

# ICES REPORT 11-11

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April 2011

## **B-spline goal-oriented error estimators for geometrically nonlinear rods**

by

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*Reference: Luca Dede and Hugo A.F.A. Santos , "B-spline goal-oriented error estimators for geometrically nonlinear rods ", ICES REPORT 11-11, The Institute for Computational Engineering and Sciences, The University of Texas at Austin, April 2011.*

## Report Documentation Page

*Form Approved*  
*OMB No. 0704-0188*

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1. REPORT DATE <b>APR 2011</b>	2. REPORT TYPE	3. DATES COVERED <b>00-00-2011 to 00-00-2011</b>	
4. TITLE AND SUBTITLE <b>B-spline goal-oriented error estimators for geometrically nonlinear rods</b>		5a. CONTRACT NUMBER	
		5b. GRANT NUMBER	
		5c. PROGRAM ELEMENT NUMBER	
6. AUTHOR(S)		5d. PROJECT NUMBER	
		5e. TASK NUMBER	
		5f. WORK UNIT NUMBER	
7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES) <b>University of Texas at Austin, Institute for Computational Engineering and Sciences, Austin, TX, 78712</b>		8. PERFORMING ORGANIZATION REPORT NUMBER	
9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)		10. SPONSOR/MONITOR'S ACRONYM(S)	
		11. SPONSOR/MONITOR'S REPORT NUMBER(S)	
12. DISTRIBUTION/AVAILABILITY STATEMENT <b>Approved for public release; distribution unlimited</b>			
13. SUPPLEMENTARY NOTES			
14. ABSTRACT <b>We consider goal-oriented a posteriori error estimators for the evaluation of the errors on quantities of interest associated with the solution of geometrically nonlinear curved elastic rods. For the numerical solution of these nonlinear one-dimensional problems, we adopt a B-spline based Galerkin method, a particular case of the more general Isogeometric Analysis. We propose error estimators using higher order enhanced solutions, which are based on the concept of enrichment of the original B-spline basis by means of the pure k-refinement procedure typical of Isogeometric Analysis. We provide several numerical examples for linear and nonlinear output functionals, corresponding to the rotation, displacements and strain energy of the rod, and we compare the effectiveness of the proposed error estimators.</b>			
15. SUBJECT TERMS			
16. SECURITY CLASSIFICATION OF:			17. LIMITATION OF ABSTRACT
a. REPORT <b>unclassified</b>	b. ABSTRACT <b>unclassified</b>	c. THIS PAGE <b>unclassified</b>	<b>Same as Report (SAR)</b>
			18. NUMBER OF PAGES <b>27</b>
			19a. NAME OF RESPONSIBLE PERSON

# B-spline Goal-oriented Error Estimators for Geometrically Nonlinear Rods

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14<sup>th</sup> April 2011

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## Abstract

We consider goal-oriented a posteriori error estimators for the evaluation of the errors on quantities of interest associated with the solution of geometrically nonlinear curved elastic rods. For the numerical solution of these nonlinear one-dimensional problems, we adopt a B-spline based Galerkin method, a particular case of the more general Isogeometric Analysis. We propose error estimators using higher order “enhanced” solutions, which are based on the concept of enrichment of the original B-spline basis by means of the “pure”  $k$ -refinement procedure typical of Isogeometric Analysis. We provide several numerical examples for linear and nonlinear output functionals, corresponding to the rotation, displacements and strain energy of the rod, and we compare the effectiveness of the proposed error estimators.

**Keywords:** *Geometrically nonlinear rods; Isogeometric Analysis; B-spline basis; goal-oriented a posteriori error estimation; error estimator.*

## 1 Introduction

The study of large deflections of thin beams, or rods, has received a growing interest in many engineering and science problems. Examples of these problems include framed structures [36, 37], compliant mechanisms [11, 44] and nanoscale structures [45].

The simplest geometrically nonlinear bending theory of planar elastic rods is the *Elastica theory*, mathematically formulated by L. Euler in 1744 [31]. In this theory a rod is thought of as an inextensible line of particles which resists bending according to a law given by a linear constitutive relation; no restrictions on the magnitude of displacements or angles of rotation are considered. Since then, several variants have been proposed, in particular, theories including dynamical effects, extensibility of the rod, shear deformation, plasticity, follower loads, etc., see *e.g.* [3] and the references therein. Also, different approaches have been considered in the literature for the analysis of elastic thin beams: (i) the elliptic integral approach first proposed by [9], which gives closed-form solutions only for simple loading cases and boundary conditions [33], (ii) the numerical integration approach with iterative shooting techniques (*e.g.* [29, 32, 13]), and

(iii) the incremental Finite Element method with Newton–Raphson iteration techniques [43, 22, 21].

Of these approaches, the Finite Element method (*e.g.* [14, 40, 25]) is indeed the most popular approach, mainly due to its versatility to the analysis of problems with complex topologies and geometries. As a result, numerous geometrically nonlinear planar beam elements have been developed over the past few decades. Among others, see *e.g.* [17, 19, 18, 24, 41, 27, 36, 47, 12, 30, 23, 37, 42].

However, the Finite Element method only provides approximate solutions whose quality depends on the discretization procedure. The problem of how to measure the quality of these numerical solutions, assessing the accuracy of the Finite Element approximations, is essential for a reliable application of these problems.

Nevertheless, if, on the one hand, error estimation offers no major challenges in the linear analysis of one–dimensional beam problems, since it is possible to employ certain elements which can model the linear problem exactly, even with one element per member, on the other hand, approaches based on *a posteriori* error estimation [2] for geometrically nonlinear beams have received very little attention. Exceptions to this are the works presented in [28] and [34].

Furthermore, although the error estimation on the solution of a problem represents an important aspect of the numerical approximation, it is also important to properly evaluate quantities of interest associated with such solution, often referred to as *output functionals* (see *e.g.* [4]). For the rod problem, these quantities of interest, can be defined by local quantities, such as, for instance, displacements, rotations, forces and bending moments, or by global quantities, such as the total strain energy. In this context, *a posteriori* error estimation approaches, are often referred to as *goal-oriented* approaches, as they are particularly suited for estimating the error on quantities of interest, rather than the solution itself; the introduction of the dual (adjoint) problem allows the quantification of the sensitivity of the output functionals with respect to the perturbations on the solution. Several contributions have been made in this field, with special emphasis on the Finite Element method, for both linear and nonlinear problems, see *e.g.* [2, 8, 35, 20, 5].

It is the main goal of this work to propose and discuss goal-oriented *a posteriori* error estimators for the evaluation of the errors on quantities of interest involving the solution of geometrically nonlinear rods problems. With this aim, we consider a numerical approximation scheme based on a B–spline basis [38] for the approximation space. This choice represents a particular case of the Isogeometric Analysis method [26, 15], a Galerkin approximation method based on the isoparametric concept in which the basis of the approximation space is the same as the one used to represent the geometry and which can be represented by B–splines, NURBS (Non–Uniform Rational B–splines) [38] or eventually T–splines [6]. High order,  $C^k$  globally continuous basis can be generated while maintaining the exactness of the representation of the geometry in the analysis; moreover, the basis possesses useful properties for the approximation of solutions independently of the geometrical construction. Error analysis methods [7] and *a posteriori* error estimates with T–splines [16] have already been proposed in the literature, also in the goal-oriented framework [46].

The proposed error estimators are constructed on a B–spline basis in which the “enhanced” approximated solutions, typically employed to evaluate the estimators, are not only generated by means of a mesh refinement strategy, as proposed in [46] for two–dimensional B–splines and T–splines, but also by means of higher order approximations. In particular, we build the “enhanced” higher order B–spline basis by performing one step of the “pure”  $k$ –refinement procedure typical of Isogeometric Analysis [15] (order

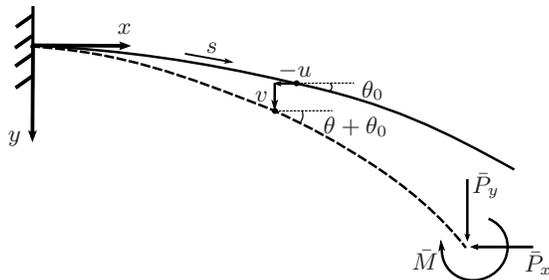


Figure 1: Cantilever rod model.

elevation without internal knots insertion); in this manner, an higher order B-spline basis with increased global continuity is obtained by introducing only an additional degree of freedom with respect to the original one. As a result, the corresponding estimators and, therefore, the errors associated with the outputs, can be evaluated at a relatively small computational cost. The case of the classical Finite Element method with the standard Lagrangian polynomial linear basis is obtained and discussed as a particular case of the B-spline basis of order one.

As the proposed error estimators are formulated in a general framework, they can be straightforwardly applied to the analysis of other nonlinear problems, even multidimensional.

The paper is organized as follows. In Sec.2 we introduce the boundary value problem; in Sec.3 we reformulate the problem in an abstract setting by introducing its corresponding weak form and recall goal-oriented a posteriori error estimates. In Sec.4 we describe the B-spline based approximation and propose the error estimators. In Sec.5 we provide numerical tests for the rod problem and discuss the obtained results. Conclusions follow.

## 2 Boundary-value problem

We confine attention to the statics of cantilever rods having a planar initially curved reference configuration subjected to a pair of concentrated loads  $\bar{P}_x$  and  $\bar{P}_y$  and a bending moment  $\bar{M}$  applied at the tip, as represented in Fig.1. The governing differential equation of these type of rods is given as follows [31]:

$$EI \frac{d^2\theta}{ds^2} + \bar{P}_x \sin(\theta + \theta_0) + \bar{P}_y \cos(\theta + \theta_0) = 0. \quad (1)$$

where  $s \in \Omega = (0, L)$  represents the arch-length of the rod (curvilinear abscissa) in the undeformed configuration, with  $L$  the length of the rod;  $\theta_0 = \theta_0(s)$  stands for the initial slope angle of the rod,  $\theta = \theta(s)$  represents the rotation angle of the normal to rod axis, and  $EI$  is the bending stiffness of the beam, which we assume as constant, being  $E$  the Young modulus and  $I$  the cross-sectional moment of inertia. The boundary conditions for the differential equation (1) are:

$$\begin{aligned} \theta(0) &= 0, \\ EI \frac{d\theta}{ds} \Big|_{s=L} &= \bar{M}. \end{aligned} \quad (2)$$

As it is well known, the boundary–value problem defined by Eqs.(1) and (2) may exhibit multiple solutions, very often referred in the literature to as *elastica shapes*. Each shape corresponds to a critical point of the total potential energy functional defined by  $\Pi_p(\cdot) : \mathcal{V} \rightarrow \mathcal{R}$ :

$$\Pi_p(\theta) := U(\theta) + W(\theta) \quad (3)$$

where  $U$  and  $W$  represent the strain (internal) and the external energies of the rod element, respectively:

$$U(\theta) := \int_{\Omega} \frac{1}{2} EI \left( \frac{d\theta}{ds} \right)^2 ds, \quad (4)$$

$$W(\theta) := \int_{\Omega} (\bar{P}_x \cos(\theta + \theta_0) - \bar{P}_y \sin(\theta + \theta_0)) ds \\ + \bar{P}_x(x_0(0) - x_0(L)) - \bar{P}_y(y_0(0) - y_0(L)) - \bar{M}\theta(L), \quad (5)$$

with  $\mathcal{V}$  the kinematically admissible (functional) space defined as:

$$\mathcal{V} := \{\theta \in H^1(\Omega) : \theta(0) = 0\}, \quad (6)$$

where  $H^1(\Omega)$  represents a standard Hilbert space [1]; the pairs  $(x_0(0), y_0(0))$  and  $(x_0(L), y_0(L))$  represent the initial coordinates of the cantilever at  $s = 0$  and  $s = L$ , respectively.

The horizontal and vertical displacements of the rod, herein denoted by  $u = u(s)$  and  $v = v(s)$ , respectively (see Fig.1), are shown to obey the following differential equations:

$$\frac{du}{ds} = \cos(\theta + \theta_0) - \frac{dx_0}{ds}, \\ \frac{dv}{ds} = \sin(\theta + \theta_0) - \frac{dy_0}{ds}, \quad (7)$$

where:

$$\frac{dx_0}{ds} = \cos(\theta_0), \\ \frac{dy_0}{ds} = \sin(\theta_0), \quad (8)$$

together with the boundary conditions:

$$u(0) = v(0) = 0. \quad (9)$$

We are interested in evaluating quantities of interest associated with the solution  $\theta(s)$  of problem (1)–(2), in particular, the strain energy  $U(\theta)$  defined by (4), the rotation at the tip of the cantilever rods  $\theta(L)$ , and the horizontal and vertical displacements at the tip of the cantilever rods,  $u(L)$  and  $v(L)$ . The displacements can be obtained from the integration of equations (7) and (9) as:

$$u(L) = \int_{\Omega} (\cos(\theta + \theta_0) - \cos(\theta_0)) ds. \\ v(L) = \int_{\Omega} (\sin(\theta + \theta_0) - \sin(\theta_0)) ds. \quad (10)$$

### 3 Goal-oriented a posteriori error estimation

In this Section we recall and discuss the so-called goal-oriented analysis; with this aim, we reformulate the problem discussed in the previous Section in an abstract setting by introducing its weak form and the adopted Galerkin approximation scheme.

