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On Round-off Error for Adaptive Finite Element Methods

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Abstract

Round-off error analysis has been historically studied by analyzing the condition number of the associated matrix. By controlling the size of the condition number, it is possible to guarantee a prescribed round-off error tolerance. However, the opposite is not true, since it is possible to have a system of linear equations with an arbitrarily large condition number that still delivers a small round-off error. In this paper, we perform a round-off error analysis in context of 1D and 2D *hp*-adaptive Finite Element simulations for the case of Poisson equation. We conclude that boundary conditions play a fundamental role on the round-off error analysis, specially for the so-called 'radical meshes'. Moreover, we illustrate the importance of the right-hand side when analyzing the round-off error, which is independent of the condition number of the matrix.

Keywords: Finite Element Methods (FEM), hp-adaptivity, round-off error, condition number.

1. Introduction

The study of round-off error is crucial when solving a linear system of equations, since it may pollute and even destroy the solution of the problem. Round-off error is of particular concern in adaptive *hp*-finite element (FE) computations, where h denotes the element size and p the polynomial order of approximation, both varying locally throughout the computational grid. There is a potential for large round-off errors when using heavy mesh-refinements in a *hp*-adaptive FE discretization to approximate a particular feature of the solution.

During the last decades, several studies have been devoted to analyze round-off error in the context of FE computations. Historically, most researchers have analyzed the round-off error appearing in the solution of a general linear system of equations by studying the condition number of the associated matrix. Thus, the pioneering works of Neumann and Goldstine [1] in 1947; [2] in 1951, and Turing [3] in 1948, analyzed the problem of round-off error and introduced its relationship to the conditioning of the problem. A further important development in the study of

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condition number was performed by Wilkinson [4] and Isaacson [5]. In this work, Isaacson bounds the sensitivity of the solution with respect to perturbations in the right-hand side by using the condition number of the matrix.

For the case of linear systems of equations arising from uniform h-refined meshes in FE computations of second order differential operators, the condition number κ is known to be of the form $O(h^{-2})$, where h is the size of smallest element in the mesh with respect to the domain size. For non-uniform meshes, the above result constitutes an upper bound of the condition number of the matrix, although in some cases, it can be improved.

Since the condition number controls the round-off error, a natural approach to minimize error is by decreasing the condition number. One way to achieve this is by performing an optimal scaling of basis functions, addressed in the past by [6]. A particularly important case of non-uniform meshes is the so-called 'radical mesh' [7, 8], where heavy refinements are performed towards some fixed point. This situation often occurs in practical applications when the problem exhibits a singularity, and adaptive grids are employed to properly approximate the solution around the singularity. In Figure 1 we show 1D and 2D radical meshes after some 'radical' refinements.

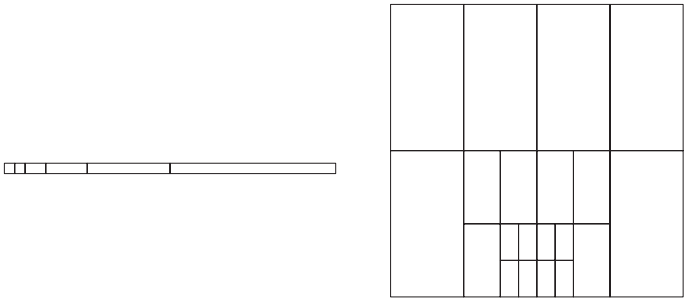

Figure 1: Left: Radical Mesh in 1D. Right: Radical Mesh in 2D.

In context of FE methods, it is possible to re-scale the basis functions as described in [9] to minimize the condition number. While this is an effective idea, the re-scaling of basis functions is not implemented in most FEM codes, perhaps because such implementation is not in general a trivial task. Furthermore, we observed that round-off error in our adaptive hp-FE computations is in fact *not* significant, even when we omitted the use of re-scaled basis functions.

