Accurate upper and lower error bounds by solving flux-free local problems in "stars"

Pedro Díez – Núria Parés – Antonio Huerta

Universitat Politècnica de Catalunya
Departament de Matemàtica Aplicada III
E.T.S. de Ingenieros de Caminos, Canales y Puertos
E.U. de Ingenieros Técnicos Industriales de Barcelona
E-08034 Barcelona, Spain

pedro.diez@upc.es

ABSTRACT. *Two implicit residual type estimators yielding upper bounds of the error are presented which do not require flux equilibration. One of them is based on the ideas introduced in [MAC 00, CAR 99, MOR 03, PRU 02]. The new approach introduced here is based on using the estimated error function rather than the estimated error norms. Once the upper bounds are computed, also lower bounds for the error are obtained with little supplementary effort.*

RÉSUMÉ. *On présente deux estimateurs d'erreur qui ne nécessitent point d'équilibration locale de flux (contraintes) et qui fournissent des bornes supérieures de l'erreur. Le premier se base dans les idées introduites dans [MAC 00, CAR 99, MOR 03, PRU 02]. L'estimateur introduit ici suit la même philosophie mais se base dans l'estimation des fonctions d'erreur et pas seulement celle des normes. Une fois les estimateurs en borne supérieure calculés, des bornes inférieures peuvent être obtenues avec un petit effort supplémentaire.*

KEYWORDS: *error estimation, flux-free estimates, adaptivity, upper and lower bounds of the error.*

MOTS-CLÉS : *estimation d'erreur, estimateurs sans flux, adaptivité, bornes supérieures (majorations) et inférieures (minorations) de l'erreur.*

1. Introduction

The goal of the application of computational mechanics to engineering practice is often the evaluation of particular quantities of interest. These quantities are also denoted as engineering outputs of the problem. The goal of an adaptive procedure is to control efficiently the accuracy of these outputs, which represent the relevant engineering quantities. Recently, a number of researchers have addressed the problem of assessing and controlling the error of the numerical solution in these outputs of interest, instead of the classical energy norm error estimation.

It is worth noting that goal oriented error estimates have the attractive feature of being directly computable from energy estimates of the error. It suffices to apply them to the approximations of the primal and dual (with respect to the output) problems. In order to bound the error in the quantity of interest, simultaneous lower and upper bounds of the energy error are needed.

Many approaches for computing bounds on outputs, as [PAR 97] and [PRU 99], are based in this important property, thus, based on the obtention of accurate upper and lower bounds for the energy norm of the error.

In this work, a new approach to obtain simultaneous upper and lower bounds of the energy norm of the error is presented. The main advantage is that it does not require neither flux jumps computations nor equilibration strategies. It is therefore well-suited for assessing the error in a 3D context, where the equilibration and the computation of fluxes is very expensive.

The approach described in this paper uses the solution associated with a fine *truth* mesh as a reference solution. The reference mesh is much finer than the current original mesh and therefore the reference solution is much closer to the unknown exact solution than the computed with the original mesh. Thus, a reference error e_{ref} is introduced as an alternative to the exact error e. The reference and the exact errors are practically identical, being the reference error slightly lower than the exact error. The error estimates introduced below are indeed upper and lower bounds of the error. However, the overestimation (upper bound) is only proved with respect to the reference error, not with respect to the exact error. It may happen that the error estimate ranges between the reference and the exact errors. In that case, paradoxically, the *upper bound* is underestimating the exact error. Some work has been devoted to obtain upper bounds with respect to the exact solution [BON 02]. These approaches are based on solving the local equations using equilibrium methods. Nevertheless, this *problem* arises only if the estimate is extremely sharp and the introduced overestimation with respect to the reference error is lower than the difference between the reference and the exact solution. In practice, this happens rarely.

2. Model problem and error equations

The model problem is stated as follows: find $u \in H^1_{\Gamma_D}(\Omega)$ such that

$$a(u, v) = l(v), \quad \forall v \in H^1_0(\Omega),$$ [1]

where $H^1_{\Gamma_D}(\Omega)$ and $H^1_0(\Omega)$ are the standard Sobolev spaces satisfying the Dirichlet and homogeneous boundary conditions respectively.