### 3.1 Weak form

The weak form associated with the primal boundary–value problem introduced in the preceding Section reads:

$$\text{find } \theta \in \mathcal{V} : a(\theta)(\phi) = f(\phi) \quad \forall \phi \in \mathcal{V}, \quad (11)$$

with the form  $a(\cdot)(\cdot) : \mathcal{V} \times \mathcal{V} \rightarrow \mathbb{R}$  semilinear in the second argument (nonlinear in the first) and differentiable in Fréchet sense, and the functional  $f(\cdot) : \mathcal{V} \rightarrow \mathbb{R}$  linear and continuous. We assume that suitable hypothesis for the existence and local uniqueness of the solutions of problem (11) hold. Additionally, in view of the error estimation, it is convenient to introduce the primal residual  $R^{pr}(\cdot)(\cdot) : \mathcal{V} \times \mathcal{V} \rightarrow R$  as:

$$R^{pr}(\theta)(\phi) := f(\phi) - a(\theta)(\phi). \quad (12)$$

Associated with the solution of problem (11), we desire to evaluate quantities of interest  $q_i$  represented by output functionals:

$$q_i = l_i(\theta) \quad i = 1, \dots, N, \quad (13)$$

with  $l_i(\theta) : \mathcal{V} \rightarrow R$  suitable differentiable linear or nonlinear functionals.

By introducing the finite dimensional approximation space  $\mathcal{V}_h \subset \mathcal{V}$ , the Galerkin approximated primal problem reads:

$$\text{find } \theta_h \in \mathcal{V}_h : a(\theta_h)(\phi_h) = f(\phi_h) \quad \forall \phi_h \in \mathcal{V}_h, \quad (14)$$

with the associated approximated output functionals  $q_{i,h}$ :

$$q_{i,h} = l_i(\theta_h) \quad i = 1, \dots, N. \quad (15)$$

If we refer to the problem (1)–(2), we have that  $\mathcal{V} = \{v \in H^1(\Omega) : v(0) = 0\}$  and:

$$\begin{aligned} a(\theta)(\phi) &= \int_{\Omega} \left( EI \frac{d\theta}{ds} \frac{d\phi}{ds} - \bar{P}_x \sin(\theta + \theta_0) \phi - \bar{P}_y \cos(\theta + \theta_0) \phi \right) ds, \\ f(\phi) &= \bar{M} \phi(L). \end{aligned} \quad (16)$$

We are interested in evaluating the following output functionals

$$\begin{aligned} q_1 = l_1(\theta) &:= U(\theta), & q_2 = l_2(\theta) &:= \theta(L), \\ q_3 = l_3(\theta) &:= u(L), & q_4 = l_4(\theta) &:= v(L), \end{aligned} \quad (17)$$

where  $l_1(\theta)$  is quadratic in  $\theta$ ,  $l_2(\theta)$  is linear in  $\theta$  and  $l_3(\theta)$  and  $l_4(\theta)$  are nonlinear trigonometric functionals. Note that, in general,  $q_2 = \theta(s_0)$  can be represented as follows  $l_2(\theta) = \int_{\Omega} \theta(s) \delta(s - s_0) ds$ , with  $\delta(s)$  the delta Dirac function and  $s_0 \in \Omega$ .

### 3.2 A posteriori error estimation

A posteriori error estimation in the goal–oriented framework represents a well established tool for errors associated with output functionals, see *e.g.* [8, 35, 20, 5], especially in the linear case. In this Section we recall results for nonlinear problems in view of the definition of the error estimators.

We introduce the dual variables  $z_i \in \mathcal{V}$ , representing the solutions of the following dual problems:

$$\text{find } z_i \in \mathcal{V} : a'(\theta)(z, \phi) = l'_i(\theta)(\phi) \quad \forall \phi \in \mathcal{V}, \quad i = 1, \dots, N, \quad (18)$$

which depend on the primal solution  $\theta \in \mathcal{V}$  (11) and on the output functionals  $l_i(\theta)$  (13). The notations  $a'(\cdot)(\cdot, \cdot) : \mathcal{V} \times \mathcal{V} \times \mathcal{V} \rightarrow R$  and  $l'_i(\cdot)(\cdot) : \mathcal{V} \times \mathcal{V} \rightarrow R$  indicate the first Fréchet differentials in  $\theta$  of the form  $a(\theta)(\cdot)$  and functionals  $l_i(\theta)$ . Note that, for a given  $\theta \in \mathcal{V}$ , the form  $a'(\theta)(\cdot, \cdot) : \mathcal{V} \times \mathcal{V} \rightarrow \mathbb{R}$  and the functionals  $l'_i(\theta)(\cdot) : \mathcal{V} \rightarrow \mathbb{R}$  are linear; it follows that the dual problems (18) are linear with respect to the dual variables. Similar considerations follow for higher order differentials. Additionally, it is convenient to introduce the dual residuals  $R_i^{du}(\cdot)(\cdot, \cdot) : \mathcal{V} \times \mathcal{V} \times \mathcal{V} \rightarrow R$  as:

$$R_i^{du}(\theta)(z_i, \phi) := l'(\theta)(\phi) - a'(\theta)(z_i, \phi) \quad i = 1, \dots, N. \quad (19)$$

The Galerkin approximation of the dual problems (18) reads:

$$\text{find } z_{i,h} \in \mathcal{V}_h : a'(\theta_h)(z_h, \phi_h) = l'_i(\theta_h)(\phi_h) \quad \forall \phi_h \in \mathcal{V}_h, \quad i = 1, \dots, N, \quad (20)$$

with  $\theta_h \in \mathcal{V}_h$  the solution of the primal problem (14).

The goal of the a posteriori error estimation consists in properly estimate the errors on the output functionals

$$|q_i - q_{i,h}| \quad i = 1, \dots, N, \quad (21)$$

once the approximated primal  $\theta_h \in \mathcal{V}$  is provided. With this aim, we recall from [8] the following Propositions, in which the Galerkin orthogonality property has been taken into account:

**Proposition 3.1** *For the Galerkin approximated primal (14) and dual (20) problems, we have:*

$$q_i - q_{i,h} = \mathcal{E}_{q_i} + \mathcal{R}_i \quad i = 1, \dots, N, \quad (22)$$

with:

$$\mathcal{E}_{q_i} = \mathcal{E}_{q_i}(\theta, z_i) := \frac{1}{2} R^{pr}(\theta_h)(z_i) + \frac{1}{2} R_i^{du}(\theta_h)(z_{i,h}, \theta), \quad (23)$$

the remainder terms:

$$\begin{aligned} \mathcal{R}_i := & \frac{1}{2} \int_0^1 \{ l_i'''(\theta_h + te^{pr})(e^{pr}, e^{pr}, e^{pr}) - a'''(\theta_h + te^{pr})(e^{pr}, e^{pr}, e^{pr}, z_h + te^{du}) \\ & - 3a''(\theta_h + te^{pr})(e^{pr}, e^{pr}, e_i^{du}) \} t(t-1) dt \end{aligned} \quad (24)$$

and the primal and dual errors defined as  $e^{pr} := \theta - \theta_h$  and  $e^{du} := z_i - z_{i,h}$ .

**Proposition 3.2** *Let us assume that  $\widehat{\theta}_h \in \widehat{\mathcal{V}}_h \subset \mathcal{V}$  is an improved (enhanced) approximated solution with respect to  $\theta_h \in \mathcal{V}_h$ , then:*

$$q_i - q_{i,h} = \widehat{\mathcal{E}}_{q_i} + \widehat{\mathcal{R}}_i \quad i = 1, \dots, N, \quad (25)$$

with:

$$\widehat{\mathcal{E}}_{q_i} = \widehat{\mathcal{E}}_{q_i}(z_i) := R^{pr}(\theta_h)(z_i), \quad (26)$$

and the remainder terms such that:

$$\left| \widehat{\mathcal{R}}_i \right| \leq \max_{v_h \in \overline{\theta, \widehat{\theta}_h, \theta_h}} |l_i''(v_h)(\widehat{e}^{pr}, e^{pr}) - a''(v_h)(\widehat{e}^{pr}, e^{pr}, z)|, \quad (27)$$

being  $\overline{\theta, \widehat{\theta}_h, \theta_h}$  the “triangle” spanned in  $\mathcal{V}$  by the functions  $\theta$ ,  $\widehat{\theta}_h$  and  $\theta_h$  and  $\widehat{e}_{pr} := \theta - \widehat{\theta}_h$ .

Let us observe that:

1. the a posteriori error estimates (22) and (25) are not computable, since they involve the exact solutions  $\theta \in \mathcal{V}$  and  $z_i \in \mathcal{V}$ ;
2. the remainder terms  $\mathcal{R}_i$  in Eq.(24) are null for at most quadratic functionals  $l_i(\theta)$  and bilinear form  $a(\theta)(\cdot) = a(\theta, \cdot)$ ;
3. in the case of linear functionals  $l_i(\theta)$  and bilinear form  $a(\theta)(\cdot) = a(\theta, \cdot)$ , the remainder terms  $\mathcal{R}_i$  and  $\widehat{\mathcal{R}}_i$  in Eqs.(24) and (27) are null and the errors  $q_i - q_{i,h} = \mathcal{E}_{q_i} \equiv \widehat{\mathcal{E}}_{q_i}$ ;
4. if the differentials of the form  $a(\theta)(\cdot)$  and functionals  $l_i(\theta)$  can be bounded for  $\theta \in \mathcal{V}$ , the remainder terms  $\mathcal{R}_i$  and  $\widehat{\mathcal{R}}_i$  converge to zero with order 3 and 2, respectively, in the errors  $e^{pr}$  and  $e_i^{du}$ ;
5. for the rod problem under consideration (see Eqs.(16) and (17)), the remainder terms  $\mathcal{R}_i$  and  $\widehat{\mathcal{R}}_i$  can be bounded, since the functionals involved are at most quadratic or depend on trigonometric functions which are  $C^\infty$  continuous and bounded; similar properties hold for the form  $a(\theta)(\cdot)$ ;
6. the terms  $\mathcal{E}_{q_i}$  and  $\widehat{\mathcal{E}}_{q_i}$  in the estimates (22) and (25) can be used to evaluate the errors  $|q_i - q_{i,h}|$  if the remainder terms  $\mathcal{R}_i$  and  $\widehat{\mathcal{R}}_i$  are “sufficiently” small; eventually, they can be used to correct the output functionals  $s_{i,h}$  as  $\widetilde{q}_{i,h} = q_{i,h} + \mathcal{E}_{q_i}$  or  $\widehat{q}_{i,h} = q_{i,h} + \widehat{\mathcal{E}}_{q_i}$ .

## 4 Error estimators with B–spline basis

In this Section, following from the goal-oriented a posteriori error estimates recalled in Sec.3, we propose the error estimators for the Galerkin approximation method with the use of a B–spline basis.

### 4.1 Numerical approximation: B–spline basis

We use univariate B–spline basis for the construction of the approximation space  $\mathcal{V}_h$ ; we refer the reader to [38] and also to [15] for a general overview of the definition and construction of B–spline basis as well as their properties. We consider B–spline basis defined in a parametric domain, hereafter denoted by  $\overline{\Omega} = (0, 1)$ , with associated knot vectors  $\Xi = \{\xi_j\}_{j=1}^m$ , with  $\xi_j$  the  $j^{\text{th}}$  knot, for some  $m = n + p + 1$ , where  $n$  is the total number of degrees of freedom and  $p$  is the polynomial order under consideration. Specifically, we consider open knots vectors  $\Xi$  with internal equally spaced  $N_e$  knot spans, for which the total number of degrees of freedom is  $n = N_e + p$ ;  $N_e$  can be interpreted as the number of “elements”  $e = 1, \dots, N_e$  of size  $h$  in which  $\overline{\Omega}$  is partitioned. In this case,  $\Xi \equiv \Xi_{h,p} := \{\{0\}^{p+1}, \dots, \xi_j, \dots, \{1\}^{p+1}\}$  with  $\xi_j = (j - p - 1)h$  for  $j = p + 2, \dots, n$  with  $h := 1/N_e$ .

The  $j^{\text{th}}$  B–spline basis function,  $B_{h,p,j}(\xi)$ , is defined in  $\overline{\Omega}$  by using the knot vector  $\Xi$  with the Cox–de Boor recursion formula (see [38] and [15]); the subscripts  $h$  and  $p$  in the basis functions refer to the number of internal knot spans ( $N_e$  “elements”) and their polynomial order  $p$ . Examples of such basis functions for  $p = 1, 2, 3$  are highlighted in Fig.2(top–right), (bottom–left) and (bottom–right), respectively, in the case  $N_e = 5$ .