The main objective of this work is to analyze round-off error when different boundary conditions (and hence, different right-hand sides) are considered, and specifically, to explain why we do not observe a degradation in the solution when we employ conventional (not re-scaled) basis functions with radical meshes. In this context, the main contribution of this paper is to observe that the round-off error is *not* always related to the condition number. Rather, a new ingredient needs to be introduced to fully understand round-off error, namely, the right-hand side. This was also observed by Rice [10], who concluded that the condition number does not always provide a reliable guide to study the effects of round-off error. In this paper, we perform a more detailed analysis in context of hp-FE computations. Via an eigenvalue analysis, we observe that the right-hand side may excite only a few of the eigenvalues of the associated matrix. This results in smaller round-off error than that predicted by the condition number.

Another contribution of the paper is to exhibit that round-off error is affected by a particular choice of the right-hand side. Finally, we also consider the case of p refinements. Taking into account that the choice of basis functions can significantly affect the condition number [11, 12, 13, 14, 15] and round off-error, we briefly analyze the impact of this choice using hierarchical Peano [16, 17, 18] and Integrated Legendre Polynomials (ILP) [19] basis functions.

Due to the intrinsic complexity associated with the theoretical and implementation analysis within the hp-adaptive FEM, we restrict our analysis to the Poisson equation. This work is organized as follows: Section 2 introduces the model problem and solution methodology. Section 3 explains how it is possible to obtain small round-off errors even in the presence of large condition numbers. In Section 4 the numerical results are shown, and finally the conclusions are outlined in Section 5.

2. Model Problem and Solution Method

In this section we introduce the mathematical problem to be solved. We also discuss the variational formulation and the method we shall use to solve it: *hp*-adaptive Finite Element Method (FEM). The main advantage of this method is that with an optimal sequence of *hp* refinements, exponential convergence is achieved. In 1D this was proved by Gui and Babuska [20] and in 2D by Babuska and Guo [21], and Schwab [22].

2.1. Model Problem: Poisson Equation

Our model problem is given by the Poisson equation:

$$-\Delta\, u(\boldsymbol{x}) = f \tag{1}$$

where f is the right-hand side, u is the solution and Δ is the Laplace operator in 1D or 2D.

We will analyze both, 1D and 2D problems, Ω being the computational domain, corresponding to $[0, 1]$ in 1D and to $[0, 1]^2$ in 2D. We introduce essential (Dirichlet) boundary conditions in some region Γ_D of the boundary Γ, and natural (Neumann) boundary conditions in some region Γ_N. To facilitate the round-off error analysis, we will select two *a priori* solutions.

$$1D: \begin{cases} u_1(x) = 1 \\ u_2(x) = \begin{cases} u(x) = \dfrac{1}{x_0^2}(x - x_0)^2, & x \in (0, x_0) \\ u(x) = 0, & \text{otherwise.} \end{cases} \end{cases} \qquad 2D: u(x, y) = 1, \tag{2}$$

Figure 2 shows the shape of $u_2(x)$ solution for different values of x_0, where x_0 is a real constant between zero and one.

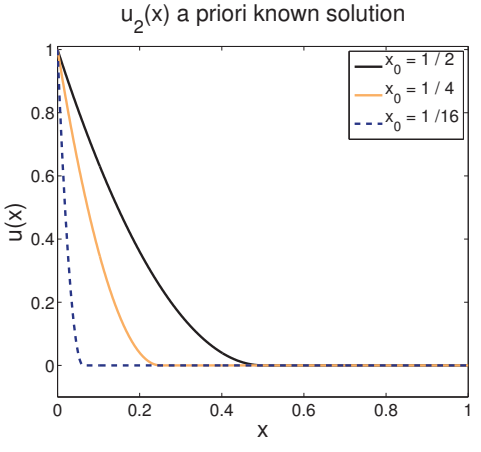

Figure 2: Representation of $u_2(x)$ for different values of x_0.

