $u_h \in V_h$ be defined by

$$u_h - \Phi_\xi \in V_h', \qquad \int_\Omega e(u_h)\cdot\sigma(v)\rho\,dx = l(v), \quad \forall v \in V_h', \tag{31}$$

By the same arguments as in the proof of Lemma 2 we have

Lemma 3. *There exists a unique solution $u_h \in V_h$ of the discrete problem (31).*

We have the following Galerkin orthogonality:

Lemma 4. *Suppose that u and u_h satisfy (21) and (31), respectively. Then*

$$\int_\Omega e(u_h - u)\cdot\sigma(v)\rho\,dx = 0, \quad \forall v \in V_h'.$$

Proof. Let $v \in V_h' \subset V$. Then by (21) and (31),

$$\begin{aligned}\int_\Omega e(u_h-u)\cdot\sigma(v)\rho\,dx &= \int_\Omega e(u_h)\cdot\sigma(v)\rho\,dx - \int_\Omega e(u)\cdot\sigma(v)\rho\,dx\\ &= l(v) - l(v) = 0.\end{aligned}$$ □

2.2 A classical estimate

Throughout this section, we will assume that $\rho = 1$ and that A is smooth on each simplex of the mesh $\mathcal{T}$. In particular, this enables local application of the Green's formula. We also suppose that $l(v)$ is bounded on $L^2(\Omega)$. Let $f \in L^2(\Omega)$ be such that $l(v) = (f, v)$ for all $v \in V \subset H^1(\Omega)$. Furthermore, we assume that $\pi(f) = f$.

Recall that q is assumed to be a bounded linear functional on V and we are interested in the error $\mathcal{E}_q = q(u_h) - q(u)$, where u and u_h solve (21) and (31), respectively. To this end, we let $\Psi \in V$ be the solution of the adjoint problem

$$\Psi \in V, \quad \int_\Omega e(\Psi) \cdot \sigma(v)\, dx = q(v), \qquad \forall v \in V. \tag{32}$$

We recall the following formulation of the Green's formula. For $u, v \in H^1(\Omega)$ and if $\sigma(v)$ is smooth, we have

$$\int_{\partial\Omega} u \cdot F(v)\, dx = \int_\Omega e(u) \cdot \sigma(v)\, dx + \int_\Omega u \cdot (\nabla \cdot \sigma(v))\, dx, \tag{33}$$

where $F(v) := \sigma(v)\nu$ and ν is the outward unit normal of Ω (see for example [24]).

This is the classical estimate in n dimensions. See for example [6], for an exposition of the 2-dimensional case.

Proposition 1. *Let u and u_h be the solutions of (21) and (31), respectively. Suppose that $A_{|K}$ is smooth for all $K \in \mathcal{T}$. Assume that $l(v)$ is bounded in $L^2(\Omega)$. Then there is a positive constant $C = C(\Omega, \gamma, \nu_1)$ such that*

$$\mathcal{E}_q^2 \le C\, ||q||_{V^*}^2 \sum_{K \in \mathcal{T}} R_K.$$

where $R_K = h_K^2\, ||\nabla \cdot \sigma(u_h) + f||_{L^2(K)}^2 + h_K\, ||J_K(F(u_h))||_{L^2(\partial K)}^2$.

Proof. By the assumptions on V, V_h', $l(v)$, A and Ω, we have by Lemma 2 and Lemma 3, that u and u_h are well defined. Since $q(v)$ is a bounded linear functional on V, the element Ψ in (32) is well defined by Lemma 2. We note that, by the Korn inequality (Theorem 2 with $\rho = 1$), equation (32), and the first inequality in (20),

$$\begin{aligned} ||\Psi||_{H^1(\Omega)}^2 &\le C(\Omega)\, ||e(\Psi)||_{H^1(\Omega)}^2 = C(\Omega) \int_\Omega e(\Psi) \cdot e(\Psi)\, dx \\ &= C(\Omega, \nu_1) q(\Psi) \le C(\Omega, \nu_1)\, ||q||_{V^*}\, ||\Psi||_{H^1(\Omega)}. \end{aligned}$$

That is

$$||\Psi||_{H^1(\Omega)} \le C(\Omega, \nu_1)\, ||q||_{V^*}. \tag{34}$$

Let $\Psi_\pi = \Psi - \pi(\Psi)$. By equation (32), the Galerkin orthogonality

(Lemma 4), and $\pi(\Psi) \in V_h'$, we have

$$\begin{aligned}
\mathcal{E}_q &= q(u_h) - q(u) = q(u_h - u) = \int_\Omega e(\Psi) \cdot \sigma(u_h - u)\, dx \\
&= \int_\Omega e(\Psi) \cdot \sigma(u_h - u)\, dx - \int_\Omega e(\pi(\Psi)) \cdot \sigma(u_h - u)\, dx \\
&= \int_\Omega e(\Psi_\pi) \cdot \sigma(u_h)\, dx - \int_\Omega e(\Psi_\pi) \cdot \sigma(u)\, dx \\
&= \int_\Omega e(\Psi_\pi) \cdot \sigma(u_h)\, dx - l(\Psi_\pi) = \int_\Omega (e(\Psi_\pi) \cdot \sigma(u_h) - \Psi_\pi \cdot f)\, dx \\
&= \sum_{K \in \mathcal{T}} \int_K (e(\Psi_\pi) \cdot \sigma(u_h) - \Psi_\pi \cdot f)\, dx.
\end{aligned}$$

Since $A_{|K}$ is smooth, we have that $\sigma(u_h)_{|K}$ is smooth. An application of Green's formula on a simplex $K \in \mathcal{T}$ gives

$$\int_K e(\Psi_\pi) \cdot \sigma(u_h)\, dx = \int_{\partial K} \Psi_\pi \cdot F(u_h)\, dx - \int_K \Psi_\pi \cdot \nabla \cdot \sigma(u_h)\, dx.$$

By the Cauchy-Schwarz inequality, and the interpolation inequalities (8) and (9), we have that

$$\begin{aligned}
&\sum_{K \in \mathcal{T}} \int_K (e(\Psi_\pi) \cdot \sigma(u_h) - \Psi_\pi \cdot f)\, dx \\
&\quad = \sum_{K \in \mathcal{T}} \left(\int_{\partial K} \Psi_\pi \cdot F(u_h)\, dx - \int_K \Psi_\pi \cdot (\nabla \cdot \sigma(u_h) + f)\, dx \right) \\
&\quad = \sum_{K \in \mathcal{T}} \left(\frac{1}{2} \int_{\partial K} \Psi_\pi \cdot J_K(F(u_h))\, dx - \int_K \Psi_\pi \cdot (\nabla \cdot \sigma(u_h) + f)\, dx \right) \\
&\quad \leq C(\Omega, \gamma)\, ||\Psi||_{H^1(\Omega)} \left(\Big(\sum_{K \in \mathcal{T}} h_K^2\, ||\nabla \cdot \sigma(u_h) + f||^2_{L^2(K)} \Big)^{\frac{1}{2}} \right. \\
&\qquad\qquad \left. + \left(\sum_{K \in \mathcal{T}} h_K\, ||J_K(F(u_h))||^2_{L^2(\partial K)} \right)^{\frac{1}{2}} \right),
\end{aligned}$$

where we in the last equality used that summing $F(u_h)$ over all edges is the same as summing the jumps of $F(u_h)$ over all edges up to a factor two with corrections for the boundary of Ω. By (34), it follows that

$$\begin{aligned}
\mathcal{E}_q \leq C(\Omega, \gamma, \nu_1)\, ||q||_{V^*} &\left(\Big(\sum_{K \in \mathcal{T}} h_K^2\, ||\nabla \cdot \sigma(u_h) + f||^2_{L^2(K)} \Big)^{\frac{1}{2}} \right. \\
&\qquad \left. + \Big(\sum_{K \in \mathcal{T}} h_K\, ||J_K(F(u_h))||^2_{L^2(\partial K)} \Big)^{\frac{1}{2}} \right),
\end{aligned}$$

which implies

$$\mathcal{E}_q^2 \leq C\,||q||_{V^*}^2 \left(\sum_{K\in\mathcal{T}} h_K^2\,||\nabla\cdot\sigma(u_h)+f||_{L^2(K)}^2 \right.$$
$$\left. + \sum_{K\in\mathcal{T}} h_K\,||J_K(F(u_h))||_{L^2(\partial K)}^2 \right),$$

where $C = C(\Omega, \gamma, \nu_1)$. By the definition of R_K, the proof is complete. □