The finite element interpolation space and the finite element solution are denoted by V^h and u_h respectively, and the energy norm is denoted by $\|\cdot\|$. Let x^i, $i = 1 \ldots n_{\mathrm{node}}$ denote the nodes of the mesh and $\phi^i \in V^h$ the corresponding shape functions. The support of ϕ^i is denoted by ω^i and it is called the star centered in or associated with node x^i.

Note that the shape functions are a partition of unity,

$$\sum_{i=1}^{n_{\mathrm{node}}} \phi^i(x) = 1, \qquad \forall x \in \Omega. \tag{2}$$

This essential property is used in the following to define residual estimators based in stars. Similar approaches have been used in references [BAB 78], [CAR 99] and [MOR 03].

We address the problem of assessing the error, $e := u - u_h \in H^1_0(\Omega)$.

The global equation for the error is

$$a(e, v) = l(v) - a(u_h, v) =: R(v), \qquad \forall v \in H^1_0(\Omega), \tag{3}$$

where $R(\cdot)$ stands for the weak residual associated to u_h.

In practice, the exact error e is replaced by its projection into the reference space, $e_{\mathrm{ref}} \in V^{\mathrm{ref}}_0 := V^{\mathrm{ref}} \cap H^1_0(\Omega)$. The new interpolation space, V^{ref}, is obtained either by h-refinement or by p-refinement from V^h (that is, either $\widetilde{h} < h$ or $\widetilde{p} > p$).

3. Upper bounds estimators in stars

In this section, two estimates are presented, both providing an upper bound of the energy norm of the reference error.

The first strategy introduces a local approximation $e_{\mathrm{u}}^{\omega^i} \in V^{\mathrm{ref}}_{0,\omega^i}$ of the contribution of the star ω^i to the reference error, where $V^{\mathrm{ref}}_{0,\omega^i}$ denote the local restriction of the reference space to the star ω^i, that is, $V^{\mathrm{ref}}_{0,\omega^i} := V^{\mathrm{ref}}_0 \cap H^1(\omega^i)$. Then $e_{\mathrm{u}}^{\omega^i}$ is defined to be the solution of

$$a_{\omega^i}(e_{\mathrm{u}}^{\omega^i}, v) = R(\phi^i v), \qquad \forall v \in V^{\mathrm{ref}}_{0,\omega^i}, \tag{4}$$

where $a_{\omega^i}(\cdot, \cdot)$ is the restriction of the bilinear form $a(\cdot, \cdot)$ to the star ω^i.

A global estimate of the error is defined adding the local contributions, that is

$$e_{\mathrm{u}} := \sum_{i=1}^{n_{\mathrm{node}}} e_{\mathrm{u}}^{\omega^i}. \tag{5}$$

Note that e_{u} belongs to the "broken" space, that is, $e_{\mathrm{u}} \in V_{\mathrm{brok}}^{\mathrm{ref}} := \bigoplus V_{0,\Omega_k}^{\mathrm{ref}}$, where $V_{0,\Omega_k}^{\mathrm{ref}}$ is the restriction of the reference space to the element Ω_k. In other words, the restriction of e_{u} to an element belongs to the reference space, and hence is continuous, but it is generally discontinuous across interelement boundaries.

The following theorem states that e_{u} defined in Eq. (5) behaves as an upper bound residual type error estimator based in a flux equilibration technique, see references [BAN 85] and [AIN 93].

Theorem 1. *The estimate $e_{\mathrm{u}} \in V_{\mathrm{brok}}^{\mathrm{ref}}$ introduced in Eq. (5) verifies*

$$a(e_{\mathrm{u}}, v) = a(e_{\mathrm{ref}}, v), \qquad \forall v \in V_0^{\mathrm{ref}}. \tag{6}$$

Thus, the norm of e_{u} is an upper bound of the energy norm of the reference error, that is

$$\varepsilon^+ (e_{\mathrm{u}}) := \|e_{\mathrm{u}}\|^2 \geq \|e_{\mathrm{ref}}\|^2. \tag{7}$$

To derive the second estimate a weighted version of the bilinear form $a(\cdot, \cdot)$ is introduced, $a^{\phi^i}(\cdot, \cdot)$. That is, if

$$a(u, v) = \int f(u, v) \quad \implies \quad a^{\phi^i}(u, v) := \int \phi^i f(u, v), \tag{8}$$

and its induced norm is denoted by $\|\cdot\|_{\phi^i}$.