To obtain the variational formulation, we multiply equation (1) by a test function $\xi \in H^1_D(\Omega)$, where $H^1_D(\Omega) = \{u \in L^2(\Omega) : u|_{\Gamma_D} = 0, \nabla u \in L^2(\Omega)\}$ is the space of admissible test functions and u^D the value of the solution on Γ_D. Then, integrating by parts, the following variational formulation is obtained:

$$\begin{cases} \text{Find} \quad \tilde{u} \in H^1_D(\Omega) \text{ such that:} \\ \displaystyle\int_\Omega \boldsymbol{\nabla}\tilde{u} \cdot \boldsymbol{\nabla}\xi d\boldsymbol{x} = \int_\Omega f\xi d\boldsymbol{x} + \int_{\Gamma_N} g\xi dS - \int_\Omega \boldsymbol{\nabla}u^D \cdot \boldsymbol{\nabla}\xi d\boldsymbol{x} \quad \forall \xi \in H^1_D(\Omega), \end{cases} \tag{3}$$

where u^D is a lift of the Dirichlet boundary condition data u^D (denoted with the same symbol). The solution then is the sum of u and the lift: $\tilde{u} + u^D$ while $g = \dfrac{\partial u}{\partial n}$ is a function defined on Γ_N, $\dfrac{\partial u}{\partial n}$ is the normal derivative of u (flux).

2.2. The hp-adaptive Finite Element Method

The *hp*-adaptive finite element method (*hp*-FEM) is a general version of the finite element method (FEM) with a special choice of basis functions. Here, a piecewise-polynomial approximation is employed, as before, h is the element size and p the polynomial degree of approximation.

Taking a finite dimensional space $V_{hp} \in V$, where V is the Sovolev space of order one, H^1, (3) can be discretized as:

$$\begin{cases} \text{Find} \quad u_{hp} \in u_{hp}^D + V_{hp} \quad \text{such that:} \\ b(u_{hp}, v_{hp}) = l(v_{hp}) \quad \forall v_{hp} \in V_{hp}, \end{cases} \tag{4}$$

where subscript 'hp' denotes an hp discretization. The mesh consists of a collection of K elements, where the bilinear form is expressed as:

$$b(u_{hp}, v_{hp}) = \sum_K b_K(u_{hp}, v_{hp}) = \sum_K \int_{\Omega_K} \boldsymbol{\nabla} u_{hp} \cdot \boldsymbol{\nabla} v_{hp} d\boldsymbol{x}, \tag{5}$$

and the linear form

$$l(v_{hp}) = \sum_K l_K(v_{hp}) = \sum_K \left(\int_{\Omega_K} f v_{hp} d\boldsymbol{x} + \int_{\Gamma_{N_K}} g v_{hp} dS - \int_{\Gamma_{D_K}} u^D v_{hp} dS \right). \tag{6}$$

This leads to a linear system of N equations (being $N = dim(V_{hp})$):

$$Bd = l. \tag{7}$$

Here, B is a sparse, symmetric and positive definite matrix, d is the vector of unknown coefficients that define the disctrete solution of our problem, and l is the load vector the right-hand side. To solve the linear system arising from the Galerkin discretization, one of the most populars direct solvers is used: MUMPS [23].

Note that in this work the following definition of the condition number is used:

$$\kappa(B) = \lambda_{max}/\lambda_{min}, \tag{8}$$

where λ_{max} and λ_{min} are the biggest and smallest eigenvalues of matrix B, respectively.

3. Round-off Error and Conditioning

It is commonly believed that the condition number determines the behavior of the round-off error. It is true that, up to a constant, the condition number is an upper bound of the round-off error, but these numbers are not equivalent. For instance, despite its huge condition number, solving the following linear system of equations with a direct method returns an exact solution.

$$\begin{pmatrix} 1 & 0 \\ 0 & 10^{-32} \end{pmatrix} \begin{pmatrix} d_1 \\ d_2 \end{pmatrix} = \begin{pmatrix} 1 \\ 1 \end{pmatrix} \tag{9}$$

This simple example illustrates why it is interesting to study the relation between conditioning and round-off error. To do this, we now give some intuition about how a particular right-hand side can minimize the round-off error without improving the condition number. Following the argument of [24], let δd be the error produced in the solution when the right-hand side of (7) is perturbed by $\ell + \delta\ell$. Then,

$$\delta d = B^{-1} \delta\ell. \tag{10}$$

Expanding $\delta\ell$ in terms of the eigenvectors $v_1, ..., v_N$ of B, as

$$\delta\ell = \sum_{i=1}^{N} c_i v_i, \tag{11}$$

and inserting this expression into (10), one obtains that

$$\delta d = \sum_{i=1}^{N} c_i v_i / \lambda_i, \tag{12}$$

where λ_i are the eigenvalues (strictly positive) of B. From (12), if the right-hand side of the problem is a collection of few eigenvectors ($c_i = 0$ for several i), then the expected error seems to be smaller.