Remark 1. *In case $\pi(f) \neq f$, approximations of f give rise to a data oscillation term in the residual. See for example [7]. If the domain Ω is not exactly covered by the mesh, an extra term for that approximation appears as well. If the tensor A is not exactly representable in the descretized space, another extra term appears.*

2.3 An estimate via local problems

In the previous subsection, we assumed that the tensor A was smooth on the simplexes of the mesh $\mathcal{T}$. Here, A is again assumed to be general and instead we are a bit more restrictive on the properties of the goal function q. Still, we are interested in estimating the error $\mathcal{E}_q$. This leads to an estimate which is not exactly computable in the sense of Section 2.2. However, it does not contain any unknown constants which was the case above. The extra assumptions on q also have an effect on the finite element space V_h'.

Eventhough, we are mainly interested in the case where $\rho = 1$ as in Section 1.3, we will use a general weight function ρ throughout this section.

Let $\{U_i\}$ be a finite open cover of Ω such that for all U_i there exists an $M \subset \mathcal{T}$ for which

$$U_i = \operatorname{Int} \bigcup_{K\in M} \overline{K}.$$

In that sense, the cover $\{U_i\}$ matches the simplicial subdivision of Ω. Let $\{\varphi_i\}$ be a partition of unity subject to the cover $\{U_i\}$. By this we mean that each φ_i is a positive continuous function on U_i, which vanishes outside U_i. Moreover, we naturally assume that

$$\sum_i \varphi_i = 1.$$

We will consider local problems on the elements of the cover $\{U_i\}$. The corresponding local spaces will be of the following type. For each i, suppose that V_i is a closed subspace of $H^1(U_i;\,\rho)$ such that

(L1) $V_i \cap \mathcal{R} = \{0\}$,

(L2) $V_i \cap (v_{|U_i} + \mathcal{R}) \neq \emptyset, \quad \forall v \in V$.

Let V_i be equipped with the norm

$$||v||_{V_i} := ||v||_{E,\varphi_i\rho,U_i} = \left(\int_{U_i} e(v)\cdot\sigma(v)\varphi_i\rho\,dx\right)^{\frac{1}{2}}. \tag{35}$$

This norm is equivalent to the norm on $H^1(U_i;\,\varphi_i\rho)$ due to (L1) by Lemma 1. The condition (L1) guarantees that V_i is not too big, and the condition (L2) guarantees that V_i is not too small, for our purpose.

Let q be a bounded linear functional on V, where V is the space of Section 2.1. For each i, let Ψ_i^q be defined by

$$\Psi_i^q \in V_i, \qquad \int_{U_i} e(\Psi_i^q)\cdot\sigma(v)\varphi_i\rho\,dx = q(\varphi_i v), \quad \forall v\in V_i. \tag{36}$$

Lemma 5. *The element Ψ_i^q is well defined by (36).*

Proof. Fix i. The space V_i satisfies the conditions on V in Lemma 2, where $\varphi_i\rho$ is used as the weight function. Now we have to show that $v\mapsto q(\varphi_i v)$ is a bounded linear functional on V_i. The linearity and boundedness follows from the fact that these properties are preserved under composition of maps. We have that q and $v\mapsto\varphi_i v$ are linear and bounded. So by Lemma 2 with $\xi=0$, we are done. □

Remark 2. *Note that the condition (L2) was not necessary to establish the existence of Ψ_i^q in Lemma 5. However, the condition (L1) was used.*

Lemma 6. *Let u and u_h be the solutions of the respective problems (21) and (31). Let q be a linear functional on $H^1(\Omega;\,\rho)$ which is bounded on V. Moreover, assume that for each i, $q(\varphi_i\mathcal{R})=\{0\}$. Then*

$$\mathcal{E}_q^2 \le ||u_h-u||_{E,\rho}^2 \sum_i ||\Psi_i^q||_{V_i}^2. \tag{37}$$

Remark 3. *Observe that $||u_h-u||_{E,\rho} = ||u_h-u||_{E,\rho,\Omega}$ in (37).*

Proof of Lemma 6. For each i let $r_i\in\mathcal{R}$ be such that $(u_h-u)_{|U_i}+r_i\in V_i$. This is possible by (L2), since $u_h-u\in V$. Note that $q(\varphi_i r_i)=0$ by hypothesis. Since

$$\sum_i \varphi_i = 1,$$

and q is linear, we can write

$$\begin{aligned} q(u_h-u) &= q\Big((u_h-u)\Big(\sum_i\varphi_i\Big)\Big) = \sum_i q\left(\varphi_i(u_h-u)\right) \\ &= \sum_i\left(q\left(\varphi_i(u_h-u)\right)+q(\varphi_i r_i)\right) = \sum_i q\left(\varphi_i(u_h-u+r_i)\right). \end{aligned}$$

Now, for each i, we have by (36), and by making use of the Cauchy-Schwarz inequality, that

$$\begin{aligned} q(\varphi_i(u_h - u + r_i)) &= \int_{U_i} e(\Psi_i^q) \cdot \sigma(u_h - u + r_i)\varphi_i \rho \, dx \\ &\le \int_{U_i} \left| \varphi_i^{\frac{1}{2}} \rho^{\frac{1}{2}} A^{\frac{1}{2}} e(\Psi_i^q) \right| \left| \varphi_i^{\frac{1}{2}} \rho^{\frac{1}{2}} A^{\frac{1}{2}} e(u_h - u + r_i) \right| \, dx \\ &\le ||\Psi_i^q||_{V_i} \, ||u_h - u + r_i||_{V_i} \, . \end{aligned}$$

Therefore,

$$\begin{aligned} &\mathcal{E}_q = q(u_h) - q(u) = q(u_h - u) \le \sum_i ||\Psi_i^q||_{V_i} \, ||u_h - u + r_i||_{V_i} \\ &\le \left(\sum_i ||\Psi_i^q||_{V_i}^2 \right)^{\frac{1}{2}} \left(\sum_i ||u_h - u + r_i||_{V_i}^2 \right)^{\frac{1}{2}} \\ &= ||u_h - u + r_i||_{E,\rho} \left(\sum_i ||\Psi_i^q||_{V_i}^2 \right)^{\frac{1}{2}} = ||u_h - u||_{E,\rho} \left(\sum_i ||\Psi_i^q||_{V_i}^2 \right)^{\frac{1}{2}}, \end{aligned}$$

where we in the last step used that $e(r_i) = 0$, since $r_i \in \mathcal{R} = \ker(e)$. The assertion (37) immediately follows. □

In order to estimate $||u_h - u||_{E,\rho}$, which appears in Lemma 6, we consider the quantity of interest q_e defined on $H^1(\Omega)$ by

$$q_e(v) = \int_\Omega e(u_h - u) \cdot \sigma(v) \rho \, dx. \tag{38}$$

Note that by the assumptions on u, we can calculate $q_e(v)$ for a given v:

$$q_e(v) = \int_\Omega e(u_h) \cdot \sigma(v)\rho \, dx - \int_\Omega e(u) \cdot \sigma(v)\rho \, dx = \int_\Omega e(u_h) \cdot \sigma(v)\rho \, dx - l(v).$$

For q_e, the condition $q(\varphi_i \mathcal{R}) = \{0\}$ can be realized by imposing the finite element space V_h' to contain certain functions.