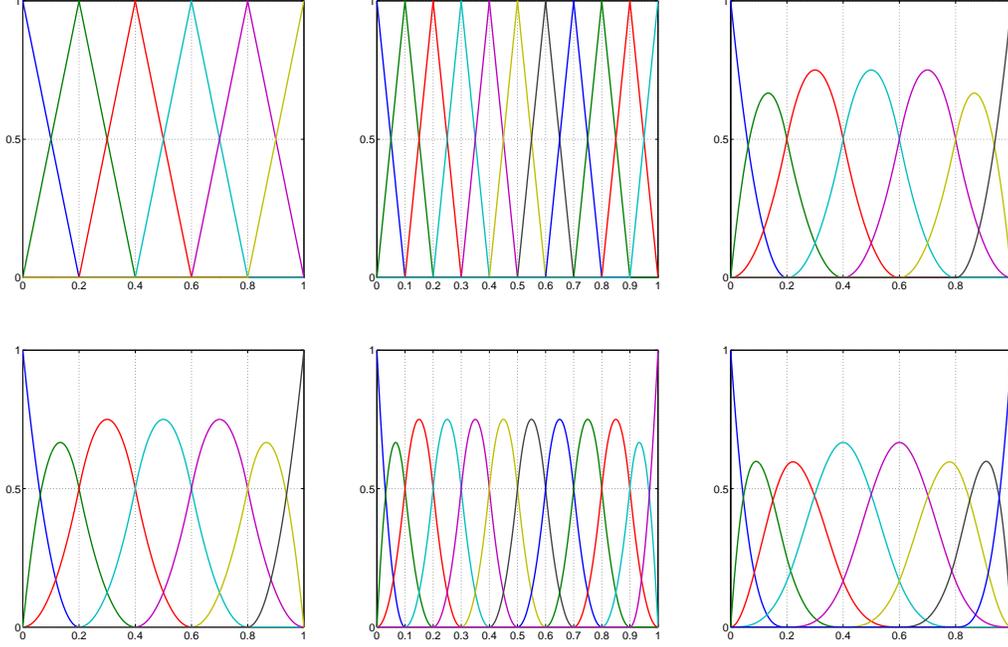


Figure 2: B-spline basis  $\{B_{h,p,j}(\xi)\}_{j=1}^{N_e+p}$  (left) and enhanced basis  $\{B_{2h,p,j}(\xi)\}_{i=1}^{2N_e+p}$  (center) and  $\{B_{h,p+1,j}(\xi)\}_{i=1}^{N_e+p+1}$  (right) for  $p = 1$  (top) and  $p = 2$  (bottom) with  $\xi \in \overline{\Omega}$ ;  $N_e = 5$  is considered.

We observe that globally high-order continuous B-spline basis functions with compact support can be easily constructed by introducing a relatively small number of additional degrees of freedom; indeed,  $n = N_e + p$  with respect to the classic Finite Element method for which  $C^0$  globally continuous basis yields  $n = pN_e + 1$  degrees of freedom. Specifically, the basis functions so far constructed are  $C^{p-1}$  globally continuous and  $C^\infty$  in each “element”. Additionally, we have that the support of each basis function is  $p+1$  knot spans (“elements”).

**Remark 4.1** For a given knot vector  $\Xi$ , the B-spline basis of order  $p = 1$  ( $\{B_{h,1,j}(\xi)\}_{j=1}^{N_e+1}$ ) coincides with the classic linear Finite Element Lagrangian basis.

The geometrical map from the parametric domain  $\overline{\Omega}$  to the physical domain  $\Omega$ ,  $s(\xi) : \overline{\Omega} \rightarrow \Omega$ , is defined by using the B-spline basis  $\{B_{h,p,j}(\xi)\}_{j=1}^n$  and  $n$  control points  $\zeta_j \in \mathbb{R}$  as  $s(\xi) := \sum_{j=1}^n B_{h,p,j}(\xi)\zeta_j$ . We assume that  $\zeta_{j+1} > \zeta_j$  for  $j = 1, \dots, n$

in order to have an invertible map, with  $\zeta_1 = 0$  and  $\zeta_n = L$ ; it is convenient for this one-dimensional problem to distribute the control points  $\zeta_j$  such that a linear map is obtained.

The functional space  $\overline{\mathcal{X}}_{h,p} := \text{span}(\{B_{h,p,j}(\xi)\}_{j=1}^{n_{h,p}})$  of dimension  $n_{h,p} = N_e + p$  is originated by the B-spline basis for  $\xi \in \overline{\Omega}$ , for which a generic function  $\overline{v}_{h,p}(\xi) \in \overline{\mathcal{X}}_{h,p}$

reads  $\bar{v}_{h,p}(\xi) = \sum_{j=1}^n B_{h,p,j}(\xi)v_j$  for some control variables  $v_j \in \mathbb{R}$ . The function  $\bar{v}_{h,p}(\xi)$

mapped in the physical domain  $\Omega$  reads  $v_{h,p}(s) = \bar{v}_{h,p}(\xi) \circ s(\xi)^{-1}$ . Due to the invertibility of the geometrical map, the functions  $v_{h,p}$  and  $\bar{v}_{h,p}$  will be indifferently interchanged as well for the space  $\bar{\mathcal{X}}_{h,p}$  with its correspondent  $\mathcal{X}_{h,p}$  in  $\Omega$ .

It follows that the Galerkin approximated solutions of the primal and dual problems (Eqs.(11) and (18)), which we will indicate as  $\theta_{h,p}$ ,  $z_{i,h,p}$  in order to highlight their dependency on the “element” size  $h$  and order  $p$ , belongs to the functional space  $\mathcal{V}_{h,p} := \left\{ v_{h,p} \in \mathcal{X}_{h,p} : v_{h,p}|_{\Gamma_D} = 0 \right\} \subset \mathcal{V}$  of dimension  $n_{\mathcal{V}_{h,p}} \leq n_{h,p}$ ; note that with this new notation, the space  $\mathcal{V}_h \equiv \mathcal{V}_{h,p}$  and the output functionals  $q_{i,h} \equiv q_{i,h,p}$ .

For a more comprehensive analysis of the use of B-splines basis (eventually NURBS basis) and the related advantages in the context of analysis, we refer the reader to [7] and [15] (and to the references therein indicated).

We solve the nonlinear primal problem (14) by means of the Newton–Raphson method [39]. In particular, the approximated solution  $\theta_{h,p} \in \mathcal{V}_{h,p}$  is achieved by means of a converging sequence of intermediate solutions  $\theta_{h,p}^k \in \mathcal{V}_{h,p}$ , obtained by solving for  $k = 0, 1, \dots$  the following tangent (linear) problem with the consequent update:

$$\begin{aligned} \text{find } \delta\theta_{h,p}^k \in \mathcal{V}_{h,p} : a'(\theta_{h,p}^k)(\delta\theta_{h,p}^k, \phi_{h,p}) &= -R^{pr}(\theta_{h,p}^k)(\phi_{h,p}) \quad \forall \phi_{h,p} \in \mathcal{V}_{h,p}, \\ \theta_{h,p}^{k+1} &= \theta_{h,p}^k + \delta\theta_{h,p}^k, \end{aligned} \quad (28)$$

where  $\theta_{h,p}^0 \in \mathcal{V}_{h,p}$  is a prescribed initial guess of the solution “sufficiently” close to the solution  $\theta_{h,p}$ ; the bilinear form  $a'(\theta)(\cdot, \cdot)$  is given in Eq.(18), while the primal residual  $R^{pr}(\cdot)(\cdot)$  in Eq.(12). The satisfaction of the stopping criterium  $\|\mathbf{R}^{k+1}\| < \text{tol}_{NR}\|\mathbf{R}^0\|$  terminates the procedure for some  $\text{tol}_{NR} \ll 1$ , where  $\mathbf{R}^k := \{R^{pr}(\theta_{h,p}^k)(B_{h,p,j})\}_{j=1}^{n_{\mathcal{V}_{h,p}}}$ .

## 4.2 Error estimators

We propose and consider the error estimators for the output functionals  $q_i$  for  $i = 1, \dots, N$  by using the a posteriori error estimates (22) and (25) with the approximation method presented in the previous Section. Due to the difficulties in properly evaluating the remainder terms  $\mathcal{R}_i$  and  $\widehat{\mathcal{R}}_i$  of Eqs.(24) and (27), we derive error estimators by using only the terms  $\mathcal{E}_i$  and  $\widehat{\mathcal{E}}_i$  of Eqs.(23) and (26).

We remark that while the terms  $\mathcal{E}_i = \mathcal{E}_i(\theta, z_i)$  depend on both the exact primal and dual solutions,  $\widehat{\mathcal{E}}_i = \widehat{\mathcal{E}}_i(z_i)$  depends only on the exact dual solutions. In both cases, in order to derive and evaluate the error estimators, we need computable variables in place of the exact primal and dual solutions. The most natural choice for replacing the exact solutions with the approximated ones  $\theta_{h,p}$  and  $z_{i,h,p} \in \mathcal{V}_{h,p}$  is, however, not effective, since  $\mathcal{E}_i(\theta_h, z_{i,h,p}) = \widehat{\mathcal{E}}_i(z_{i,h,p}) \equiv 0$  due to the Galerkin orthogonality property of the primal and dual problems (11) and (18) (see also [5]). For this reason the exact solutions need to be replaced by computable enhanced approximated solutions; see *e.g.* [8] for a wider discussion<sup>1</sup>.

A first couple of error estimators is obtained by considering enhanced dual solutions for the terms  $\widehat{\mathcal{E}}_i(z_i)$ . A first, standard choice, consists in building the enhanced functional space  $\mathcal{V}_{2h,p}$  by uniformly refining the knot spans internal to  $\Xi$  such that the dimension

<sup>1</sup>An alternative possibility consists in using approximated solutions (or gradients of the solutions) recovered from  $\theta_{h,p}$  and  $z_{i,h,p} \in \mathcal{V}_{h,p}$ ; see *e.g.* [10].

of the enhanced space  $\mathcal{X}_{2h,p}$  is  $n_{2h,p} = 2N_e + p = 2n_{h,p} - p$ ; this procedure is called knot insertion ([38]) and we can regard it as “mesh” refinement. However, knot insertion does not coincide with the  $h$ -refinement of the Finite Element method of order  $p$ , since the new basis obtained is  $C^{p-1}$  continuous through the newly inserted knots and not  $C^0$ ; they do coincide only for the case  $p = 1$ .

As alternative, we propose to use a higher order enhanced dual solution with respect to the order  $p$  considered for the primal solution  $\theta_{h,p} \in \mathcal{V}_{h,p}$ . With this aim, in order to build the higher order enhanced space  $\mathcal{V}_{h,p+1}$ , we consider the *order elevation* of the original B-spline basis, but without increasing the multiplicity of the internal knots of the original knot vector  $\Xi_{h,p}$  ([38]); only the multiplicity of the external knots  $\{0\}$  and  $\{1\}$  is increased by one to obtain the new knot vector  $\Xi_{h,p+1} := \{\{0\}^{p+2}, \dots, \xi_j, \dots, \{1\}^{p+2}\}$ . The result is a B-spline basis with increased  $C^p$  continuity through the internal knots  $\xi_j$  of the knot vector  $\Xi_{h,p+1}$ <sup>2</sup>. This procedure corresponds to a step of the “pure”  $k$ -refinement approach introduced for Isogeometric Analysis [15]; however, this can not be identified with the standard  $p$ -refinement of the Finite Element method which would maintain  $C^0$  continuity through the knots. Finally, the higher order enhanced space reads  $\mathcal{V}_{h,p+1} := \left\{ v_{h,p+1} \in \mathcal{X}_{h,p+1} : v_{h,p+1}|_{\Gamma_D} = 0 \right\}$ , where the space  $\mathcal{X}_{h,p+1}$  assumes dimension  $n_{h,p+1} = N_e + p + 1 = n_{h,p} + 1$ .

Examples of the so obtained enhanced B-spline basis are displayed in Fig.2 for the cases  $p = 1, 2$  and  $N_e = 5$ .

The enhanced dual solutions  $z_{i,2h,p} \in \mathcal{V}_{2h,p}$  and  $z_{i,h,p+1} \in \mathcal{V}_{h,p+1}$  are obtained by solving the following dual problems, respectively:

$$\text{find } z_{i,2h,p} \in \mathcal{V}_{2h,p} : a'(\theta_{h,p})(z_{i,2h,p}, \phi_{2h,p}) = l'_i(\theta_{h,p})(\phi_{2h,p}) \quad \forall \phi_{2h,p} \in \mathcal{V}_{2h,p}, \quad (29)$$

$$\text{find } z_{i,h,p+1} \in \mathcal{V}_{h,p+1} : a'(\theta_{h,p})(z_{i,h,p+1}, \phi_{h,p+1}) = l'_i(\theta_{h,p})(\phi_{h,p+1}) \quad \forall \phi_{h,p+1} \in \mathcal{V}_{h,p+1}, \quad (30)$$

for  $i = 1, \dots, N$ , where  $\theta_{h,p} \in \mathcal{V}_{h,p}$  is the approximated solution of the primal problem (not enhanced).