Then a new family of local estimates, $\eta_{\mathrm{u}}^{\omega^i} \in V_{0,\omega^i}^{\mathrm{ref}}$, are defined as the solution of

$$a^{\phi^i}\big(\eta_{\mathrm{u}}^{\omega^i}, v\big) = R\big(\phi^i v\big), \qquad \forall v \in V_{0,\omega^i}^{\mathrm{ref}}. \tag{9}$$

Also a global estimate, $\eta_u \in V_{\mathrm{brok}}^{\mathrm{ref}}$, is considered

$$\eta_u := \sum_{i=1}^{n_{\mathrm{node}}} \eta_{\mathrm{u}}^{\omega^i}. \tag{10}$$

Theorem 2. *Let η_u be the global estimate defined in Eq. (10). Then an upper bound is computed from η_u using the weighted norms as*

$$\varepsilon^+ (\eta_u) := \sum_{i=1}^{n_{\mathrm{node}}} \|\eta_{\mathrm{u}}^{\omega^i}\|_{\phi^i}^2 \geq \|e_{\mathrm{ref}}\|^2. \tag{11}$$

REMARK.— Note that upper bound estimates are obtained without any flux recovery or flux splitting technique. The effect of the flux jumps across each edge of the mesh is implicitly taken into account because the support of the local problems are the stars, which include the interelement edges. There is no need of computing and postprocessing the fluxes of the finite element solution, u_h, along the interelement edges.

4. Lower bound recovering

The idea of obtaining a lower bound by a simple post-processing of the upper bound error estimate, is to construct continuous estimates from them. A simple averaging technique can be considered [DIE 03]. However, in this case, the particular form of the estimates e_{u} and η_u can be taken into account in order to improve the lower bounds.

The idea is that the local estimates, $e_{\mathrm{u}}^{\omega^i}$ and $\eta_{\mathrm{u}}^{\omega^i}$, are discontinuous along the boundary of the star ω^i. In order to enforce continuity it suffices to consider $\phi^i e_{\mathrm{u}}^{\omega^i}$ and $\phi^i \eta_{\mathrm{u}}^{\omega^i}$.

Therefore e_{w} and η_{w} given by

$$
e_{\mathrm{w}} := \sum_{i=1}^{\mathrm{n_{node}}} \phi^i e_{\mathrm{u}}^{\omega^i}, \qquad \eta_{\mathrm{w}} := \sum_{i=1}^{\mathrm{n_{node}}} \phi^i \eta_{\mathrm{u}}^{\omega^i}, \qquad [12]
$$

are continuous global estimates.

Theorem 3. *Let $e_{\mathrm{u}}^{\omega^i}, \eta_{\mathrm{u}}^{\omega^i} \in V_{0,\omega^i}^{\mathrm{ref}}$, $i = 1 \ldots \mathrm{n_{node}}$ be the estimates obtained solving Eqs. (4) and (9) respectively. Then the continuous estimates e_{w} and η_{w} defined in Eq. (12) yield lower bounds of the energy norm of the exact error:*

$$
\varepsilon^- (e_{\mathrm{w}}) := \frac{\left(\sum\limits_{i=1}^{\mathrm{n_{node}}} \| e_{\mathrm{u}}^{\omega^i} \|_{\phi^i}^2 \right)^2}{\| e_{\mathrm{w}} \|^2} \quad \text{and} \quad \varepsilon^- (\eta_{\mathrm{w}}) := \frac{\left(\sum\limits_{i=1}^{\mathrm{n_{node}}} \| \eta_{\mathrm{u}}^{\omega^i} \|_{\phi^i}^2 \right)^2}{\| \eta_{\mathrm{w}} \|^2} = \frac{\varepsilon^+ (\eta_u)^2}{\| \eta_{\mathrm{w}} \|^2},
$$

where $\|\cdot\|_{\omega^i}$ stands for the norm associated to the local bilinear form $a_{\omega^i}(\cdot, \cdot)$, $\|v\|_{\omega^i}^2 = a_{\omega^i}(v, v)$. That is

$$
\varepsilon^- (e_{\mathrm{w}}) \leq \| e \|^2 \qquad \text{and} \qquad \varepsilon^- (\eta_{\mathrm{w}}) \leq \| e \|^2. \qquad [13]
$$