Lemma 7. *Suppose that $\varphi_i \mathcal{R} \subset V_h'$. Then $q(\varphi_i \mathcal{R}) = \{0\}$.*

Proof. For any i and any $r \in \mathcal{R}$, we have by hypothesis that $\varphi_i r \in V_h'$. Therefore

$$q_e(\varphi_i r) = \int_\Omega e(u_h - u) \cdot \sigma(\varphi_i r) \rho \, dx = 0,$$

by the Galerkin orthogonality (Lemma 4). □

Theorem 3. *Let u and u_h be the solutions of the respective problems (21) and (31). Let q_e be defined by (38). Moreover, assume that $q(\varphi_i \mathcal{R}) = \{0\}$. Then*

$$||u_h - u||^2_{E,\rho} \leq \sum_i ||\Psi_i^{q_e}||^2_{V_i} .$$

Proof. The function q_e is linear on $H^1(\Omega;\, \rho)$. It is also bounded on V since for $v \in V$,

$$\begin{aligned} |q_e(v)| &= \int_\Omega e(u_h - u) \cdot \sigma(v) \rho \, dx \leq \nu_2 \int_\Omega |\rho^{\frac{1}{2}} e(u_h - u)||\rho^{\frac{1}{2}} e(v)| \, dx \\ &\leq \nu_2 \, ||e(u_h - u)||_{0,\rho} \, ||e(v)||_{0,\rho} \leq \nu_2 \, ||e(u_h - u)||_{0,\rho} \, ||\nabla v||_{0,\rho} \\ &\leq C(\nu_2, u, u_h) \, ||v||_{H^1(\Omega;\, \rho)} \, . \end{aligned}$$

By Lemma 5 with $q = q_e$, for all i there exists a unique element $\Psi_i^{q_e}$ that satisfies (36). So by Lemma 6 we conclude that

$$\mathcal{E}^2_{q_e} \leq ||u_h - u||^2_{E,\rho} \sum_i ||\Psi_i^{q_e}||^2_{V_i} . \tag{39}$$

By definition,

$$\begin{aligned} \mathcal{E}_{q_e} &= q_e(u_h) - q_e(u) = q_e(u_h - u) \\ &= \int_\Omega e(u_h - u) \cdot \sigma(u_h - u) \rho \, dx = ||u_h - u||^2_{E,\rho} . \end{aligned}$$

Thus, by (39),

$$||u_h - u||^4_{E,\rho} \leq ||u_h - u||^2_{E,\rho} \sum_i ||\Psi_i^{q_e}||^2_{V_i} ,$$

which implies

$$||u_h - u||^2_{E,\rho} \leq \sum_i ||\Psi_i^{q_e}||^2_{V_i} .$$

Theorem 3 is proved. □

By using Lemma 3, we find the following estimate for $\mathcal{E}_q$:

Theorem 4. *Suppose that the conditions of Theorem 3 are fulfilled. Let V be equipped with the energy norm $||\cdot||_{E,\rho}$ defined by (6). With q_e defined by (38) and $\Psi_i^{q_e}$ defined by (36) with $q = q_e$, we have*

$$\mathcal{E}^2_q \leq ||q||^2_{V^*} \sum_i ||\Psi_i^{q_e}||^2_{V_i} .$$

Proof. Let $\Psi \in V$ be the solution of problem (32). Then we can write

$$\mathcal{E}_q = q(u_h) - q(u) = q(u_h - u) = \int_\Omega e(\Psi) \cdot \sigma(u_h - u)\rho \, dx$$
$$\leq \int_\Omega \left|\rho^{\frac{1}{2}} A^{\frac{1}{2}} e(\Psi)\right| \left|\rho^{\frac{1}{2}} A^{\frac{1}{2}} e(u_h - u)\right| \, dx \leq ||\Psi||_{E,\rho} \, ||u_h - u||_{E,\rho} \, .$$

Since V is equipped with the energy norm $||\cdot||_{E,\rho}$ we have

$$||\Psi||^2_{E,\rho} = \int_\Omega e(\Psi) \cdot \sigma(\Psi)\rho \, dx = q(\Psi) \leq ||q||_{V^*} \, ||\Psi||_{E,\rho} \, ,$$

and thus

$$||\Psi||_{E,\rho} \leq ||q||_{V^*} \, .$$

Now by Theorem 3,

$$\mathcal{E}_q^2 \leq ||q||^2_{V^*} \sum_i ||\Psi_i^{q_e}||^2_{V_i} \, . \qquad \square$$

Remark 4. *One natural cover is* $\{\omega_z\}_{z\in\mathcal{N}}$ *which can be paired with the partition of unity consisting of the first order finite element functions* $\{\phi_z\}_{z\in\mathcal{N}}$*.*

3 Estimates for the effective properties

In this section, we will apply the results of the previous section to estimate the error occurring when approximating the effective elastic properties. Recall the domain $\Omega \subset \mathbf{R}^n$ defined in Section 1.3.

For the weighted space, we define a space corresponding to $H^1_{\text{per}}(\Omega)$. Let $H^1_{\text{per}}(\Omega;\, \rho)$ be the set of $H^1(\Omega;\, \rho)$ functions which is Ω-periodic in the sense of traces. Now let

$$\widehat{H}^1_{\text{per}}(\Omega;\, \rho) := \left\{ u \in H^1_{\text{per}}(\Omega;\, \rho) : \int_\Omega u\rho \, dx = 0 \right\}.$$

First we observe that $\widehat{H}^1_{\text{per}}(\Omega;\, \rho)$ satisfies the conditions of V in Section 2.1. That gives that the equations (17) and (18) is of the same kind as the equations (21) and (31), respectively.

Lemma 8. *Let* Y *and* Ω *be a cell and a domain in* $\mathbf{R}^n$*,* $n \geq 2$*, of the type of Section 1.3. Then* $\widehat{H}^1_{\text{per}}(\Omega;\, \rho)$ *is a closed subspace of* $H^1_{\text{per}}(\Omega;\, \rho)$*. Moreover, it is the algebraic complement of* $\mathcal{R}$*:*

$$H^1_{\text{per}}(\Omega;\, \rho) = \widehat{H}^1_{\text{per}}(\Omega;\, \rho) \oplus \mathcal{R}.$$

Proof. Clearly, $\widehat{H}^1_{\text{per}}(\Omega;\,\rho)$ is a closed subspace of $H^1_{\text{per}}(\Omega;\,\rho)$.