We can intuitively illustrate this idea in the following way. Let us eigendecompose matrix B. Then,

$$VDV^{-1}d = l, \tag{13}$$

where V is the matrix containing the eigenvectors of B and D is the diagonal matrix containing its eigenvalues. Being B symmetric positive definite, V contains the orthonormalized eigenvectors, and multiplying on the left by V^{-1}, as $V^{-1} = V^T$ (orthogonal eigenvectors), we have

$$DV^T l = V^T l, \tag{14}$$

which can be rewritten as

$$Dy = z, \tag{15}$$

if $y = DV^T$ and $z = V^T l$.

The idea of having a small error when the right-hand side is a combination of few eigenvectors returns. In particular, if we consider a unique eigenvector in (12), it means having $z = (0 \cdots 0 \cdots c \cdots 0 \cdots 0)$, being $c \in \mathbb{R}$. With this choice of z and since D is a diagonal matrix, then only one contribution of y (the corresponding to the nonzero entry of z) needs to be computed.

$$y_i = z_i/\lambda_i, \quad \text{or} \quad y_i = c/\lambda_i. \tag{16}$$

The remaining eigenvalues of the matrix do *not* contribute to the round-off errror.

4. Numerical Results

4.1. 1D, Example 1: $u(x) = 1$

$$-\Delta u = 0 \quad \text{on: } \Omega = [0,1], \quad u = 1 \quad \text{on } \Gamma_D, \quad \partial_n u = 0 \quad \text{on } \Gamma_N. \tag{17}$$

We consider two sets of boundary conditions to analyze their impact in the round-off error and in the condition number of the stiffness matrix:

$$\begin{cases} \Gamma_1 : \Gamma_D = \{x \in \Omega : x = 0 \quad \text{or} \quad x = 1\} \\ \Gamma_2 : \Gamma_D = \{x \in \Omega : x = 1\} \end{cases} \tag{18}$$

being $\Gamma_N = \partial\Omega \setminus \Gamma_D$. In Figure 3 we compare the condition numbers and round-off errors for both types of boundary conditions and two different meshes, namely: a uniformly refined grid, and a 'radical' mesh.

In the left panels of Figure 3, which correspond to uniform grid refinements, we observe a strong correlation between round-off error and conditioning of the matrix, independently of the selected boundary conditions. However, the results from the radical meshes (Figure 3 (right)) are dramatically different. The condition number and the round-off error do *not* behave equally. In particular, we see that for the first set of boundary conditions, where the condition number is extremely large, the round-off error remains small.

It is commonly thought that an enormous condition number always implies a large round-off error and therefore, an inaccurate solution. However, in some cases, we are able to properly solve systems of linear equations (and obtain small round-off errors) despite having very large condition numbers. This is due to the effect of the right-hand side, which has been explained in the previous section. Namely, the right-hand side does not excite all eigenvalues of the problem and because of this, the performance may be better what the worst case scenario predicted by the condition number.

Of particular interest is our test problem with a radical mesh, which often appears in practical engineering applications where a singularity arises at the boundary. That singularity is mathematically expressed as an infinite value of the derivative, which is necessarily prescribed by a Dirichlet BC (since a Neumann BC cannot be set to infinity). For this case, we observe that the round-off error remains small despite the huge condition number. Moreover, the case of a Neumann BC implies that the value of the derivative at that point is finite, which means that no singularity is present, making the use of a radical mesh unnecessary in any practical application. Thus, it is not a coincidence that adaptive methods for Laplace equation typically exhibit a small round-off error in most engineering applications, despite the appearance of heavy refinements, which indicate a large condition number.