On this basis, from Eq.(26), we define the error estimators  $\widehat{\Delta}_{i,2h,p}$  and  $\widehat{\Delta}_{i,h,p+1}$  as, respectively:

$$\widehat{\Delta}_{i,2h,p} := \widehat{\mathcal{E}}_i(z_{i,2h,p}) \quad i = 1, \dots, N, \quad (31)$$

$$\widehat{\Delta}_{i,h,p+1} := \widehat{\mathcal{E}}_i(z_{i,h,p+1}) \quad i = 1, \dots, N, \quad (32)$$

where the  $i^{\text{th}}$  index refer to the output functional  $q_i$ . The error estimator  $\widehat{\Delta}_{i,2h,p}$  coincides with the one considered in [46], proposed for two-dimensional B-splines and T-splines.

We provide two additional error estimators from the term  $\mathcal{E}_i(\theta, z_i)$  of Eq.(23), for which the concept of enhanced dual solutions introduced so far can be extended to the primal solution  $\theta_{h,p} \in \mathcal{V}_{h,p}$ . However, we observe that in order to obtain such enhanced solutions  $\theta_{2h,p} \in \mathcal{V}_{2h,p}$  and  $\theta_{h,p+1} \in \mathcal{V}_{h,p+1}$ , nonlinear problems need to be solved by means of the Newton-Raphson method. In order to avoid this inefficiency in the evaluation of the errors on the outputs  $q_i$  associated with the current primal solution  $\theta_{h,p} \in \mathcal{V}_{h,p}$ , we propose an alternative approach based on the tangent problem (28) of the Newton-Raphson method. In particular, we obtain the enhanced primal solutions  $\widetilde{\theta}_{2h,p} \in \mathcal{V}_{2h,p}$  and  $\widetilde{\theta}_{h,p+1} \in \mathcal{V}_{h,p+1}$  by solving the following tangent (linear) problems,

<sup>2</sup>In the standard order elevation procedure the multiplicity of the internal knots is increased in order to preserve the discontinuity of the derivatives of the enhanced basis with respect to the original one.

respectively:

$$\begin{aligned} \text{find } \delta\tilde{\theta}_{2h,p} \in \mathcal{V}_{2h,p} : a'(\theta_{h,p})(\delta\tilde{\theta}_{2h,p}, \phi_{2h,p}) &= -R^{pr}(\theta_{h,p})(\phi_{2h,p}) \quad \forall \phi_{2h,p} \in \mathcal{V}_{2h,p}, \\ \tilde{\theta}_{2h,p} &= \Pi_{h,p}^{2h,p} \theta_{h,p} + \delta\tilde{\theta}_{2h,p}, \end{aligned} \quad (33)$$

$$\begin{aligned} \text{find } \delta\tilde{\theta}_{h,p+1} \in \mathcal{V}_{h,p+1} : a'(\theta_{h,p})(\delta\tilde{\theta}_{h,p+1}, \phi_{h,p+1}) &= -R^{pr}(\theta_{h,p})(\phi_{h,p+1}) \quad \forall \phi_{h,p+1} \in \mathcal{V}_{h,p+1}, \\ \tilde{\theta}_{h,p+1} &= \Pi_{h,p}^{h,p+1} \theta_{h,p} + \delta\tilde{\theta}_{h,p+1}, \end{aligned} \quad (34)$$

for the given solution of the primal problem  $\theta_{h,p} \in \mathcal{V}_{h,p}$ ;  $\Pi_{h,p}^{2h,p} : \mathcal{V}_{h,p} \rightarrow \mathcal{V}_{2h,p}$  and  $\Pi_{h,p}^{h,p+1} : \mathcal{V}_{h,p} \rightarrow \mathcal{V}_{h,p+1}$  represent projection operators of functions  $v_{h,p} \in \mathcal{V}_{h,p}$  into the spaces  $\mathcal{V}_{2h,p}$  and  $\mathcal{V}_{h,p+1}$ , respectively.

By recalling Eq.(23) and the enhanced dual solutions of Eqs.(29) and (30), we define the error estimators  $\Delta_{i,2h,p}$  and  $\Delta_{i,h,p+1}$  as:

$$\Delta_{i,2h,p} := \mathcal{E}_i(\tilde{\theta}_{2h,p}, z_{i,2h,p}) \quad i = 1, \dots, N, \quad (35)$$

$$\Delta_{i,h,p+1} := \mathcal{E}_i(\tilde{\theta}_{h,p+1}, z_{i,h,p+1}) \quad i = 1, \dots, N. \quad (36)$$

We remark that the error estimators can be conveniently and immediately adopted in the case of linear problems.

**Remark 4.2** *Following from Remark 4.1, the error estimators  $\widehat{\Delta}_{i,2h,p}$  and  $\Delta_{i,2h,p}$  for  $p = 1$  can be directly used to estimate errors associated with the classic Finite Element method with linear basis.*

We note that the error estimators do not represent rigorous error bounds for the errors on the output functionals  $|q_i - q_{i,h}|$ , since the remainder terms  $\mathcal{R}_i$  and  $\widehat{\mathcal{R}}_i$  are not included in the estimators and the exact primal and dual solutions are replaced with enhanced solutions. In order to evaluate the capability of the error estimators (31), (32), (35) and (36) to bound and provide indications of the error (21), we introduce the following effectivity indexes:

$$\begin{aligned} \widehat{\eta}_{i,2h,p} &:= \frac{\widehat{\Delta}_{i,2h,p}}{|q_i - q_{i,h,p}|}, & \widehat{\eta}_{i,h,p+1} &:= \frac{\widehat{\Delta}_{i,h,p+1}}{|q_i - q_{i,h,p}|}, \\ \eta_{i,2h,p} &:= \frac{\Delta_{i,2h,p}}{|q_i - q_{i,h,p}|}, & \eta_{i,h,p+1} &:= \frac{\Delta_{i,h,p+1}}{|q_i - q_{i,h,p}|}, \end{aligned} \quad (37)$$

for  $i = 1, \dots, N$ . Effectivity indexes larger than 1 indicate the capability of the error estimator to bound the error; however, sharp estimators should exhibit effectivity indexes close to 1. Asymptotic effectivity indexes are obtained for large number of degrees of freedom  $n_{\mathcal{V}_{h,p}}$ .

**Remark 4.3** *Although we are only dealing with a one-dimensional problem, it is still interesting to discuss the computational costs associated with the evaluation of the estimators. With this respect, the estimator  $\widehat{\Delta}_{i,h,p+1}$  is the most convenient one, since the primal residual is evaluated with the enhanced dual solutions  $z_{i,h,p+1}$  for which only an additional degree of freedom is added with respect to  $\theta_{h,p}$ . Conversely, the estimator  $\Delta_{i,2h,p}$  is the most expensive to evaluate since both the primal and dual residuals need to be evaluated with the enhanced primal and solutions  $\tilde{\theta}_{2h,p}$  and  $z_{i,2h,p}$ , each containing*

Test	$EI$	$L$	$P_x$	$P_y$	$M$
1.1	10.0	1.00	0.0	100	0.0
1.2	"	"	$\frac{1}{2} \frac{\pi^2 EI}{AL^2}$	10.0	"
1.3	"	"	$\frac{3}{2} \frac{\pi^2 EI}{AL^2}$	"	"
2	$3.60 \cdot 10^3$	$\pi$	-2.062648	0.0	0.0
3.1	0.50	4.00	0.150	-1.00	$-\frac{1}{10} \frac{\pi EI}{L}$
3.2	0.50	4.00	1.00	0.0	0.0
4	10.0	$(2\pi - \alpha)R$	50.0	0.0	0.0

Table 1: Data for the Test problems 1.1–1.3, 2, 3.1–3.2 and 4.

Test	$\theta_0(s)$	"Exact"	$N_e = 2$	4	8	16	32	64	128
1.1	$\pi s$	5	5, 5	5, 5	5, 5	5, 5	5, 5	5, 5	5, 5
1.2	"	5	5, 5	5, 5	5, 5	5, 5	5, 5	5, 5	5, 5
1.3	"	4	5, 5	5, 5	5, 5	5, 5	5, 5	5, 5	5, 5
2	$-\pi s$	4	4, 4	4, 4	4, 4	4, 4	4, 4	4, 4	4, 4
3.1	$-\pi s$	7	10, 16	11, 13	10, 6	7, 7	7, 7	7, 7	7, 7
3.2	$\pi/2 s$	5	4, 4	4, 4	5, 5	5, 5	5, 5	5, 5	5, 5
4	$-\cos(\pi s)$	5	4, 6	5, 7	5, 6	5, 5	5, 5	5, 5	5, 5

Table 2: Number of Newton–Raphson iterative steps starting from the initial solution  $\theta_0(s)$  for the “exact“ solution and the approximate ones with  $N_e \in \{2^r\}_{r=2}^7$  ( $p = 1$ ,  $p = 2$ ) for the Test problems 1.1–1.3, 2, 3.1–3.2 and 4; the pairs in the entries of the table indicate the steps for  $p = 1$  and  $p = 2$ .

a number of degrees of freedom about  $(2N_e + p)/(N_e + p)$  times higher. Among these, intermediate costs are obtained with  $\widehat{\Delta}_{i,2h,p}$  and  $\Delta_{i,h,p+1}$ . Indeed,  $\widehat{\Delta}_{i,2h,p}$  only require the evaluation of the primal residual but with the enhanced dual solution  $z_{i,2h,p}$ , while  $\Delta_{i,h,p+1}$  evaluates both the primal and dual residuals with the enhanced primal and dual solutions  $\widetilde{\theta}_{h,p+1}$  and  $z_{i,h,p+1}$ . In general, the cost associated with  $\widehat{\Delta}_{i,2h,p}$  could be higher than the one for  $\Delta_{i,h,p+1}$  for a sufficiently large  $N_e$ .

Additionally, the cost associated with the computations of the enhanced primal and dual solutions should be taken into account. With this respect the estimators  $\widehat{\Delta}_{i,2h,p}$  and  $\widehat{\Delta}_{i,h,p+1}$  only require the solution of the linear dual problems (29) and (30), while for  $\Delta_{i,2h,p}$  and  $\Delta_{i,h,p+1}$ , also the enhanced primal ones (33) and (34) need to be solved, with consequent increased computational costs.

## 5 Results and discussion

In this Section we report the numerical results obtained using the proposed error estimators applied to the solution of various Test problems of the same type as the one introduced in Sec.2. The error estimators are evaluated and analyzed in terms of their effectivity indexes; a discussion follows from these results.

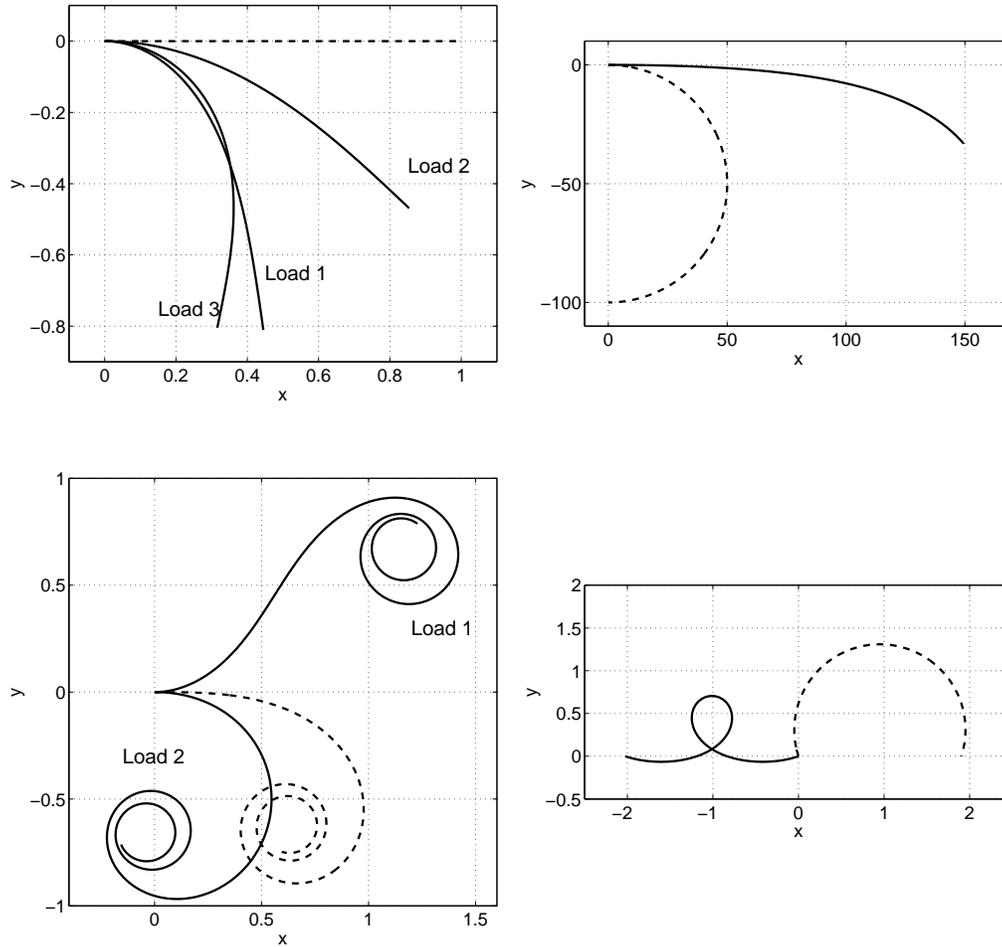


Figure 3: Undeformed configuration (dashed line,  $--$ ) and deformed ones (continuous lines,  $-$ ) for Tests 1.1–1.3 (top-left), 2 (top-right), 3.1–3.2 (bottom-left) and 4 (bottom-right).