Let $u \in H^1_{\text{per}}(\Omega;\,\rho)\cap\mathcal{R}$. Then $u \in H^1_{\text{per}}(\Omega)$ since $\mathcal{R} \subset H^1_{\text{per}}(\Omega)$. Moreover, since $u \in \mathcal{R}$ we have by (2) that there exist $a \in \mathbf{R}^n$, $b \in \mathbf{K}^n$ such that $u = a + bx$. Moreover, since $u \in \widehat{H}^1_{\text{per}}(\Omega)$,

$$u_{|x_i=-\frac{l_i}{2}} = u_{|x_i=\frac{l_i}{2}},$$

for $i = 1, \dots, n$. This together with $u = a + bx$ implies that $b = 0$. Furthermore, since $u \in \widehat{H}^1_{\text{per}}(\Omega)$, we have

$$\int_\Omega u\,dx = \int_\Omega a\,dx = |\Omega|a,$$

which implies that $a = 0 \in \mathbf{R}^n$. Therefore, we must have $u = 0 \in H^1_{\text{per}}(\Omega;\,\rho)$.

Now let $u \in H^1_{\text{per}}(\Omega;\,\rho)$ and put

$$r = \frac{\int_\Omega u\rho\,dx}{\int_\Omega \rho\,dx}.$$

Then clearly $r \in \mathcal{R} \cap H^1_{\text{per}}(\Omega;\,\rho)$. Set $v = u - r$. Then v is periodic since $u, r \in H^1_{\text{per}}(\Omega;\,\rho)$. Moreover,

$$\begin{aligned}\int_\Omega v\rho\,dx &= \int_\Omega u\rho\,dx - \int_\Omega r\rho\,dx \\ &= \int_\Omega u\rho\,dx - \Big(\int_\Omega \rho\,dx\Big)^{-1}\int_\Omega \Big(\int_\Omega u\rho\,dx\Big)\rho\,dx \\ &= \int_\Omega u\rho\,dx - \int_\Omega u\rho\,dx = 0.\end{aligned}$$

Thus $v \in \widehat{H}^1_{\text{per}}(\Omega;\,\rho)$. That proves that $\widehat{H}^1_{\text{per}}(\Omega;\,\rho)$ and $\mathcal{R}$ span $H^1_{\text{per}}(\Omega;\,\rho)$. Moreover, that the decomposition $u = v + r$ is unique for all $u \in H^1_{\text{per}}(\Omega;\,\rho)$ with $v \in \widehat{H}^1_{\text{per}}(\Omega;\,\rho)$ and $r \in \mathcal{R}$. □

Put $\rho = 1$, $l(v) = 0$. By Lemma 8, clearly $\widehat{H}^1_{\text{per}}(\Omega) \cap \mathcal{R} = \{0\}$ holds. Thus we are in the setting of Section 2.1. Therefore, the elements u and u_h are well defined by (17) and (18), respectively, by Lemma 2.

In three dimensions ($n = 3$), we have by the symmetry assumptions in (ii), that there are in general 21 unknown elements of A^* to be calculated. In terms of the Voight representation (see for example [5]), let ξ_m be the mth canonical basis vector in $\mathbf{R}^6$. Then the components of A^* can be found by solving (17) with $\xi = \xi_i$ and then use (15). The corresponding approximations are found by solving (18). For example, by (15), we have

$$a^*_{1111} = \frac{p_1}{|Y|}\int_\Omega \sigma(u)\,dx, \quad \text{for } \xi_1. \tag{40}$$

The rest of the components can be calculated using the various ξ_i and different projections p_j in (40). We are therefore interested in the quantity of interest q_j defined by

$$q_j(v) := \frac{p_j}{|Y|} \int_\Omega \sigma(v)\, dx,$$

and the error

$$\mathcal{E}_{q_j} = q_j(u_h) - q_j(u),$$

for j in the set $\{1, \ldots, 6\}$.

Proposition 2. *Suppose that u_h and u are the solutions of the respective problems (17) and (18). Let $j \in \{1, \ldots, 6\}$. Then there exists a positive constant $C = C(Y, \Omega, \gamma, \nu_1, \nu_2)$ such that*

$$\mathcal{E}_{q_j}^2 \leq C \sum_{K \in \mathcal{T}} Q_K,$$

where

$$Q_K = h_K^2 \,||\nabla \cdot \sigma(u_h)||_{L^2(K)}^2 + h_K \,||J_K(F(u_h))||_{L^2(\partial K)}^2 . \tag{41}$$

Proof. We show that q_j is a quantity function satisfying the conditions of Proposition 1. The function q_j is clearly linear on $\widehat{H}^1_{\text{per}}(\Omega)$. Moreover, for $v \in \widehat{H}^1_{\text{per}}(\Omega)$ and $j \in \{1, \ldots, 6\}$, we have by the second inequality in (20),

$$\begin{aligned} |q_i(v)| &= \left| \frac{p_i}{|Y|} \int_\Omega \sigma(v)\, dx \right| \leq \frac{1}{|Y|} \int_\Omega |\sigma(v)|\, dx \leq \frac{\nu_2}{|Y|} \int_\Omega |e(v)|\, dx \\ &\leq \frac{\nu_2 \sqrt{|\Omega|}}{|Y|} \,||e(v)||_{L^2(\Omega)} \leq \frac{\nu_2 \sqrt{|\Omega|}}{|Y|} \,||v||_{H^1(\Omega)} = \frac{\nu_2 \sqrt{|\Omega|}}{|Y|} \,||v||_{\widehat{H}^1_{\text{per}}(\Omega)} , \end{aligned}$$

which shows that q_j is bounded on $\widehat{H}^1_{\text{per}}(\Omega)$. Therefore,

$$||q_j||_{(\widehat{H}^1_{\text{per}}(\Omega))^*} = \sup \left\{ |q_j(v)| : v \in \widehat{H}^1_{\text{per}}(\Omega), ||v||_{\widehat{H}^1_{\text{per}}(\Omega)} = 1 \right\} \leq \frac{\nu_2 \sqrt{|\Omega|}}{|Y|}.$$

So by Proposition 1, there exists a constant $C = C(\Omega, \gamma, \nu_1)$ such that

$$\mathcal{E}_{q_j}^2 \leq C \frac{\nu_2^2 |\Omega|}{|Y|^2} \sum_{K \in \mathcal{T}} Q_K = C(Y, \Omega, \gamma, \nu_1, \nu_2) \sum_{K \in \mathcal{T}} Q_K,$$

where Q_K is defined by equation (41). $\square$

In view of equation (15), the diagonal components a^*_{iijj} of the effective elastic tensor can be expressed as a constant multiple of the elastic energy of u. In fact, for two-dimensional problems with high order of symmetry, this holds for all components of the effective tensor. Therefore, a natural goal function is

$$q_E(v) := \frac{q_e(v)}{2} = \frac{1}{2}\int_\Omega e(u_h - u)\cdot\sigma(v)\,dx.$$

Recall that the elastic energy is defined by (12). Note that by equation (17), $q_E(u) = 0$. Therefore,

$$\begin{aligned}\mathcal{E}_{q_E} &:= q_E(u_h) - q_E(u) = q_E(u_h)\\ &= \frac{1}{2}\int_\Omega e(u_h - u)\cdot\sigma(u_h)\,dx = W(u_h) - W(u),\end{aligned}$$

which is the error in the energy, see equation (12).

Proposition 3. *Suppose that u_h and u are the solutions of the respective problems (17) and (18). Then there exists a positive constant $C = C(\Omega,\gamma,\nu_1)$ such that*

$$\mathcal{E}_{q_E} \le C\sum_{K\in\mathcal{T}} Q_K,$$

where Q_K is defined by (41).