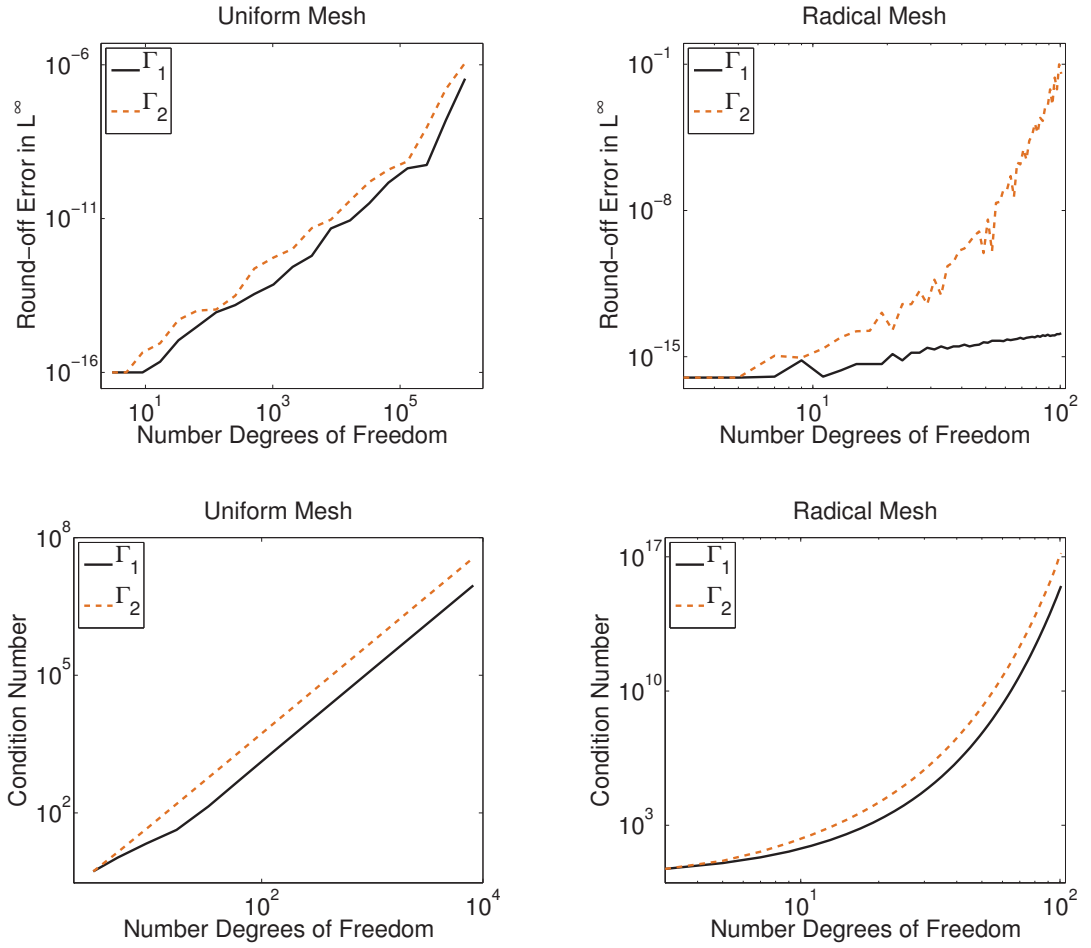

Figure 3: Log-Log representation of the condition number and round-off error for 1D Laplace problem discretized with a uniform grid (left) and a radical mesh (right). ILP shape functions of order $p = 2$ are used.

For both kind of meshes, a peculiar, but different, behavior of the eigenvalues is also observed. There exists some grouping between them. This grouping depends on the number of elements and on the polynomial order of approximation.

4.2. 1D, Example 2: $u(x) = u_2(x)$

$$-\Delta u = f \quad \text{on: } \Omega = [0, 1] \tag{19}$$

Dirichlet boundary conditions are considered in both edges (according with the definition of (2), one on the left and zero on the right). $f(x) = -2x_0^{-2}$, for $x < x_0$ (otherwise 0). Selecting different values of x_0 corresponds to different

right-hand sides of the problem. The stiffness matrix, and hence the condition number, remains invariant. Therefore, if different round-off errors are obtained is because the right-hand side $f(x)$ has been modified.