To improve this lower bounds, once the continuous estimate is computed, a global error assessment is introduced to take into account pollution errors [HUE 00]. Following this strategy, two new estimates, $e_{\mathrm{w}}^{\mathrm{G}}$ and $\eta_{\mathrm{w}}^{\mathrm{G}}$, are obtained using e_{w} and η_{w}. Both $e_{\mathrm{w}}^{\mathrm{G}}$ and $\eta_{\mathrm{w}}^{\mathrm{G}}$ are continuous and provide new lower bounds for the error. The lower bounds provided by $e_{\mathrm{w}}^{\mathrm{G}}$ and $\eta_{\mathrm{w}}^{\mathrm{G}}$ are sharper than the lower bounds provided by e_{w} and η_{w}.

5. Numerical examples

In this section, the behavior of the estimates introduced in the previous sections is analyzed using two numerical examples: one thermic (scalar unknown) and one mechanical (vectorial unknown).

The quality of the error estimates is measured with the index ρ, defined by

$$\rho := \frac{\text{estimated error}}{\text{reference error}} - 1, \qquad [14]$$

that is, ρ is the effectivity index minus one. The quality of the estimates is given by the absolute value of ρ and the sign of ρ indicates if the estimate is an upper (positive ρ) or a lower bound (negative ρ).

In the examples bilinear finite elements are used ($p = 1$), and the reference space V^{ref} is obtained refining the initial mesh (h-refinement).

Four error estimates are considered: two upper-bound estimates, e_{u} and η_u, and two continuous estimates $e_{\mathrm{w}}^{\mathrm{G}}$ and $\eta_{\mathrm{w}}^{\mathrm{G}}$, which provide lower bounds for the error.

5.1. Example 1: thermal problem

The Poisson equation is solved in a squared domain, Ω, with boundary conditions Dirichlet homogeneous on $\Gamma_D := \{(x,0); 0 \le x \le 1\}$ and Neumann homogeneous elsewhere on $\partial\Omega$. The source term s is taken such that the exact solution has the following analytical expression (Figure (1))

$$u(x,y) = \frac{1}{2000}x^2(1-x)^2\left(e^{10x^2}-1\right)y^2(1-y)^2\left(e^{10y^2}-1\right). \qquad [15]$$
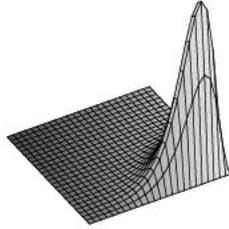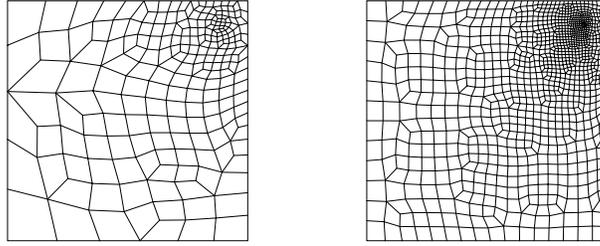

Figure 1. *Example 1: exact solution*

Two different non-uniform meshes have been considered (Figure (2)). The reference space is obtained dividing each element of the mesh into 4^2 new elements.

| ndof	$\|e_{\text{ref}}\|$	$\rho(\varepsilon^+(e_{\mathrm{u}}))$	$\rho(\varepsilon^+(\eta_u))$	$\rho(\varepsilon^-(e_{\mathrm{w}}^{\mathrm{G}}))$	$\rho(\varepsilon^-(\eta_{\mathrm{w}}^{\mathrm{G}}))$
240	.2447	.0123	.3174	.0066	.0259
1081	.1164	.0024	.2727	.0016	.0292