## 5.1 Numerical results

We study four Test problems, Tests 1–4; Tests 1.1–1.3 and 3.1–3.2 represent the same problems but with different load conditions. The data used for the various Test problems are reported in Table 1 (see Sec.2 for the definition of the notation). We note that Test 4 does not correspond to a cantilever problem, but to a simply supported rod problem. However, as both  $\bar{P}_y$  and  $\bar{M}$  are set to zero, we can make use of the equations for the cantilever problem with no changes; in particular, for this Test we choose  $\alpha = 4\pi/5$  and  $R = 1$ . The “exact” solutions of the Test problems are plotted in Fig.3 in terms of the displacements  $u(s)$  and  $v(s)$ . Such solutions are obtained using the Newton–Raphson method with initial solutions as the ones indicated with  $\theta_0(s)$  in Table 2.

We solve the Test problems using B-spline bases of orders  $p = 1$  and  $p = 2$  for

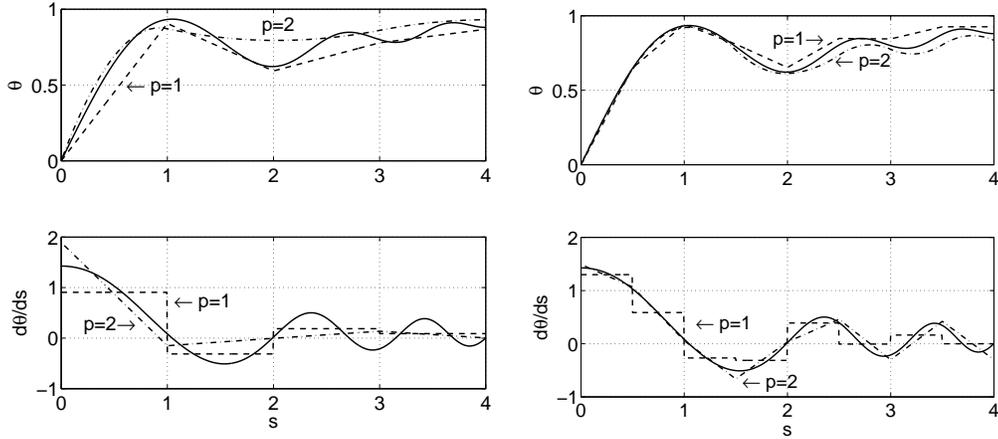


Figure 4: Test 3.2. Comparison of the approximated solutions  $\theta_{h,p}$  (top) and their derivatives  $\frac{d\theta_{h,p}}{ds}$  (bottom) with the “exact” ones (continuous lines, —) for  $p = 1$  (dashed lines, --) and  $p = 2$  (dash-dotted lines, -·);  $N_e = 4$  (left) and  $N_e = 8$  (right).

decreasing values of  $h = 1/N_e$ ; in particular, we assume  $N_e = 2, 4, 8, \dots, 128$  ( $N_e \in \{2^r\}_{r=2}^7$ ). A 7-point Gauss quadrature rule is used for the evaluation of the integrals in each element  $e = 1, \dots, N_e$ . Also, the tolerance for the stopping criterion of the Newton–Raphson method (28) is set to  $tol_{NR} = 10^{-12}$ .

Additionally, we assume the approximated solutions obtained by solving the primal problem with a B-spline basis of order  $p = 4$  with an open knot vector  $\Xi$  partitioned into  $N_e = 1,024$  equally spaced “elements” as the “exact” solutions.

In Fig.4 we compare the approximated solutions and their derivatives, obtained for Test 3.2 with  $p = 1, 2$  and  $N_e = 4, 8$ , against the “exact” solutions.

In Table 2 we report the number of Newton–Raphson iterative steps required for convergence to the approximate primal solutions  $\theta_{h,p} \in \mathcal{V}_{h,p}$  in comparison to those obtained for convergence to the “exact” solution. We can observe that the obtained number of steps is equal to the one obtained for convergence to the “exact” solution in most of the cases, with the exception of Tests 3 and 4 when a small number of “elements”  $N_e$  is considered.

In Tables 3–9 we report the effectivity indexes (37) of the error estimators associated with all the Test problems and output functionals  $q_i$  for  $i = 1, \dots, N = 4$  (the index  $i$  is dropped in the effectivity indexes, since deducible from the context) for all the approximations  $\mathcal{V}_{h,p}$  obtained with  $N_e \in \{2^r\}_{r=2}^7$  and  $p = 1, 2$ . The values of the “exact” output functionals  $q_i$  are reported as well as the asymptotic convergence orders of the errors  $|q_i - q_{i,h,p}|$  with respect to  $h$ ; these correspond to about 2 and 4 in the cases  $p = 1$  and  $p = 2$ , respectively. The output functional  $q_4$  is not discussed for Test 4 since in this case  $q_4 \equiv 0$  and  $q_{4,h,p} = 0$  except for round-off errors.

$p = 1$

$N_e$	$ q_1 - q_{1,h,p} $	$\widehat{\eta}_{2h,p}$	$\widehat{\eta}_{h,p+1}$	$\eta_{2h,p}$	$\eta_{h,p+1}$
2	1.3257e+00	0.79	1.18	0.79	0.60
4	3.2983e-01	0.89	2.05	0.89	1.38
8	8.0124e-02	0.95	2.68	0.95	1.83
16	1.9863e-02	0.97	3.00	0.97	2.03
32	4.9551e-03	0.97	3.15	0.97	2.12
64	1.2381e-03	0.97	3.22	0.97	2.16
128	3.0949e-04	0.98	3.26	0.98	2.18

Conv. Order = 2.00

$p = 2$

$N_e$	$ q_1 - q_{1,h,p} $	$\widehat{\eta}_{2h,p}$	$\widehat{\eta}_{h,p+1}$	$\eta_{2h,p}$	$\eta_{h,p+1}$
2	1.3831e-01	0.51	0.97	0.51	1.73
4	5.4334e-03	0.42	1.65	0.42	6.83
8	3.1742e-04	0.40	1.63	0.40	8.32
16	1.9405e-05	0.39	1.60	0.39	8.04
32	1.1957e-06	0.39	1.59	0.39	7.70
64	7.4366e-08	0.39	1.58	0.39	7.49
128	4.6413e-09	0.39	1.58	0.39	7.38

Conv. Order = 4.00

$N_e$	$ q_2 - q_{2,h,p} $	$\widehat{\eta}_{2h,p}$	$\widehat{\eta}_{h,p+1}$	$\eta_{2h,p}$	$\eta_{h,p+1}$
2	4.5317e-02	0.75	0.82	0.75	0.93
4	1.0614e-02	0.75	0.96	0.75	1.11
8	2.6207e-03	0.75	0.99	0.75	1.15
16	6.5324e-04	0.75	1.00	0.75	1.16
32	1.6319e-04	0.75	1.00	0.75	1.17
64	4.0791e-05	0.75	1.00	0.75	1.17
128	1.0197e-05	0.75	1.00	0.75	1.17

Conv. Order = 2.00

$N_e$	$ q_2 - q_{2,h,p} $	$\widehat{\eta}_{2h,p}$	$\widehat{\eta}_{h,p+1}$	$\eta_{2h,p}$	$\eta_{h,p+1}$
2	9.0134e-04	0.92	0.66	0.92	0.18
4	7.9694e-05	0.93	0.96	0.93	0.83
8	5.3464e-06	0.94	0.99	0.94	1.01
16	3.3891e-07	0.94	1.00	0.94	0.87
32	2.1228e-08	0.94	1.00	0.94	0.75
64	1.3272e-09	0.94	1.00	0.94	0.69
128	8.2955e-11	0.94	1.00	0.94	0.66

Conv. Order = 4.00

$N_e$	$ q_3 - q_{3,h,p} $	$\widehat{\eta}_{2h,p}$	$\widehat{\eta}_{h,p+1}$	$\eta_{2h,p}$	$\eta_{h,p+1}$
2	2.7692e-02	0.72	0.98	0.72	0.68
4	6.3033e-03	0.74	1.05	0.74	0.50
8	1.5299e-03	0.75	1.02	0.75	0.41
16	3.7993e-04	0.75	1.01	0.75	0.37
32	9.4829e-05	0.75	1.00	0.75	0.36
64	2.3698e-05	0.75	1.00	0.75	0.36
128	5.9239e-06	0.75	1.00	0.75	0.36

Conv. Order = 2.00

$N_e$	$ q_3 - q_{3,h,p} $	$\widehat{\eta}_{2h,p}$	$\widehat{\eta}_{h,p+1}$	$\eta_{2h,p}$	$\eta_{h,p+1}$
2	2.0920e-05	1.64	9.74	1.64	62.5
4	8.2291e-06	1.02	0.45	1.02	39.6
8	4.5144e-08	0.92	3.78	0.92	526
16	6.1625e-09	0.91	0.39	0.91	228
32	5.7855e-10	0.93	0.89	0.93	143
64	4.0226e-11	0.94	0.97	0.94	124
128	2.5867e-12	0.94	0.99	0.93	119

Conv. Order = 3.96

$N_e$	$ q_4 - q_{4,h,p} $	$\widehat{\eta}_{2h,p}$	$\widehat{\eta}_{h,p+1}$	$\eta_{2h,p}$	$\eta_{h,p+1}$
2	4.3420e-02	0.81	0.88	0.81	0.75
4	1.0687e-02	0.77	0.97	0.77	0.67
8	2.6301e-03	0.75	1.00	0.75	0.64
16	6.5463e-04	0.75	1.00	0.75	0.62
32	1.6348e-04	0.75	1.00	0.75	0.62
64	4.0858e-05	0.75	1.00	0.75	0.61
128	1.0214e-05	0.75	1.00	0.75	0.61

Conv. Order = 2.00

$N_e$	$ q_4 - q_{4,h,p} $	$\widehat{\eta}_{2h,p}$	$\widehat{\eta}_{h,p+1}$	$\eta_{2h,p}$	$\eta_{h,p+1}$
2	2.0822e-03	0.98	0.93	0.98	0.28
4	8.4967e-05	0.95	1.08	0.95	2.82
8	5.0163e-06	0.94	1.03	0.94	3.87
16	3.0663e-07	0.94	1.01	0.94	3.72
32	1.8916e-08	0.94	1.00	0.94	3.51
64	1.1771e-09	0.94	1.00	0.94	3.37
128	7.3478e-11	0.94	1.00	0.94	3.29

Conv. Order = 4.00

$$q_1 = 17.954, \quad q_2 = 1.4303, \quad q_3 = -0.55500, \quad q_4 = 0.81061$$

Table 3: Test 1.1. Errors and effectivity indexes  $\widehat{\eta}_{2h,p}$ ,  $\widehat{\eta}_{h,p+1}$ ,  $\eta_{2h,p}$  and  $\eta_{h,p+1}$  for the output functionals  $q_1$ ,  $q_2$ ,  $q_3$  and  $q_4$  with  $N_e \in \{2^r\}_{r=2}^7$  and  $p = 1, 2$ ; the asymptotic convergence orders and “exact” values of the output functionals are reported.