Proof. The function q_E is linear on $\widehat{H}^1_{\text{per}}(\Omega)$. By the second inequality in (20), for any $v \in \widehat{H}^1_{\text{per}}(\Omega)$,

$$\begin{aligned}|q_E(v)| = \left|\frac{1}{2}\int_\Omega e(u_h-u)\cdot\sigma(v)\,dx\right| &\le \frac{1}{2}\int_\Omega |\sigma(u_h-u)||e(v)|\,dx\\ &\le \frac{1}{2}\left|\left|A^{\frac{1}{2}}e(u_h-u)\right|\right|_{L^2(\Omega)}||e(v)||_{L^2(\Omega)}\\ &\le \frac{1}{2}\left|\left|A^{\frac{1}{2}}e(u_h-u)\right|\right|_{L^2(\Omega)}||v||_{\widehat{H}^1_{\text{per}}(\Omega)}.\end{aligned}$$

Thus q_E is bounded on $\widehat{H}^1_{\text{per}}(\Omega)$. We note that

$$\begin{aligned}\left|\left|A^{\frac{1}{2}}e(u_h-u)\right|\right|^2_{L^2(\Omega)} &= \int_\Omega e(u_h-u)\cdot\sigma(u_h-u)\,dx\\ &= 2q(u_h-u) = 2(q(u_h)-q(u)) = 2\mathcal{E}_{q_E}.\end{aligned}$$

Therefore,

$$|q_E(v)| \le \sqrt{\frac{\mathcal{E}_{q_E}}{2}}\,||v||_{\widehat{H}^1_{\text{per}}(\Omega)}.$$

We find

$$||q_E||_{(\widehat{H}^1_{\text{per}}(\Omega))^*} = \sup\left\{|q_E(v)| : v\in\widehat{H}^1_{\text{per}}(\Omega), ||v||_{\widehat{H}^1_{\text{per}}(\Omega)} = 1\right\} \le \sqrt{\frac{\mathcal{E}_{q_E}}{2}}.$$

By Proposition 1, there exists a constant $C = C(\Omega, \gamma, \nu_1)$ such that

$$\mathcal{E}_{q_E}^2 \le C\mathcal{E}_{q_E} \sum_{K\in\mathcal{T}} Q_K,$$

where Q_K is defined by equation (41). It follows that

$$\mathcal{E}_{q_E} \le C(\Omega, \gamma, \nu_1) \sum_{K\in\mathcal{T}} Q_K. \qquad \square$$

Now we apply the results of Section 2.3 to the same linear functions of interest. To this end we define the space $\widehat{H}^1(\Omega;\, \rho)$ by

$$\widehat{H}^1(\Omega;\, \rho) := \left\{ v \in H^1(\Omega;\, \rho) : \int_\Omega v\rho\, dx = \int_\Omega w(v)\rho\, dx = 0 \right\},$$

where w is the skew-symmetric part of the gradient (see Section 1.1). We note that we have the following decomposition. The proofs of the following two lemmas will follow the route of Brenner and Scott (see [6]) and extend it to $\mathbf{R}^n$ and the weighted spaces.

Lemma 9. *Let Ω be a domain in $\mathbf{R}^n$, $n \ge 2$. Then the space $\widehat{H}^1(\Omega;\, \rho)$ is a closed subspace of $H^1(\Omega;\, \rho)$. Moreover, it is the algebraic complement of $\mathcal{R}$:*

$$H^1(\Omega;\, \rho) = \widehat{H}^1(\Omega;\, \rho) \oplus \mathcal{R}.$$

Proof. Clearly, $\widehat{H}^1(\Omega;\, \rho)$ is a closed subspace of $H^1(\Omega;\, \rho)$. Suppose that $u \in \widehat{H}^1(\Omega;\, \rho) \cap \mathcal{R}$. Moreover, since $u \in \mathcal{R}$ we have by Lemma 2 that there exist $a \in \mathbf{R}^n$, $b \in \mathbf{K}^n$ such that $u = a + bx$. Since $u \in \widehat{H}^1(\Omega;\, \rho)$ we have

$$\int_\Omega \left(\frac{\partial u_i}{\partial x_j} - \frac{\partial u_j}{\partial x_i} \right) \rho\, dx = 0, \quad \forall i, j.$$

This combined with $u = a+bx$ implies $b = 0$. Moreover, since $u \in \widehat{H}^1(\Omega;\, \rho)$,

$$0 = \int_\Omega u\rho\, dx = a \int_\Omega \rho\, dx,$$

which implies $a = 0$ since $\int_\Omega \rho\, dx > 0$. Therefore, we must have $u = 0$.

So if $\widehat{H}^1(\Omega;\, \rho)$ and $\mathcal{R}$ span $H^1(\Omega;\, \rho)$, we have for all $u \in H^1(\Omega;\, \rho)$, the decomposition $u = v + r$ is unique, where $v \in \widehat{H}^1(\Omega;\, \rho)$ and $r \in \mathcal{R}$. Let $u \in H^1(\Omega;\, \rho)$ and put $r = a + bx$ with

$$b = \frac{\int_\Omega w(u)\rho\, dx}{\int_\Omega \rho\, dx}, \qquad a = \frac{\int_\Omega (u - bx)\rho\, dx}{\int_\Omega \rho\, dx}.$$

Then clearly $r \in \mathcal{R}$. Now let $v = u - r$. Then

$$\begin{aligned}
&\int_\Omega v\rho\,dx \\
&= \int_\Omega u\rho\,dx - \int_\Omega r\rho\,dx = \int_\Omega u\rho\,dx - \int_\Omega a\rho\,dx - \int_\Omega bx\rho\,dx \\
&= \int_\Omega u\rho\,dx - \Big(\int_\Omega \rho\,dx\Big)^{-1} \int_\Omega \Big(\int_\Omega (u - bx)\rho\,dx\Big)\,dx - \int_\Omega bx\rho\,dx \\
&= \int_\Omega u\rho\,dx - \int_\Omega (u - bx)\rho\,dx - \int_\Omega bx\rho\,dx \\
&= 0.
\end{aligned}$$

Moreover,

$$\begin{aligned}
\int_\Omega w(v)\rho\,dx &= \int_\Omega w(u)\rho\,dx - \int_\Omega w(r)\rho\,dx \\
&= \int_\Omega w(u)\rho\,dx - \int_\Omega w(a + bx)\rho\,dx \\
&= \int_\Omega w(u)\rho\,dx - \int_\Omega b\rho\,dx \\
&= \int_\Omega w(u)\rho\,dx - \Big(\int_\Omega \rho\,dx\Big)^{-1} \int_\Omega \Big(\int_\Omega w(u)\rho\,dx\Big)\,dx \\
&= 0.
\end{aligned}$$

Thus $v \in \widehat{H}^1(\Omega;\,\rho)$ and the proof is comlete. □

We need to specify the spaces V_i and we choose $V_i = \widehat{H}^1(U_i;\,\varphi_i)$. Note that $\widehat{H}^1(U_i;\,\varphi_i)$ is here equipped with the norm (35), that is $||\cdot||_{\widehat{H}^1(U_i;\,\varphi_i)} = ||\cdot||_{E,\varphi_i,U_i}$ since we have $\rho = 1$ here. Let $\Psi_i^{q_e}$ be defined by (36).