Table 1. *Estimates obtained in example 1*

Figure 2. *Example 1: initial meshes for example 1*

Paradoxically, in this example, the lower bounds provide positive values of the parameter ρ. This is because $\varepsilon^- \left(e_{\mathrm{w}}^{\mathrm{G}} \right)$ and $\varepsilon^- \left(\eta_{\mathrm{w}}^{\mathrm{G}} \right)$ are lower than the exact error but not necessarily lower than the reference error which is used to compute ρ. A similar phenomenon occurs for $\varepsilon^+ \left(e_{\mathrm{u}} \right)$. The estimate $\varepsilon^+ \left(e_{\mathrm{u}} \right)$ is larger than the reference error but not necessarily larger than the exact error. Then, even if $\|e_{\mathrm{ref}}\|^2 \leq \varepsilon^+$ and $\varepsilon^- \leq \|e\|^2$ stands, it may happen, see table, that $\varepsilon^+ \left(e_{\mathrm{u}} \right) < \varepsilon^- \left(\eta_{\mathrm{w}}^{\mathrm{G}} \right)$. This can be avoided projecting the continuous functions $e_{\mathrm{w}}^{\mathrm{G}}$ and $\eta_{\mathrm{w}}^{\mathrm{G}}$ into V^{ref} by a simple nodal interpolation. In this case, $\varepsilon^- \left(e_{\mathrm{w}}^{\mathrm{G}} \right)$ and $\varepsilon^- \left(\eta_{\mathrm{w}}^{\mathrm{G}} \right)$ are lower bounds for the squared energy norm of the reference error $\|e_{\mathrm{ref}}\|^2$, and thus $\varepsilon^- \leq \|e_{\mathrm{ref}}\|^2 \leq \varepsilon^+$.

The local effectivity indexes associated with e_{u} are analyzed in the histogram in Figure (3), which shows the occurrences of the local effectivity indexes. Only elements with a significant contribution to the error are considered. The elements such that the corresponding local error is lower than 1% of $\|e\|/\mathtt{n_{el}}$ (being $\mathtt{n_{el}}$ the number of elements) are not taken into account (62.319% of the elements). The histogram is concentrated around 100% and therefore the local behavior of the estimate is good. The global upper bound property is also recovered in a large number of elements.
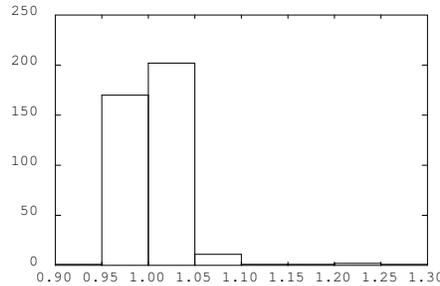
Figure 3. *Effectivity index histogram of the estimate $\varepsilon^+ \left(e_{\mathrm{u}} \right)$ for the mesh with 1081 ndof*

In Figure (4) the spatial distributions of the estimate e_{u} and reference error are shown. Note that the estimate performs well and the plots are practically identical.

7
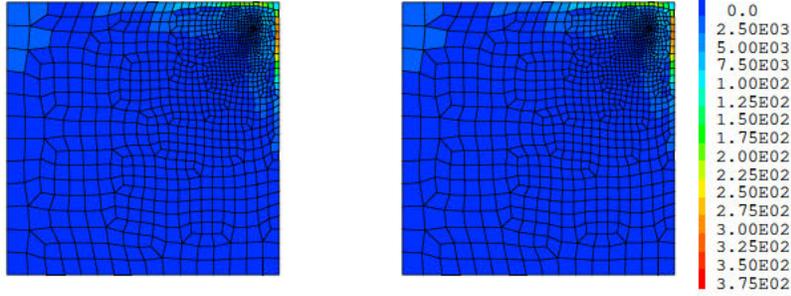
Figure 4. *Example 1: spacial distribution of the reference error (left) and the estimated error $\varepsilon^+(e_u)$ (right) for the mesh with 1081 ndof*

5.2. *Example 2: plane mechanical problem*

In this section the behavior of the estimate $\varepsilon^+(e_u)$ introduced above and the associated upper and lower bounds is analyzed in a plane-stress linear elasticity problem. The domain is a one-fourth of a symmetrically loaded plate with two rectangular holes, as shown in Figure (5). A horizontal unit distributed force is applied along Γ_0, and the symmetry is taken into account enforcing homogeneous essential boundary conditions on the normal displacements; stress-free condition apply on all other boundaries and components. The Young's modulus and Poisson ratio are taken to be 1 and 0.3, respectively.
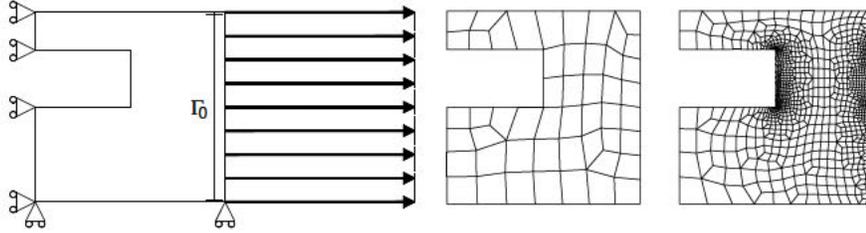

Figure 5. *Example 2: model problem and initial meshes with 70 nodes (center) and 1 294 nodal points (right)*

The considered meshes are shown in Figure (5). For the coarse mesh (70 nodes), the reference mesh is obtained dividing each element into 8^2 new ones, while for the refined one (1 294 nodes) each element is divided into 4^2 new ones.