In Figure 4 we display the round-off error corresponding to different values of x_0. We observe that round-off error depends directly on the constant we select, namely, on the right-hand side. This occurs because each $f(x)$ excites different eigenvalues of the problem. Therefore, one can conclude that round-off error depends not only on the associated stiffness matrix, but also upon the right-hand side.

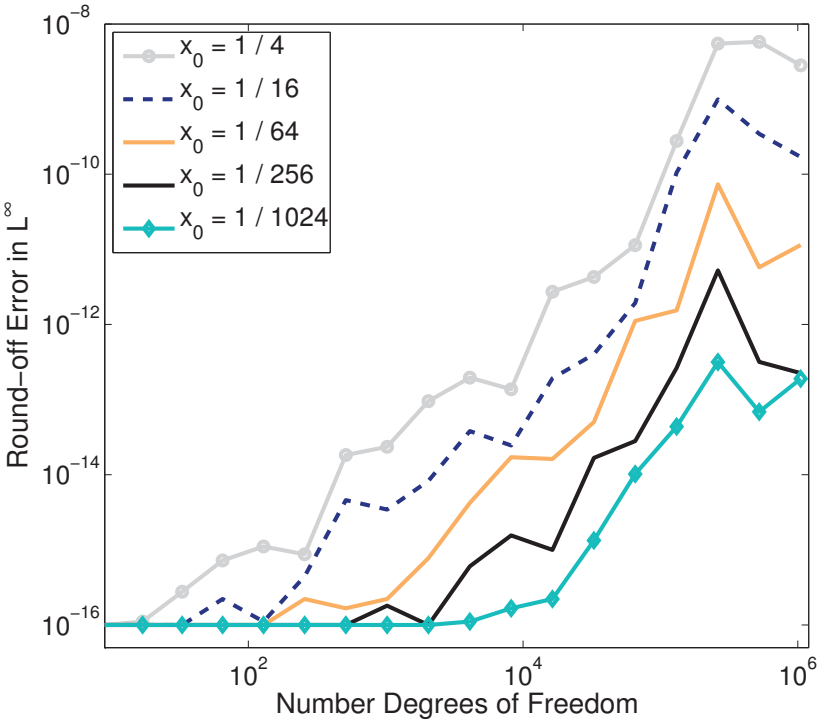

Figure 4: Round-off error for 1D Poisson problem discretized with uniform mesh. ILP shape functions of order $p = 1$ are used.

4.3. 2D, Example 1 $u(x, y) = 1$

$$\Delta u = 0 \quad \text{on: } \Omega = [0,1]^2, \quad u = 1 \quad \text{on } \Gamma_D, \quad \partial_n u = 0 \quad \text{on } \Gamma_N, \tag{20}$$

Let us consider the following two sets of boundary conditions to study how they affect round-off error and condition number of the stiffness matrix.

$$\begin{cases} \Gamma_1 : \Gamma_D = \{(x,y) \in \Omega : x = 0 \quad \text{or } x = 1 \quad \text{or } y = 0 \quad \text{or } y = 1\} \\ \Gamma_2 : \Gamma_D = \{(x,y) \in \Omega : x = 0 \quad \text{or } x = 1 \quad \text{or } y = 1\} \end{cases} \tag{21}$$

being $\Gamma_N = \partial\Omega \setminus \Gamma_D$. Notice that for Γ_1 we only consider Dirichlet boundary conditions while for Γ_2 a Neumann boundary condition is established in the refined side of the radical mesh.

Figure 5 shows a comparison between the condition number and round-off error for radical and uniform meshes for the different boundary conditions discussed above. In the case of uniform meshes, the two sets of boundary conditions deliver similar results. The round-off error grows proportionally to the matrix condition number (which for these types of grids is known to be proportional to the inverse of the mesh size squared). For radical meshes, the Neumann boundary condition produces a dramatic increase in the condition number and round-off error. However, in the 2D case, the problem is still solvable for both sets of boundary conditions, despite the large condition numbers.