$p = 1$

$N_e$	$ q_1 - q_{1,h,p} $	$\widehat{\eta}_{2h,p}$	$\widehat{\eta}_{h,p+1}$	$\eta_{2h,p}$	$\eta_{h,p+1}$
2	$2.9640e-01$	0.22	1.39	0.22	0.73
4	$7.3836e-02$	0.20	1.55	0.20	0.83
8	$1.8444e-02$	0.20	1.64	0.20	0.88
16	$4.6100e-03$	0.20	1.69	0.20	0.91
32	$1.1524e-03$	0.20	1.71	0.20	0.92
64	$2.8810e-04$	0.20	1.72	0.20	0.93
128	$7.2026e-05$	0.20	1.73	0.20	0.93

Conv. Order = 2.00

$p = 2$

$N_e$	$ q_1 - q_{1,h,p} $	$\widehat{\eta}_{2h,p}$	$\widehat{\eta}_{h,p+1}$	$\eta_{2h,p}$	$\eta_{h,p+1}$
2	$6.7273e-04$	0.54	0.72	0.54	1.82
4	$4.5086e-05$	0.58	1.21	0.58	7.38
8	$2.6654e-06$	0.57	1.33	0.57	16.7
16	$1.6335e-07$	0.57	1.37	0.57	34.5
32	$1.0153e-08$	0.57	1.38	0.57	69.9
64	$6.3364e-10$	0.57	1.39	0.57	140
128	-	-	-	-	-

Conv. Order = 4.12

$N_e$	$ q_2 - q_{2,h,p} $	$\widehat{\eta}_{2h,p}$	$\widehat{\eta}_{h,p+1}$	$\eta_{2h,p}$	$\eta_{h,p+1}$
2	$8.0199e-03$	0.82	1.15	0.82	0.68
4	$1.8738e-03$	0.77	1.04	0.77	0.48
8	$4.6054e-04$	0.75	1.01	0.75	0.34
16	$1.1464e-04$	0.75	1.00	0.75	0.27
32	$2.8631e-05$	0.75	1.00	0.75	0.23
64	$7.1557e-06$	0.75	1.00	0.75	0.21
128	$1.7888e-06$	0.75	1.00	0.75	0.20

Conv. Order = 2.00

$N_e$	$ q_2 - q_{2,h,p} $	$\widehat{\eta}_{2h,p}$	$\widehat{\eta}_{h,p+1}$	$\eta_{2h,p}$	$\eta_{h,p+1}$
2	$3.6097e-05$	0.94	0.76	0.94	11.4
4	$2.3489e-06$	0.94	0.98	0.94	60.2
8	$1.3765e-07$	0.94	1.00	0.94	146
16	$8.4227e-09$	0.94	1.00	0.94	311
32	$5.2336e-10$	0.94	1.00	0.94	639
64	$3.2659e-11$	0.94	1.00	0.94	1293
128	-	-	-	-	-

Conv. Order = 4.00

$N_e$	$ q_3 - q_{3,h,p} $	$\widehat{\eta}_{2h,p}$	$\widehat{\eta}_{h,p+1}$	$\eta_{2h,p}$	$\eta_{h,p+1}$
2	$1.7068e-02$	0.73	1.03	0.73	0.65
4	$4.3594e-03$	0.75	1.01	0.75	0.71
8	$1.0957e-03$	0.75	1.00	0.75	0.74
16	$2.7430e-04$	0.75	1.00	0.75	0.76
32	$6.8597e-05$	0.75	1.00	0.75	0.77
64	$1.7151e-05$	0.75	1.00	0.75	0.77
128	$4.2878e-06$	0.75	1.00	0.75	0.77

Conv. Order = 2.00

$N_e$	$ q_3 - q_{3,h,p} $	$\widehat{\eta}_{2h,p}$	$\widehat{\eta}_{h,p+1}$	$\eta_{2h,p}$	$\eta_{h,p+1}$
2	$7.4043e-05$	0.94	0.92	0.94	3.26
4	$4.4798e-06$	0.94	1.00	0.94	15.1
8	$2.6965e-07$	0.94	1.00	0.94	34.7
16	$1.6661e-08$	0.94	1.00	0.94	72.0
32	$1.0381e-09$	0.94	1.00	0.94	147
64	$6.4829e-11$	0.94	1.00	0.94	297
128	-	-	-	-	-

Conv. Order = 4.00

$N_e$	$ q_4 - q_{4,h,p} $	$\widehat{\eta}_{2h,p}$	$\widehat{\eta}_{h,p+1}$	$\eta_{2h,p}$	$\eta_{h,p+1}$
2	$3.0014e-02$	0.77	1.03	0.77	0.64
4	$7.4033e-03$	0.75	1.01	0.75	0.70
8	$1.8446e-03$	0.75	1.00	0.75	0.73
16	$4.6075e-04$	0.75	1.00	0.75	0.75
32	$1.1516e-04$	0.75	1.00	0.75	0.75
64	$2.8789e-05$	0.75	1.00	0.75	0.76
128	$7.1973e-06$	0.75	1.00	0.75	0.76

Conv. Order = 2.00

$N_e$	$ q_4 - q_{4,h,p} $	$\widehat{\eta}_{2h,p}$	$\widehat{\eta}_{h,p+1}$	$\eta_{2h,p}$	$\eta_{h,p+1}$
2	$3.8781e-06$	0.86	1.55	0.86	79.0
4	$7.1194e-07$	0.95	0.77	0.95	158
8	$3.8296e-08$	0.94	0.95	0.94	420
16	$2.2311e-09$	0.94	0.99	0.94	942
32	$1.3647e-10$	0.94	1.00	0.94	1967
64	$8.4783e-12$	0.94	1.00	0.94	3998
128	-	-	-	-	-

Conv. Order = 4.01

$$q_1 = 3.7685, \quad q_2 = 0.75854, \quad q_3 = -0.14608, \quad q_4 = 0.46902$$

Table 4: Test 1.2. Errors and effectivity indexes  $\widehat{\eta}_{2h,p}$ ,  $\widehat{\eta}_{h,p+1}$ ,  $\eta_{2h,p}$  and  $\eta_{h,p+1}$  for the output functionals  $q_1$ ,  $q_2$ ,  $q_3$  and  $q_4$  with  $N_e \in \{2^r\}_{r=2}^7$  and  $p = 1, 2$ ; the asymptotic convergence orders and “exact” values of the output functionals are reported. Errors and effectivity indexes for  $N_e = 128$  and  $p = 2$  are not reported since roundoff errors disrupt the convergence order.

	$p = 1$	$p = 2$																																																																																																
$q_1$	<table style="width: 100%; border-collapse: collapse;"> <thead> <tr> <th><math>N_e</math></th> <th><math> q_1 - q_{1,h,p} </math></th> <th><math>\widehat{\eta}_{2h,p}</math></th> <th><math>\widehat{\eta}_{h,p+1}</math></th> <th><math>\eta_{2h,p}</math></th> <th><math>\eta_{h,p+1}</math></th> </tr> </thead> <tbody> <tr><td>2</td><td><math>9.6686e-01</math></td><td>0.09</td><td>1.81</td><td>0.09</td><td>0.88</td></tr> <tr><td>4</td><td><math>2.2514e-01</math></td><td>0.21</td><td>2.09</td><td>0.21</td><td>0.97</td></tr> <tr><td>8</td><td><math>5.5864e-02</math></td><td>0.23</td><td>2.21</td><td>0.23</td><td>1.00</td></tr> <tr><td>16</td><td><math>1.3945e-02</math></td><td>0.24</td><td>2.27</td><td>0.24</td><td>1.01</td></tr> <tr><td>32</td><td><math>3.4849e-03</math></td><td>0.24</td><td>2.29</td><td>0.24</td><td>1.02</td></tr> <tr><td>64</td><td><math>8.7115e-04</math></td><td>0.24</td><td>2.31</td><td>0.24</td><td>1.02</td></tr> <tr><td>128</td><td><math>2.1778e-04</math></td><td>0.24</td><td>2.31</td><td>0.24</td><td>1.02</td></tr> </tbody> </table>	$N_e$	$ q_1 - q_{1,h,p} $	$\widehat{\eta}_{2h,p}$	$\widehat{\eta}_{h,p+1}$	$\eta_{2h,p}$	$\eta_{h,p+1}$	2	$9.6686e-01$	0.09	1.81	0.09	0.88	4	$2.2514e-01$	0.21	2.09	0.21	0.97	8	$5.5864e-02$	0.23	2.21	0.23	1.00	16	$1.3945e-02$	0.24	2.27	0.24	1.01	32	$3.4849e-03$	0.24	2.29	0.24	1.02	64	$8.7115e-04$	0.24	2.31	0.24	1.02	128	$2.1778e-04$	0.24	2.31	0.24	1.02	<table style="width: 100%; border-collapse: collapse;"> <thead> <tr> <th><math>N_e</math></th> <th><math> q_1 - q_{1,h,p} </math></th> <th><math>\widehat{\eta}_{2h,p}</math></th> <th><math>\widehat{\eta}_{h,p+1}</math></th> <th><math>\eta_{2h,p}</math></th> <th><math>\eta_{h,p+1}</math></th> </tr> </thead> <tbody> <tr><td>2</td><td><math>1.4633e-02</math></td><td>0.21</td><td>0.01</td><td>0.21</td><td>0.05</td></tr> <tr><td>4</td><td><math>1.8363e-03</math></td><td>0.55</td><td>1.19</td><td>0.55</td><td>0.53</td></tr> <tr><td>8</td><td><math>9.3996e-05</math></td><td>0.51</td><td>1.39</td><td>0.51</td><td>3.06</td></tr> <tr><td>16</td><td><math>5.5185e-06</math></td><td>0.50</td><td>1.44</td><td>0.50</td><td>7.78</td></tr> <tr><td>32</td><td><math>3.4011e-07</math></td><td>0.49</td><td>1.45</td><td>0.49</td><td>17.0</td></tr> <tr><td>64</td><td>–</td><td>–</td><td>–</td><td>–</td><td>–</td></tr> <tr><td>128</td><td>–</td><td>–</td><td>–</td><td>–</td><td>–</td></tr> </tbody> </table>	$N_e$	$ q_1 - q_{1,h,p} $	$\widehat{\eta}_{2h,p}$	$\widehat{\eta}_{h,p+1}$	$\eta_{2h,p}$	$\eta_{h,p+1}$	2	$1.4633e-02$	0.21	0.01	0.21	0.05	4	$1.8363e-03$	0.55	1.19	0.55	0.53	8	$9.3996e-05$	0.51	1.39	0.51	3.06	16	$5.5185e-06$	0.50	1.44	0.50	7.78	32	$3.4011e-07$	0.49	1.45	0.49	17.0	64	–	–	–	–	–	128	–	–	–	–	–
	$N_e$	$ q_1 - q_{1,h,p} $	$\widehat{\eta}_{2h,p}$	$\widehat{\eta}_{h,p+1}$	$\eta_{2h,p}$	$\eta_{h,p+1}$																																																																																												
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$$q_1 = 20.877, \quad q_2 = 1.7732, \quad q_4 = -0.68420, \quad q_3 = 0.80464$$

Table 5: Test 1.3. Errors and effectivity indexes  $\widehat{\eta}_{2h,p}$ ,  $\widehat{\eta}_{h,p+1}$ ,  $\eta_{2h,p}$  and  $\eta_{h,p+1}$  for the output functionals  $q_1$ ,  $q_2$ ,  $q_3$  and  $q_4$  with  $N_e \in \{2^r\}_{r=2}^7$  and  $p = 1, 2$ ; the asymptotic convergence orders and “exact” values of the output functionals are reported. Errors and effectivity indexes for  $N_e = 64, 128$  and  $p = 2$  are not reported since roundoff errors disrupt the convergence order.

$p = 1$

$N_e$	$ q_1 - q_{1,h,p} $	$\widehat{\eta}_{2h,p}$	$\widehat{\eta}_{h,p+1}$	$\eta_{2h,p}$	$\eta_{h,p+1}$
2	2.2404e+00	1.84	1.26	1.84	1.20
4	4.7824e-01	2.30	0.54	2.30	1.58
8	1.1172e-01	2.48	0.30	2.48	1.44
16	2.7423e-02	2.53	0.84	2.53	1.24
32	6.8241e-03	2.55	1.12	2.55	1.13
64	1.7040e-03	2.55	1.26	2.55	1.06
128	4.2589e-04	2.55	1.33	2.55	1.03

Conv. Order = 2.00

$p = 2$

$N_e$	$ q_1 - q_{1,h,p} $	$\widehat{\eta}_{2h,p}$	$\widehat{\eta}_{h,p+1}$	$\eta_{2h,p}$	$\eta_{h,p+1}$
2	1.1787e-01	0.66	0.48	0.66	2.99
4	1.0964e-02	0.15	1.53	0.15	1.00
8	6.3700e-04	0.18	1.98	0.18	1.17
16	3.8167e-05	0.21	2.14	0.21	3.37
32	2.3581e-06	0.22	2.19	0.22	7.82
64	1.4696e-07	0.22	2.22	0.22	16.7
128	9.1781e-09	0.22	2.23	0.22	34.4

Conv. Order = 4.00

$N_e$	$ q_2 - q_{2,h,p} $	$\widehat{\eta}_{2h,p}$	$\widehat{\eta}_{h,p+1}$	$\eta_{2h,p}$	$\eta_{h,p+1}$
2	1.0033e-01	0.72	0.89	0.72	0.89
4	2.7267e-02	0.74	0.98	0.74	0.97
8	6.8939e-03	0.75	1.00	0.75	0.99
16	1.7263e-03	0.75	1.00	0.75	1.00
32	4.3174e-04	0.75	1.00	0.75	1.00
64	1.0794e-04	0.75	1.00	0.75	1.00
128	2.6986e-05	0.75	1.00	0.75	1.00

Conv. Order = 2.00

$N_e$	$ q_2 - q_{2,h,p} $	$\widehat{\eta}_{2h,p}$	$\widehat{\eta}_{h,p+1}$	$\eta_{2h,p}$	$\eta_{h,p+1}$
2	5.1806e-03	0.94	0.95	0.94	0.86
4	2.5594e-04	0.94	1.11	0.94	0.98
8	1.3941e-05	0.94	1.07	0.94	0.95
16	8.4825e-07	0.94	1.02	0.94	0.84
32	5.2712e-08	0.94	1.01	0.94	0.66
64	3.2899e-09	0.94	1.00	0.94	0.31
128	2.0555e-10	0.94	1.00	0.94	0.37

Conv. Order = 4.00

$N_e$	$ q_3 - q_{3,h,p} $	$\widehat{\eta}_{2h,p}$	$\widehat{\eta}_{h,p+1}$	$\eta_{2h,p}$	$\eta_{h,p+1}$
2	6.6589e-01	0.79	0.50	0.79	0.66
4	2.5881e-01	0.76	0.80	0.76	0.88
8	7.1712e-02	0.75	0.94	0.75	0.97
16	1.8363e-02	0.75	0.98	0.75	0.99
32	4.6178e-03	0.75	1.00	0.75	1.00
64	1.1561e-03	0.75	1.00	0.75	1.00
128	2.8913e-04	0.75	1.00	0.75	1.00