The results concerning the assessment of the energy norm of the reference error are shown in table 2. In mechanical problems the obtained effectivities for $\varepsilon^+(e_u)$ are not as good as for the previous example.

nodes	$\|e_{\mathrm{ref}}\|$	$\frac{\|e_{\mathrm{ref}}\|}{\|u_h\|}$	$\rho(\varepsilon^+(e_{\mathrm{u}}))$	$\rho(\varepsilon^-(e_{\mathrm{w}}^{\mathrm{G}}))$
70	.15434	.13561	.21822	-.42410
1294	.0354100	.0308283	.16310	-.62755

Table 2. *Example 2: upper and lower bounds for* $\|e_{\mathrm{ref}}\|$
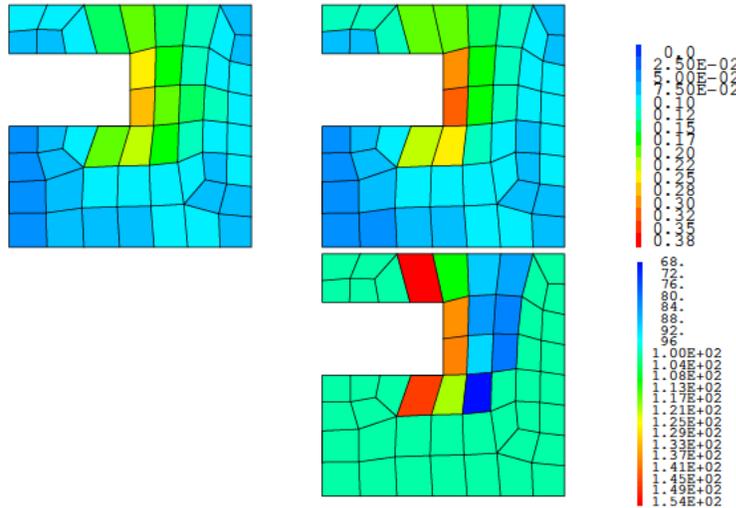
Figure 6. *Example 2: spatial distribution of the reference error (up left) and estimate (up right), and local distribution of the effectivities* $(\rho+1)\%$ *(down) for the mesh with 70 nodes*

As in the previous example, the spatial distribution and local effectivities of the estimate $\varepsilon^+(e_{\mathrm{u}})$ shown in Figure (6) provide good indicators which may be used in an adaptive procedure.

6. Concluding remarks

A general strategy to estimate the error in finite element computations has been introduced yielding both upper and lower bounds for the error. The main features of this approach are the following:

– The upper bound is obtained using a residual estimator based on solving local problems on stars (local subdomains). The local problems do not require to compute and equilibrate fluxes. The estimated error function is discontinuous across the element edges.

– A lower bound is obtained by postprocessing the approximation of the error function computed for the upper bound estimate. The error function is smoothed out

to obtain a continuous function. Then, the error estimate in energy norm is computed in a straightforward manner.

The motivation for obtaining simultaneous upper and lower bounds of the energy norm of the error arises from the necessity of estimating the error in quantities of interest, for goal oriented adaptivity. In this context, the assessment of the energy norm of the error is required for both the primal problem (the original one) and a dual problem related with the selected quantity of interest. In order to obtain accurate bounds of the error in the quantity of interest both upper and lower bounds of the energy norm of the error are required. The present approach is a simple and efficient tool for this purpose.

Compared to other approaches based in the same idea [MAC 00, CAR 99, MOR 03, PRU 02], the strategy introduced here shows a better behavior in the numerical tests, yielding sharper error estimates. Although this is demonstrated in all the studied examples (both mechanical and thermal, 2D and 3D...) a further analysis is required to obtain a general proof of this property.

7. References

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