Proposition 4. *Suppose that u_h and u are the solutions of the respective problems (17) and (18). Moreover, suppose that $q(\varphi_i\mathcal{R}) = \{0\}$. Then*

$$\mathcal{E}_{q_j}^2 \le \frac{\nu_2^2|\Omega|}{\nu_1|Y|^2} \sum_i ||\Psi_i^{q_e}||^2_{\widehat{H}^1(U_i;\,\varphi_i)}\,.$$

Proof. Directly from Lemma 9, it follows that the conditions (L1) and (L2) are satisfied, where $V = \widehat{H}^1_{\text{per}}(\Omega)$. An application of Proposition 4 yields

$$\mathcal{E}_{q_j}^2 \le ||q_j||^2_{(\widehat{H}^1_{\text{per}}(\Omega))^*} \sum_i ||\Psi_i^{q_e}||^2_{\widehat{H}^1(U_i;\,\varphi_i)}\,.$$

For $v \in \widehat{H}^1_{\text{per}}(\Omega)$,

$$|q_i(v)| = \left|\frac{p_i}{|Y|}\int_\Omega \sigma(v)\,dx\right| \le \frac{1}{|Y|}\int_\Omega |\sigma(v)|\,dx \le \frac{\sqrt{|\Omega|}}{|Y|}\frac{\nu_2}{\sqrt{\nu_1}}\,||v||_E\,.$$

Therefore,

$$||q_i||_{(\widehat{H}^1_{\text{per}}(\Omega))^*} = \sup\left\{|q_i(v)| : v \in \widehat{H}^1_{\text{per}}(\Omega), ||v||_E = 1\right\} \le \frac{\sqrt{|\Omega|}}{|Y|}\frac{\nu_2}{\sqrt{\nu_1}}.$$

It follows that

$$\mathcal{E}^2_{q_i} \le \frac{\nu_2^2|\Omega|}{\nu_1|Y|^2}\sum_i ||\Psi_i^{q_e}||^2_{\widehat{H}^1(U_i;\varphi_i)}\,. \qquad \square$$

Proposition 5. *Suppose that u_h and u are the solutions of the respective problems (17) and (18). Moreover, suppose that $q(\varphi_i\mathcal{R}) = \{0\}$. Then*

$$\mathcal{E}_{q_E} \le 2\sum_i ||\Psi_i^{q_E}||^2_{V_i}\,.$$

Proof. We note that

$$2\mathcal{E}_{q_E} = q_e(u_h - u) = ||u_h - u||^2_E\,.$$

By Lemma 3,

$$\mathcal{E}_{q_E} \le \frac{1}{2}\sum_i ||\Psi_i^{q_e}||^2_{V_i} \le 2\sum_i ||\Psi_i^{q_E}||^2_{V_i}\,. \qquad \square$$

3.1 A numerical example

Here we will demonstrate the above estimates on the task of calculating the in-plane effective bulk and shear moduli K^* and G^* of a regular triangular honeycomb.

The cross-section is showed in Figure 1(a). A Y-cell with domain Ω is showed in Figure 1(b). This cell is only one quarter of a usual cell as described in Section 1.3. Here we have used the symmetry of the domain and the local elastic tensor A, which is assumed to be homogeneous and in-plane isotropic, to calculate on the smallest possible domain.

We will use a local material with (constant) bulk and shear moduli $K = G = 1/2$. Therefore, the local elasticity tensor, written in Voight's notation, is

$$A = \begin{pmatrix} K+G & K-G & 0 \\ K-G & K+G & 0 \\ 0 & 0 & G \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1/2 \end{pmatrix}.$$

The eigenvalues of A are 1 and 1/2. So we can take $\nu_1 = 1/2$ and $\nu_2 = 1$ in (20).

The shear modulus G is the ordinary shear modulus. How the bulk modulus K is related to the corresponding three-dimensional bulk modulus depends on the application in mind. See for example [17], for the cases of plane strain and plane stress.

It can be showed that the structure is in-plane effectively isotropic due to its three-fold rotational symmetry. The effective tensor A^*, written in matrix form, is of the form

$$A^* = \begin{pmatrix} K^* + G^* & K^* - G^* & 0 \\ K^* - G^* & K^* + G^* & 0 \\ 0 & 0 & G^* \end{pmatrix},$$

where K^* is the effective in-plane bulk modulus.

The volume fraction occupied by the solid material, is 1/2, that is

$$\frac{1}{2} = \frac{|\Omega|}{|Y|}.$$

See [4] for an explicit definition of the domain $\Omega \subset \mathbf{R}^2$.

Let the unit cell be $Y' = (-\frac{\sqrt{3}}{2}, \frac{\sqrt{3}}{2}) \times (-\frac{1}{2}, \frac{1}{2})$ and let $Y = (0, \frac{\sqrt{3}}{2}) \times (0, \frac{1}{2})$ be a quarter cell (the domain shown in Figure 1(b)). Let Ω be the solid domain of Figure 1(b). We name some parts of the boundary of Ω as follows:

$$\Gamma_1 = \{x \in \partial\Omega : x_1 = 0\}, \qquad \Gamma_2 = \{x \in \partial\Omega : x_2 = 0\},$$
$$\Gamma_3 = \left\{x \in \partial\Omega : x_1 = \frac{\sqrt{3}}{2}\right\}, \quad \Gamma_4 = \left\{x \in \partial\Omega : x_2 = \frac{1}{2}\right\}.$$

The test function space takes the form

$$V' = \left\{v \in H^1(\Omega) : v_{1|\Gamma_1} = v_{1|\Gamma_3} = v_{2|\Gamma_2} = v_{2|\Gamma_4} = 0\right\}.$$

By Section 1.3 and the results in [3, 19], using the symmetry of the domain, we may solve the following problem in order to calculate an approximation of G^*: Find $u \in H^1(\Omega)$ such that

$$u_{1|\Gamma_1} = v_{2|\Gamma_2} = 0, \quad u_{1|\Gamma_3} = \frac{\sqrt{3}}{2}, \quad u_{2|\Gamma_4} = -\frac{1}{2},$$
$$\int_\Omega e(u) \cdot Ae(v)\, dx = 0, \quad \forall v \in V'. \tag{42}$$

Then

$$G^* = \frac{W(u)}{2|Y|}, \tag{43}$$

where $W(u)$ is the elastic energy of the deformation field u defined by (12). The corresponding problem of K^* is when the condition on $u_{2|\Gamma_4}$ is replaced with $u_{2|\Gamma_4} = \frac{1}{2}$ in (42) and we have

$$K^* = \frac{W(u)}{2|Y|}. \tag{44}$$

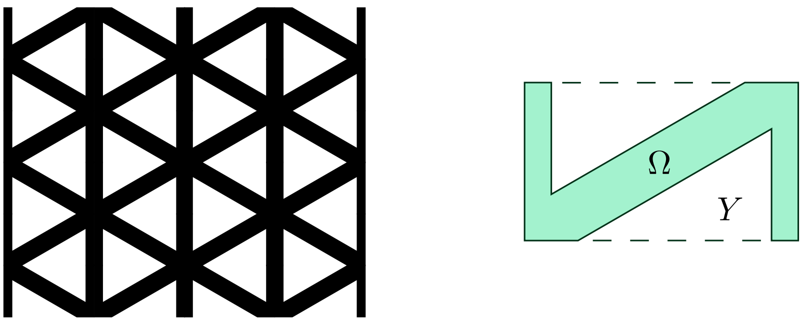
When calculating the local problem estimate we will use the natural partition of unity of the domain Ω as described in Remark 4. Denote by W_z the space $H^1(\omega_z;\, \phi_z)$. For stars $\omega_z \subset \Omega$ for which $\overline{\omega_z}$ does not intersect the Dirichlet type boundary ∂Y, we will use the local spaces

$$V_z = V_i = \widehat{H}^1(\omega_z;\, \phi_z), \quad \text{for} \quad \overline{\omega_z} \cap \partial Y = \emptyset,$$