Conv. Order = 2.00

$N_e$	$ q_3 - q_{3,h,p} $	$\widehat{\eta}_{2h,p}$	$\widehat{\eta}_{h,p+1}$	$\eta_{2h,p}$	$\eta_{h,p+1}$
2	1.6235e-01	0.99	0.79	0.99	0.99
4	1.1652e-02	0.95	0.90	0.95	1.04
8	6.7858e-04	0.94	0.98	0.94	1.10
16	4.1144e-05	0.94	1.00	0.94	1.21
32	2.5510e-06	0.94	1.00	0.94	1.43
64	1.5912e-07	0.94	1.00	0.94	1.87
128	9.9398e-09	0.94	1.00	0.94	2.74

Conv. Order = 4.00

$N_e$	$ q_4 - q_{4,h,p} $	$\widehat{\eta}_{2h,p}$	$\widehat{\eta}_{h,p+1}$	$\eta_{2h,p}$	$\eta_{h,p+1}$
2	1.0131e+00	0.77	0.71	0.77	0.10
4	2.3267e-01	0.76	0.97	0.76	0.73
8	5.6522e-02	0.75	0.99	0.75	0.93
16	1.4022e-02	0.75	1.00	0.75	0.97
32	3.4986e-03	0.75	1.00	0.75	0.98
64	8.7422e-04	0.75	1.00	0.75	0.99
128	2.1853e-04	0.75	1.00	0.75	1.00

Conv. Order = 2.00

$N_e$	$ q_4 - q_{4,h,p} $	$\widehat{\eta}_{2h,p}$	$\widehat{\eta}_{h,p+1}$	$\eta_{2h,p}$	$\eta_{h,p+1}$
2	6.5408e-03	0.55	2.51	0.55	38.1
4	3.1507e-03	0.93	0.90	0.93	3.05
8	2.2060e-04	0.94	0.97	0.94	3.05
16	1.4141e-05	0.94	0.99	0.94	6.90
32	8.8924e-07	0.94	1.00	0.94	14.8
64	5.5663e-08	0.94	1.00	0.94	30.5
128	3.4803e-09	0.94	1.00	0.94	62.1

Conv. Order = 4.00

$$q_1 = 66.987, \quad q_2 = -2.2807, \quad q_3 = 149.51, \quad q_4 = -66.795$$

Table 6: Test 2. Errors and effectivity indexes  $\widehat{\eta}_{2h,p}$ ,  $\widehat{\eta}_{h,p+1}$ ,  $\eta_{2h,p}$  and  $\eta_{h,p+1}$  for the output functionals  $q_1$ ,  $q_2$ ,  $q_3$  and  $q_4$  with  $N_e \in \{2^r\}_{r=2}^7$  and  $p = 1, 2$ ; the asymptotic convergence orders and “exact” values of the output functionals are reported.

$p = 1$

$N_e$	$ q_1 - q_{1,h,p} $	$\widehat{\eta}_{2h,p}$	$\widehat{\eta}_{h,p+1}$	$\eta_{2h,p}$	$\eta_{h,p+1}$
2	1.0620e+00	0.11	0.02	0.11	0.01
4	1.8859e-01	1.10	0.85	1.10	0.75
8	4.6160e-03	9.65	2.33	9.65	6.96
16	6.6637e-03	0.62	2.25	0.62	0.85
32	1.7265e-03	0.58	2.62	0.58	1.07
64	4.3536e-04	0.58	2.71	0.58	1.12
128	1.0908e-04	0.57	2.74	0.57	1.14

Conv. Order = 2.00

$p = 2$

$N_e$	$ q_1 - q_{1,h,p} $	$\widehat{\eta}_{2h,p}$	$\widehat{\eta}_{h,p+1}$	$\eta_{2h,p}$	$\eta_{h,p+1}$
2	7.1760e-02	0.50	1.24	0.50	1.26
4	4.5158e-02	3.33	2.07	3.33	2.37
8	3.2464e-02	0.75	0.86	0.75	0.87
16	2.4634e-04	0.24	2.41	0.24	1.36
32	1.3965e-05	0.03	2.05	0.03	1.05
64	8.1306e-07	0.01	2.00	0.01	0.82
128	4.9573e-08	0.01	1.99	0.01	0.41

Conv. Order = 4.04

$N_e$	$ q_2 - q_{2,h,p} $	$\widehat{\eta}_{2h,p}$	$\widehat{\eta}_{h,p+1}$	$\eta_{2h,p}$	$\eta_{h,p+1}$
2	3.6770e+00	0.24	0.03	0.24	0.02
4	1.2626e-01	3.00	0.46	3.00	0.57
8	6.5856e-02	1.03	1.42	1.03	1.47
16	4.4395e-03	0.78	1.51	0.78	1.84
32	1.0978e-03	0.76	1.11	0.76	1.61
64	2.7624e-04	0.75	1.03	0.75	1.56
128	6.9183e-05	0.75	1.01	0.75	1.55

Conv. Order = 2.00

$N_e$	$ q_2 - q_{2,h,p} $	$\widehat{\eta}_{2h,p}$	$\widehat{\eta}_{h,p+1}$	$\eta_{2h,p}$	$\eta_{h,p+1}$
2	1.3917e-01	0.23	0.66	0.24	0.92
4	1.0903e-01	1.83	0.69	1.83	0.84
8	4.2557e-02	1.15	0.61	1.15	0.97
16	3.2737e-04	0.98	1.37	0.98	1.13
32	8.3927e-06	0.95	1.26	0.95	1.10
64	3.8305e-07	0.94	1.08	0.94	0.08
128	2.2432e-08	0.94	1.02	0.94	2.00

Conv. Order = 4.10

$N_e$	$ q_3 - q_{3,h,p} $	$\widehat{\eta}_{2h,p}$	$\widehat{\eta}_{h,p+1}$	$\eta_{2h,p}$	$\eta_{h,p+1}$
2	8.3879e-01	0.62	0.09	0.62	0.06
4	5.9996e-02	0.15	0.96	0.15	0.27
8	2.7870e-02	0.79	1.13	0.79	0.91
16	6.4018e-03	0.75	1.06	0.75	0.80
32	1.6060e-03	0.75	1.02	0.75	0.76
64	4.0219e-04	0.75	1.00	0.75	0.75
128	1.0059e-04	0.75	1.00	0.75	0.75

Conv. Order = 2.00

$N_e$	$ q_3 - q_{3,h,p} $	$\widehat{\eta}_{2h,p}$	$\widehat{\eta}_{h,p+1}$	$\eta_{2h,p}$	$\eta_{h,p+1}$
2	4.1045e-02	0.28	0.49	0.28	0.26
4	3.0216e-02	1.13	0.67	1.13	0.87
8	1.4802e-03	1.50	0.17	1.50	0.70
16	8.7423e-05	0.96	1.24	0.96	0.69
32	3.8437e-06	0.94	1.08	0.94	1.00
64	2.1475e-07	0.94	1.02	0.94	2.13
128	1.3055e-08	0.94	1.01	0.94	4.44

Conv. Order = 4.04

$N_e$	$ q_4 - q_{4,h,p} $	$\widehat{\eta}_{2h,p}$	$\widehat{\eta}_{h,p+1}$	$\eta_{2h,p}$	$\eta_{h,p+1}$
2	1.4515e+00	0.03	0.01	0.03	0.01
4	3.1567e-01	1.29	0.63	1.29	0.53
8	3.4253e-02	0.34	0.44	0.34	0.13
16	1.7935e-02	0.74	1.01	0.74	0.83
32	4.5925e-03	0.75	1.01	0.75	0.82
64	1.1556e-03	0.75	1.00	0.75	0.81
128	2.8938e-04	0.75	1.00	0.75	0.81

Conv. Order = 2.00

$N_e$	$ q_4 - q_{4,h,p} $	$\widehat{\eta}_{2h,p}$	$\widehat{\eta}_{h,p+1}$	$\eta_{2h,p}$	$\eta_{h,p+1}$
2	2.1004e-02	1.00	3.08	0.98	5.55
4	1.3415e-03	58.2	44.3	58.2	46.4
8	4.1508e-02	1.04	0.96	1.04	1.10
16	5.5119e-04	0.95	1.20	0.95	1.14
32	2.8052e-05	0.94	1.04	0.94	1.05
64	1.6060e-06	0.94	1.01	0.94	1.35
128	9.7772e-08	0.94	1.00	0.94	2.02

Conv. Order = 4.04

$$q_1 = 1.1153, \quad q_2 = -2.7978, \quad q_3 = -1.5349, \quad q_4 = 0.63397$$

Table 7: Test 3.1. Errors and effectivity indexes  $\widehat{\eta}_{2h,p}$ ,  $\widehat{\eta}_{h,p+1}$ ,  $\eta_{2h,p}$  and  $\eta_{h,p+1}$  for the output functionals  $q_1$ ,  $q_2$ ,  $q_3$  and  $q_4$  with  $N_e \in \{2^r\}_{r=2}^7$  and  $p = 1, 2$ ; the asymptotic convergence orders and “exact” values of the output functionals are reported.

$p = 1$

$N_e$	$ q_1 - q_{1,h,p} $	$\widehat{\eta}_{2h,p}$	$\widehat{\eta}_{h,p+1}$	$\eta_{2h,p}$	$\eta_{h,p+1}$
2	$2.4354e-01$	0.11	0.07	0.11	0.01
4	$8.8545e-02$	0.18	0.76	0.18	0.60
8	$3.1482e-02$	0.14	1.30	0.14	0.56
16	$9.9188e-03$	0.03	1.80	0.03	0.92
32	$2.5746e-03$	0.02	1.92	0.02	0.98
64	$6.4948e-04$	0.02	1.95	0.02	0.99
128	$1.6274e-04$	0.02	1.96	0.02	1.00

Conv. Order = 2.00

$p = 2$

$N_e$	$ q_1 - q_{1,h,p} $	$\widehat{\eta}_{2h,p}$	$\widehat{\eta}_{h,p+1}$	$\eta_{2h,p}$	$\eta_{h,p+1}$
2	$1.6649e-01$	0.29	0.21	0.29	0.22
4	$4.7141e-02$	0.55	0.33	0.55	0.34
8	$1.0316e-02$	0.24	0.48	0.24	0.32
16	$3.8222e-04$	0.01	2.37	0.01	1.13
32	$1.7474e-05$	0.01	2.13	0.01	0.95
64	$9.9520e-07$	0.01	2.04	0.01	0.79
128	$6.0669e-08$	0.01	2.01	0.01	0.54

Conv. Order = 4.04

$N_e$	$ q_2 - q_{2,h,p} $	$\widehat{\eta}_{2h,p}$	$\widehat{\eta}_{h,p+1}$	$\eta_{2h,p}$	$\eta_{h,p+1}$
2	$1.3614e-01$	0.79	0.81	0.80	0.81
4	$1.2298e-02$	5.43	2.06	5.43	0.35
8	$4.5826e-02$	1.10	1.13	1.10	1.42
16	$1.2723e-03$	0.83	1.65	0.83	0.79
32	$2.6283e-04$	0.77	1.25	0.77	0.95
64	$6.3235e-05$	0.75	1.07	0.75	0.96
128	$1.5679e-05$	0.75	1.02	0.75	0.97

Conv. Order = 2.00

$N_e$	$ q_2 - q_{2,h,p} $	$\widehat{\eta}_{2h,p}$	$\widehat{\eta}_{h,p+1}$	$\eta_{2h,p}$	$\eta_{h,p+1}$
2	$8.9991e-03$	7.41	1.84	7.35	0.51
4	$5.0555e-02$	2.29	1.30	2.29	1.41
8	$4.4598e-02$	1.04	1.12	1.04	0.96
16	$3.0119e-05$	0.86	5.93	0.86	4.96
32	$3.2597e-06$	0.95	1.49	0.95	4.41
64	$1.6636e-07$	0.94	1.14	0.94	8.74
128	$9.3557e-09$	0.94	1.04	0.94	17.8

Conv. Order = 4.10

$N_e$	$ q_3 - q_{3,h,p} $	$\widehat{\eta}_{2h,p}$	$\widehat{\eta}_{h,p+1}$	$\eta_{2h,p}$	$\eta_{h,p+1}$
2	$5.0522e-01$	0.73	0.37	0.73	0.36
4	$1.6131e-01$	0.57	0.72	0.57	0.53
8	$6.6343e-02$	0.69	1.03	0.69	0.93
16	$1.9524e-02$	0.74	1.05	0.74	1.02
32	$5.0777e-03$	0.75	1.02	0.75	1.00
64	$1.2814e-03$	0.75	1.00	0.75	1.00
128	$3.2110e-04$	0.75	1.00	0.75	1.00