This result agrees with [9], since 2D is a special case where the re-scaling of basis functions is not necessary. However, as we showed in the 1D case and according with the theory, in 3D a disagreement between the round-off error and condition number is also expected.

In the 2D problem, a peculiar behavior in the eigenvalues is also empirically observed. There exists two clusters of eigenvalues. This clustering depends on the number of elements of the mesh and the polynomial order p.

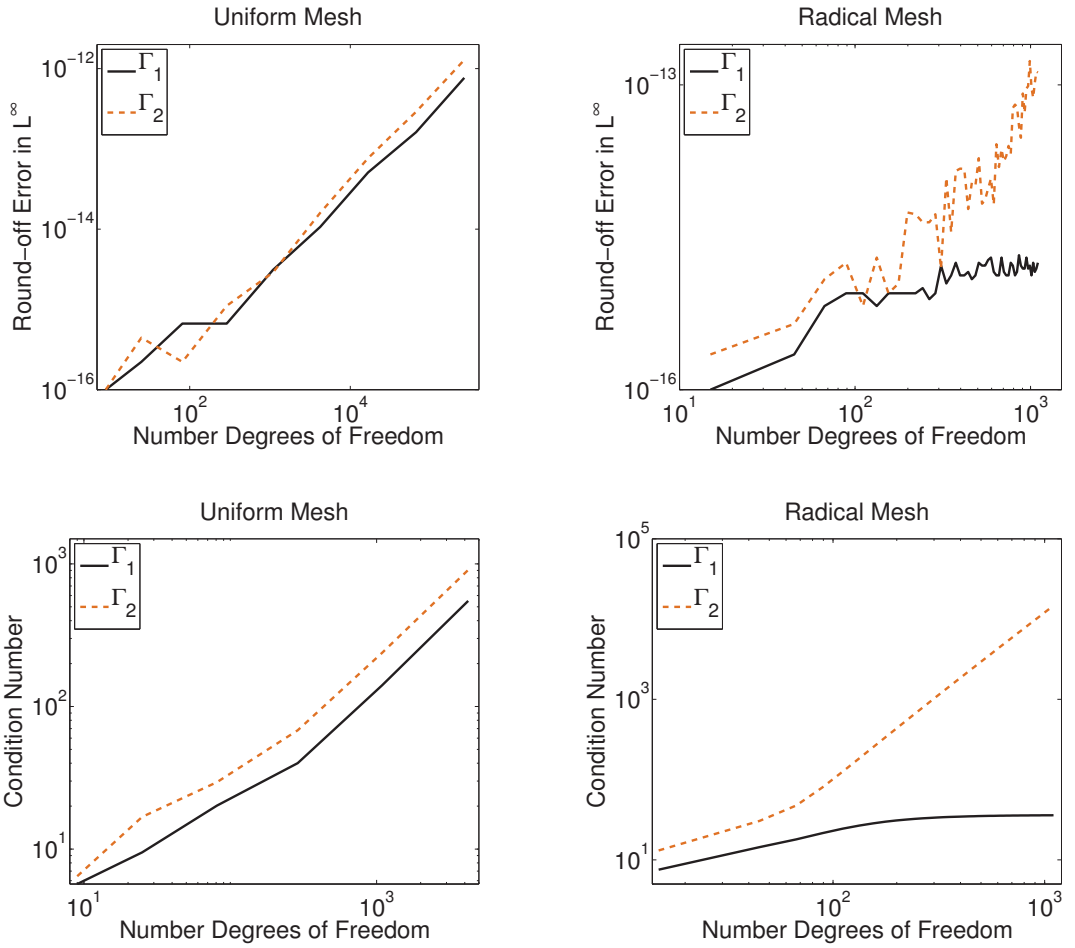

Figure 5: Log-Log representation of condition number and round-off error for 2D Laplace problem discretized with uniform grid (left) and radical mesh (right). ILP shape functions of order p = 2 are used.

4.4. 2D, Example 2 $u(x, y) = 1$

$$\Delta u = 0 \quad \text{on: } \Omega = [0,1]^2, \quad u = 1 \quad \text{on } \Gamma_D, \quad \partial_n u = 0 \quad \text{on } \Gamma_N, \tag{22}$$

where $\Gamma_D = \{(x, y) \in \Omega : x = 0 \quad \text{or } y = 0\}$ and $\Gamma_N = \partial\Omega \setminus \Gamma_D$.