and for the rest $V_z = V_\delta$, $\delta \in \{A, B, C, D, e, f, g, h\}$, where

$$\begin{aligned}
V_A &= \left\{ v \in W_z : v_{1|\Gamma_1} = v_{2|\Gamma_2} = 0 \right\}, \quad \text{for} \quad z \in \Gamma_1 \cap \Gamma_4,\\
V_B &= \left\{ v \in W_z : v_{1|\Gamma_1} = v_{2|\Gamma_2} = 0 \right\}, \quad \text{for} \quad z \in \Gamma_1 \cap \Gamma_2,\\
V_C &= \left\{ v \in W_z : v_{1|\Gamma_2} = v_{2|\Gamma_3} = 0 \right\}, \quad \text{for} \quad z \in \Gamma_2 \cap \Gamma_3,\\
V_D &= \left\{ v \in W_z : v_{1|\Gamma_3} = v_{2|\Gamma_4} = 0 \right\}, \quad \text{for} \quad z \in \Gamma_3 \cap \Gamma_4,\\
V_e &= \left\{ v \in W_z : v_{1|\Gamma_1} = \int_{\omega_z} v_2 \phi_z \, dx = 0 \right\}, \quad \text{for} \quad z \in \Gamma_1,\ z \notin \Gamma_2 \cup \Gamma_4,\\
V_f &= \left\{ v \in W_z : \int_{\omega_z} v_1 \phi_z \, dx = v_{2|\Gamma_2} = 0 \right\}, \quad \text{for} \quad z \in \Gamma_2,\ z \notin \Gamma_1 \cup \Gamma_3,\\
V_g &= \left\{ v \in W_z : v_{1|\Gamma_3} = \int_{\omega_z} v_2 \phi_z \, dx = 0 \right\}, \quad \text{for} \quad z \in \Gamma_3,\ z \notin \Gamma_2 \cup \Gamma_4,\\
V_h &= \left\{ v \in W_z : \int_{\omega_z} v_1 \phi_z \, dx = v_{2|\Gamma_4} = 0 \right\}, \quad \text{for} \quad z \in \Gamma_4,\ z \notin \Gamma_1 \cup \Gamma_3.
\end{aligned}$$

See Figure 2 for an illustration of the roles of these spaces.



(a) (b)

Figure 1: The cross-section (a) and a quarter of a unit cell (b) of a regular triangular honeycomb of volume fraction 1/2. In (a), the light space is assumed to be void and the dark area is an in-plane isotropic material with local elastic tensor A. In (b), the coloured area is the domain Ω of the local tensor A, and the whole rectangle, the cell, is Y.

These are closed subspaces of $H^1(\omega_z;\, \phi_z) = W_z$ satisfying the conditions (L1), (L2) and $V_z \cap \mathcal{R} = \{0\}$, when the second order finite element functions are used. Moreover, for q_E we have $q_E(\phi_z \mathcal{R}) = \{0\}$.

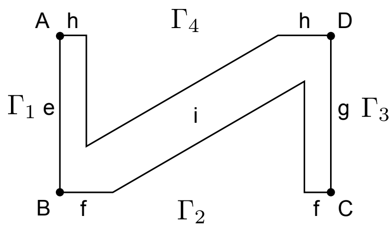


Figure 2: The symbols alongside the parts of the domain illustrate the local spaces used in the different parts. A symbol δ represents the subscript in V_z, that is $V_z = V_\delta$.

Since we do not know the exact solution of the problem, we cannot calculate the exact error in G^*. Therefore, we will use a reference value G^*_{ref} which is obtained by solving the problem numerically for a much finer mesh than in the example below. We will use $K^*_{\text{ref}} = 0.15172$ and $G^*_{\text{ref}} = 0.08796$, which we believe satisfy $0 < K^*_{\text{ref}} - K^* < 10^{-5}$ and $0 < G^*_{\text{ref}} - G^* < 10^{-5}$ (see [4]).

We use first and second order finite element function to calculate approximations u_h of the problem (42). Then the approximation G^*_h of G^* is obtained by substituting u with u_h in (43). Doing so with uniform mesh refinement yields the circle and square marked graphs in Figure 4. The degrees of freedom shown on the horizontal axis is the number of unknowns in the linear system of equations obtained by the discretization.

The estimate of Theorem 3 can be used as a basis for an adaptive method. We calculate the residuals R_K and refine those with R_K greater then some thresshold κ. We let κ be the average value of the residuals. The graphs of this method for the first and the second order finite element functions are shown as rhombus and triangle marked graphs in Figure 4. Another adaptive method is obtained by choosing κ to be the average of the residuals $||\Psi^{q_E}||_z$ in Theorem 3. This will be called the method based on local problems (on stars). The result is shown as star marked (solid) graph in Figure 4. We use second order finite element functions for this method.

We discretize each star ω_z with a finer mesh use the second order finite element method to approximate $\Psi^{q_E}_z$.

By comparing the slopes of the graphs in Figure 4 we can get an idea of the rate of convergence of the various methods in the studied interval of degrees of freedom. For comparison purposes the triangles in the figure show the slopes of the functions $x^{-1/2}$, x^{-1}, and x^{-2}, where x is the degrees of freedom. We see that all the adaptive methods give better results than their respective uniform method. In particular, the method based on the local problems estimates on stars seems to be equally good as the classical second order method (compare the triangle and star marked (solid) graphs in Figure 4). However, one can argue that more computational work is needed to calculate the residuals in the local problems estimate than in the classical estimate.

One can make the following somewhat unprecise argument about the expected rate of convergence. If the domain Ω has a smooth boundary we know that the solution u is smooth (see for example [1]). Eventhough the domain is rough, such that in our case with corners, the solution should be smooth away from the corners. In our case we cannot expect much more than the existence of one derivative of u in a neighbourhood of the corners. However, it should be some fraction greater than one. We have sharp corners in the domain of angles $\frac{3\pi}{2}$, $\frac{7\pi}{6}$, and $\frac{\pi}{3}$, where $\frac{\pi}{3}$ is the smallest and probably the most destructive in this sense. For our boundary conditions, however, in view of the work by Rössle ([27]), we can expect about 3/2 weak derivatives.

We have

$$\mathbf{dof} \sim \frac{1}{h^2}$$

Therefore, for uniform mesh refinement, in view of for example the interpolation inequality of Scott and Zhang, we expect a slope not steeper than x^{-1}. In the case of adaptive mesh refinement, we expect the refinements in the corners to compensate for the lack of smoothness and the behaviour as if we would have a smooth u. Thus the rate of convergence would be closer to x^{-2}.

Now we turn to the actual estimate obtained from the local problems. Since it does not contain any unknown constants we can find an approximation by simply summing the residuals calculated by the second order method. Suppose that μ are the error estimate obtained from the local problems on the stars. That is

$$\mu = \sum_{z \in \mathcal{N}} ||\Psi_z^{q_E}||_{V_z}^2 .$$

Note that μ for K^* and G^* are in general different because of the ξ in their respective problems. Denote by η_{K^*} and η_{G^*} the error fractions

$$\eta_{K^*} = \frac{\mu}{K_h^* - K_{\mathrm{ref}}^*}, \qquad \eta_{G^*} = \frac{\mu}{G_h^* - G_{\mathrm{ref}}^*}.$$

In Table 2, the values of η_{G^*} are shown for the meshes used in the case where G_h^* is calculated using the adaptive method based on the local problems on stars. Note also that μ here is an approximation, so we expect the true value of μ to be even greater. Although, the number of points of measure are few, it may seem to be that η_{G^*} grows with the degrees of freedom. This behavior can also be found in an example considered by Carstensen et al in [7], eventhough, in their example the effect seems to appear only for small number of degrees of freedom. In our example we have only considered small numbers of degrees of freedom.