Conv. Order = 2.00

$N_e$	$ q_3 - q_{3,h,p} $	$\widehat{\eta}_{2h,p}$	$\widehat{\eta}_{h,p+1}$	$\eta_{2h,p}$	$\eta_{h,p+1}$
2	$3.0211e-01$	0.62	0.61	0.62	0.60
4	$1.1336e-01$	0.82	0.35	0.82	0.25
8	$1.7674e-02$	0.93	0.91	0.93	0.97
16	$7.6475e-04$	0.95	1.26	0.95	1.48
32	$3.4985e-05$	0.94	1.07	0.94	1.64
64	$1.9942e-06$	0.94	1.02	0.94	2.21
128	$1.2161e-07$	0.94	1.00	0.94	3.42

Conv. Order = 4.04

$N_e$	$ q_4 - q_{4,h,p} $	$\widehat{\eta}_{2h,p}$	$\widehat{\eta}_{h,p+1}$	$\eta_{2h,p}$	$\eta_{h,p+1}$
2	$7.3282e-02$	0.98	0.36	0.98	0.38
4	$5.6749e-02$	1.09	1.04	1.09	1.11
8	$1.1139e-03$	0.99	0.18	0.99	2.35
16	$1.8407e-03$	0.77	1.03	0.77	0.89
32	$4.4339e-04$	0.76	1.01	0.76	0.95
64	$1.0988e-04$	0.75	1.00	0.75	0.97
128	$2.7413e-05$	0.75	1.00	0.75	0.99

Conv. Order = 2.00

$N_e$	$ q_4 - q_{4,h,p} $	$\widehat{\eta}_{2h,p}$	$\widehat{\eta}_{h,p+1}$	$\eta_{2h,p}$	$\eta_{h,p+1}$
2	$7.0421e-02$	1.69	1.08	1.68	1.17
4	$3.2583e-02$	1.31	1.23	1.31	1.21
8	$5.6490e-03$	1.05	1.17	1.05	1.10
16	$3.5804e-05$	0.96	0.98	0.96	0.49
32	$1.4246e-06$	0.94	1.00	0.94	3.90
64	$8.1164e-08$	0.94	1.00	0.94	9.46
128	$4.9944e-09$	0.94	1.00	0.94	19.9

Conv. Order = 4.04

$$q_1 = 0.32890, \quad q_2 = 0.87998, \quad q_3 = -0.75134, \quad q_4 = -0.034175$$

Table 8: Test 3.2. Errors and effectivity indexes  $\widehat{\eta}_{2h,p}$ ,  $\widehat{\eta}_{h,p+1}$ ,  $\eta_{2h,p}$  and  $\eta_{h,p+1}$  for the output functionals  $q_1$ ,  $q_2$ ,  $q_3$  and  $q_4$  with  $N_e \in \{2^r\}_{r=2}^7$  and  $p = 1, 2$ ; the asymptotic convergence orders and “exact” values of the output functionals are reported.

$p = 1$

$p = 2$

$N_e$	$ q_1 - q_{1,h,p} $	$\widehat{\eta}_{2h,p}$	$\widehat{\eta}_{h,p+1}$	$\eta_{2h,p}$	$\eta_{h,p+1}$	$N_e$	$ q_1 - q_{1,h,p} $	$\widehat{\eta}_{2h,p}$	$\widehat{\eta}_{h,p+1}$	$\eta_{2h,p}$	$\eta_{h,p+1}$
2	2.1779e+01	0.51	0.68	0.60	0.85	2	7.6587e+00	0.37	0.42	0.42	0.29
4	9.9297e+00	0.03	0.81	0.02	0.41	4	5.8921e-02	2.74	12.0	3.90	11.1
8	1.6917e+00	0.35	2.18	0.35	0.85	8	8.9579e-02	0.14	3.70	0.14	1.81
16	4.0822e-01	0.44	2.54	0.44	0.98	16	9.3778e-03	0.34	1.88	0.34	1.16
32	1.0397e-01	0.44	2.57	0.44	0.99	32	4.6134e-04	0.27	1.77	0.27	1.03
64	2.6120e-02	0.44	2.57	0.44	0.99	64	2.7059e-05	0.25	1.74	0.25	1.01
128	6.5381e-03	0.44	2.58	0.44	1.00	128	1.6646e-06	0.25	1.74	0.25	1.00
Conv. Order = 2.00						Conv. Order = 4.02					

$N_e$	$ q_2 - q_{2,h,p} $	$\widehat{\eta}_{2h,p}$	$\widehat{\eta}_{h,p+1}$	$\eta_{2h,p}$	$\eta_{h,p+1}$	$N_e$	$ q_2 - q_{2,h,p} $	$\widehat{\eta}_{2h,p}$	$\widehat{\eta}_{h,p+1}$	$\eta_{2h,p}$	$\eta_{h,p+1}$
2	5.1712e-01	0.96	1.28	1.33	1.04	2	1.3746e-01	0.95	0.46	3.85	6.50
4	8.9262e-03	0.72	1.31	0.41	0.39	4	8.9098e-03	0.93	0.86	0.14	2.33
8	1.3851e-03	0.65	1.22	212	482	8	6.6169e-04	0.94	1.11	9.73	18.9
16	5.9992e-04	0.73	1.03	59.0	230	16	4.2862e-05	0.94	1.03	2.73	8.03
32	1.6827e-04	0.75	1.01	4.17	15.1	32	2.5470e-06	0.94	1.01	0.55	2.65
64	4.3218e-05	0.75	1.00	1.18	5.25	64	1.5723e-07	0.94	1.00	0.21	0.94
128	1.0876e-05	0.75	1.00	0.16	2.01	128	9.7966e-09	0.94	1.00	0.57	0.13
Conv. Order = 2.00						Conv. Order = 4.00					

$N_e$	$ q_3 - q_{3,h,p} $	$\widehat{\eta}_{2h,p}$	$\widehat{\eta}_{h,p+1}$	$\eta_{2h,p}$	$\eta_{h,p+1}$	$N_e$	$ q_3 - q_{3,h,p} $	$\widehat{\eta}_{2h,p}$	$\widehat{\eta}_{h,p+1}$	$\eta_{2h,p}$	$\eta_{h,p+1}$
2	1.3144e+00	0.90	1.05	1.07	1.31	2	2.7769e-01	1.08	0.19	1.22	0.32
4	4.3784e-01	0.88	0.96	0.88	1.11	4	6.1107e-03	0.42	2.50	0.34	0.86
8	8.5190e-02	0.76	1.06	0.77	1.08	8	3.8213e-03	0.93	1.87	0.94	1.64
16	2.1252e-02	0.75	1.03	0.76	1.04	16	3.0891e-04	0.95	1.15	0.95	1.13
32	5.3832e-03	0.75	1.01	0.76	1.01	32	1.5794e-05	0.94	1.04	0.94	1.02
64	1.3504e-03	0.75	1.00	0.75	1.00	64	9.3709e-07	0.94	1.01	0.94	0.99
128	3.3788e-04	0.75	1.00	0.75	1.00	128	5.7814e-08	0.94	1.00	0.94	0.99
Conv. Order = 2.00						Conv. Order = 4.02					

$$q_1 = 45.293, \quad q_2 = 1.5882, \quad q_3 = -3.9254$$

Table 9: Test 4. Errors and effectivity indexes  $\widehat{\eta}_{2h,p}$ ,  $\widehat{\eta}_{h,p+1}$ ,  $\eta_{2h,p}$  and  $\eta_{h,p+1}$  for the output functionals  $q_1$ ,  $q_2$  and  $q_3$  with  $N_e \in \{2^r\}_{r=2}^7$  and  $p = 1, 2$ ; the asymptotic convergence orders and “exact” values of the output functionals are reported.

## 5.2 Discussion

Based on the results reported in Tables 3–9, we extrapolate the following considerations for the error estimators  $\widehat{\Delta}_{i,2h,p}$ ,  $\widehat{\Delta}_{i,h,p+1}$ ,  $\Delta_{i,2h,p}$  and  $\Delta_{i,h,p+1}$ ; see Eqs.(31), (32), (35) and (36).

1. As expected, all the error estimators could highlight poor performances when a small number of “elements”  $N_e = 2, 4$  is considered (see *e.g.* the effectivity indexes for Test 1.3 and  $q_1$ ); also, the effectivity indexes largely changes from an error estimator to an other. Even if in many cases the effectivity indexes can be considered “sufficiently” close to 1 (in particular for the estimators  $\widehat{\Delta}_{i,2h,p}$ ,  $\widehat{\Delta}_{i,h,p+1}$  and  $\Delta_{i,2h,p}$ ), the reliability of the estimators largely depends on the Test problem for  $N_e$  “small” ( $N_e = 2, 4$ ).
2. As expected, the error estimators do not represent rigorous error bounds for the errors on the output functionals  $q_1$ – $q_4$  for all the Test problems.
3. For the error estimator  $\widehat{\Delta}_{i,2h,p}$  (Eq.(31)):

- asymptotic effectivity indexes of values 0.75 and 0.94 are achieved with  $p = 1$  and  $p = 2$ , respectively, for the output functionals  $q_2$ – $q_4$  (linear and nonlinear with the trigonometric functions sine and cosine) in all the tests considered;
  - asymptotic effectivity indexes in the range 0.20–2.55 are achieved for the quadratic strain energy functional  $q_1$  with  $\widehat{\eta}_{1,h,p+1} < 1$  in all the Test problems except for Test 2 ( $p = 1$ ); for the Tests 3.1 ( $p = 2$ ) and 3.2 the error on  $q_1$  is largely underestimated even asymptotically.
4. For the error estimator  $\widehat{\Delta}_{i,h,p+1}$  (Eq.(32)):
- the asymptotic effectivity index  $\widehat{\eta}_{i,h,p+1} = 1.00$  is achieved with both  $p = 1$  and  $p = 2$  for the output functionals  $q_2$ – $q_4$  in all the Tests problems;
  - asymptotic effectivity indexes bigger than one ( $\widehat{\Delta}_{1,h,p+1} > 1.00$ ) are obtained for the quadratic strain energy functional  $q_1$  in all the Test problems; asymptotically,  $\widehat{\Delta}_{1,h,p+1}$  is in the range 1.33–2.58 for all the Test problems and differs for  $p = 1$  and  $p = 2$ .
5. For the error estimator  $\Delta_{i,2h,p}$  (Eq.(35)):
- the behavior of this estimator is very close to the one of  $\widehat{\Delta}_{i,2h,p}$  for  $p = 1$  and  $p = 2$  in many Test problems, except when a small number of “elements” is considered ( $N_e = 2, 4$ ) or as *e.g.* in Test 4 for  $q_2$ .
6. For the error estimator  $\Delta_{i,h,p+1}$  (Eq.(36)):
- asymptotic effectivity indexes are achieved only for  $p = 1$  in a range  $\eta_{1,h,p+1} = 0.20$ – $2.18$ ; these values considerably vary with the Test problem and the output functional under consideration (even if linear  $q_2$ – $q_4$ );
  - the behavior of the error estimator is quite unpredictable for  $p = 2$  for which no asymptotic effectivity indexes are achieved; very large overestimations of the errors ( $\eta_{1,h,p+1} \gg 1$ ) are obtained *e.g.* for Tests 1.1–1.3.

Based on the previous considerations and by recalling Remark 4.3 regarding the computational costs, we conclude that the estimator  $\widehat{\Delta}_{i,h,p+1}$  (31), which employs the higher order enhanced dual solution, represents the most reliable and preferable error estimator among the ones considered for the evaluation of the errors resulting from the linear, quadratic and nonlinear (with trigonometric functions sine and cosine) outputs and for  $p = 1, 2$ .

If the classic Finite Element method with linear Lagrangian basis is used (see Remarks 4.1 and 4.2), the error estimator  $\widehat{\Delta}_{i,2h,1}$  is preferable to  $\Delta_{i,2h,1}$  due to the considerations in Remark 4.3 regarding the computational costs.

## 6 Conclusions

We have proposed and studied goal-oriented a posteriori error estimators for the evaluation of the errors on quantities of interest associated with the solution of geometrically nonlinear curved elastic rods with arbitrarily large planar deflections under the so-called *Elastica* theory; for the numerical solution of these problems, a Galerkin formulation with B-spline basis of order one and two has been considered. We have introduced goal-oriented error estimators with higher order “enhanced” primal and dual solutions,

in which the enrichment of the original B-spline basis by means of “pure”  $k$ -refinement has been used. These estimators have been compared in several test cases with the most traditional ones based on the mesh refined “enhanced” primal and dual solutions. The numerical tests reveal a better performance, in terms of effectivity indexes, for the proposed error estimator based on the higher order “enhanced” dual solution with respect to one based on the mesh refined “enhanced” dual solution; while asymptotic effectivity indexes larger than one have been obtained for the quadratic functional (strain energy), unitary asymptotic effectivity indexes have been achieved for the linear and the nonlinear output functionals (rotation and displacements).

The error estimators can eventually be adopted for the analysis of other structural problems, such as *e.g.* the so-called Kirchhoff and Reissner–Simo spatial beam theories, or other more general PDEs.

## Acknowledgements

L. Dedè was partially supported by the Office of Naval Research under Contract Number N00014-08-0992. H.A.F.A. Santos acknowledges the financial support of the Fundação para a Ciência e a Tecnologia (FCT) of Portugal.

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