We now consider uniformly refined meshes, and we analyze how the round-off error behaves for different shape functions when p-refinements are performed. In Figure 6 we compare round-off error results when Peano and ILP basis functions are considered.

We observe an initial pre-asymptotic behavior (a plateau) where p method dominates, followed by an asymptotic one, where h dominates. Thus, when the number of elements grows sufficiently, the choice of basis functions is not important, since both give a similar performance in terms of round-off error. However, if we do not have enough

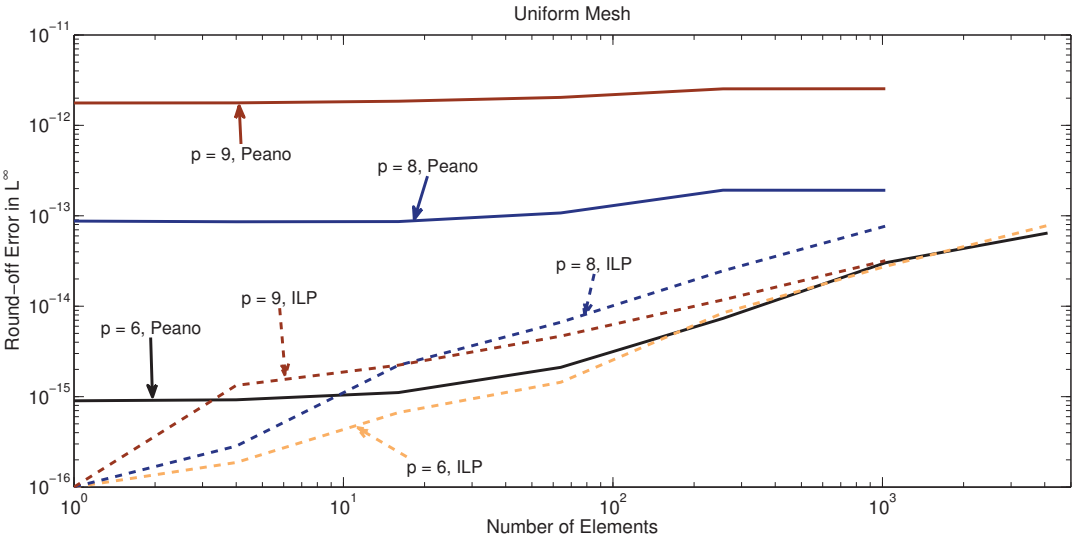

Figure 6: Round-off error for 2D Laplace problem discretized with uniform mesh.

elements and we highly increase p, Peano hierarchical shape functions provide significantly worse performance. For a more detailed study of conditioning due to the use of different boundary conditions, we refer to [11]

5. Conclusions

In this paper, we analyze the relation between condition number and round-off error. We point out that in the context of *hp*-adaptive FE, it is possible to have a system of linear equations with an arbitrarily large condition number that still brings small round-off errors. Therefore, the round-off error is not always related to the condition number and something else has to be introduced to completely understand its behavior, namely, the right-hand side of the system.

We intentionally select a particular *a priori* solution which allows us to define different right-hand sides. The associated stiffness matrix remains invariant, and therefore with the same condition number. We obtain different round off-errors, because each of the right-hand sides excites different eigenvalues of the problem. In this way the right-hand side plays a key role in round-off error.

For the case of adaptive methods, a Neumann boundary condition implies a finite value of the derivative at that point, and hence, no singularity appears at that boundary. Therefore, radical meshes are unnecessary. On the other hand, if a Dirichlet boundary condition is imposed, this may lead to a singular behavior of the solution at that boundary making convenient the use of a radical mesh, but in that case, we show numerically that the round-off error will still remain small.

Finally, we also show that for high polynomial orders, ILP provides better results than Peano hierarchical shape functions when a small number of elements is considered. However, if a sufficient number of refinements are carried out, the choice of basis functions is not important.

Acknowledgments

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