In the adaptive method, no recombination of mesh cells corresponding to very small local error indicators has been considered.

The results for the case of K^* are the same as for G^* as can be seen in Figure 3 and Table 1, where we compare the slopes of the graphs and the order of the numbers.

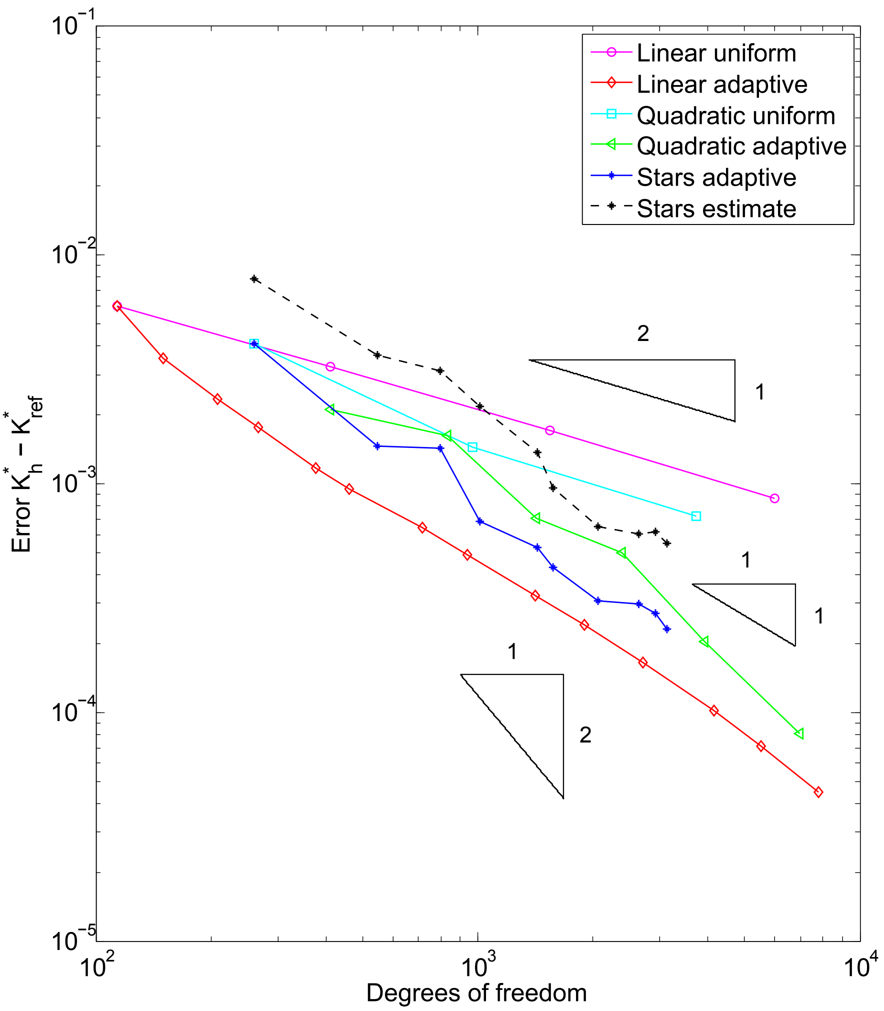


Figure 3: A log-log plot of the error in the finite element approximation K_h^* of K^*, with respect to the reference value K_{ref}^*, for the various numerical methods. The triangles indicate the slope of the functions $x^{-1/2}$, x^{-1}, and x^{-2}, where x is the number of degrees of freedom.

The numerical calculations, including mesh generation, have been carried out using the computer program MATLAB (see [20]).

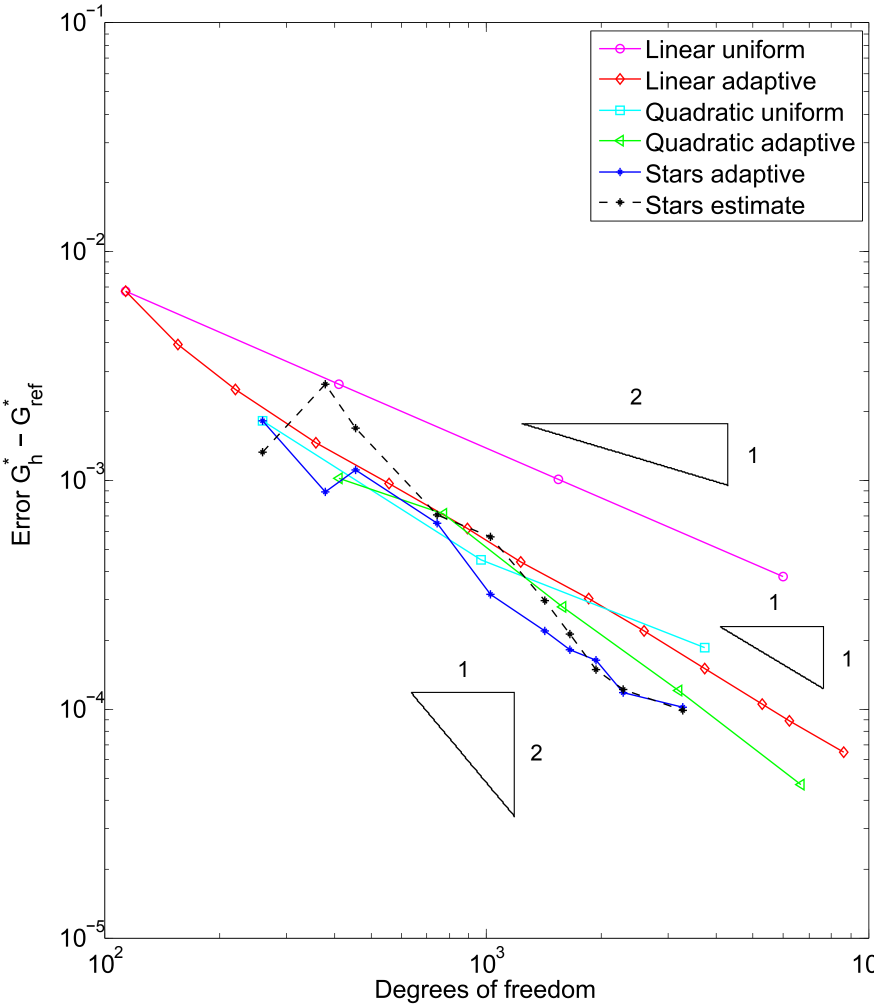


Figure 4: A log-log plot of the error in the finite element approximation G_h^* of G^*, with respect to the reference value G^*_{ref}, for the various numerical methods. The triangles indicate the slope of the functions $x^{-1/2}$, x^{-1}, and x^{-2}, where x is the number of degrees of freedom.

dof	260	546	798	1014	1432	1578	2070	2644	2916	3132
η_{K^*}	1.89	2.46	2.15	3.09	2.50	2.13	1.96	1.88	2.10	2.17

Table 1: The degrees of freedom **dof** and the error fraction η_{K^*} for the adaptive method based on local problems on stars for K^*.

dof	260	380	456	742	1024	1420	1658	1942	2284	3276
η_{G^*}	0.736	2.94	1.52	1.09	1.77	1.36	1.17	0.913	1.03	0.966

Table 2: The degrees of freedom **dof** and the error fraction η_{G^*} for the adaptive method based on local problems on stars for G^*.

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