ADAPTIVE NUMERICAL INTEGRATION ON SPHERICAL TRIANGLES

Natalia Boal and Francisco-Javier Sayas

Abstract. In this work we present an adaptive algorithm for the numerical approximation of integrals on parts of a spherical surface. The rules are constructed by dividing progressively a basic triangulation of a spherical triangle following [3] and mapping the curved triangulation to a polyhedron where integrals are approximated by simple two–dimensional rules (see [2]).

We show numerical evidence of the possibility of applying Richardson extrapolation to accelerate the convergence and to estimate the error. With arguments close to those used in [5] we give a formal justification of why this is possible and construct an adaptive algorithm by refining the triangulation where needed.

Keywords: Numerical integration, extrapolation, a posteriori estimates

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§1. Introduction

The following work deals with numerical integration over spherical polygons, i.e., connected regions of the unit sphere, S_2, bounded by maximum circles. Such integrals are interesting because they appear in an extensive variety of applications, for example, in Boundary Element Methods (where the integrand can be highly oscillating in parts of the polygon) and in Partial Differential Equations on smooth surfaces (for instance, those appearing in computation of diffraction coefficients for wedge–shaped objects). Our contribution is a first step towards construction and full theoretical justification of automatic integration rules.

If we take $\mathcal{T}_0$ a partition of a spherical polygons Ω into triangles, we can write

$$\int_\Omega \psi = \sum_{T\in\mathcal{T}_0} \int_T \psi. \tag{1}$$

Thus, the problem reduces to computing the integral of ψ on each spherical triangle T and, from now on, for simplicity, we will restrict the exposition to Ω being a spherical triangle, which will be denoted K.

We aim to approximate the integral with some degree of optimality in the number of evaluations, obtaining as much precision as we desire and controlling the error. To do that, we propose an adaptive compound integration rule on triangulations of K. These triangulations will not have the restriction of being *à la Ciarlet*: we will admit that triangles share only part of their common sides. We will also try to construct the triangulation well adapted to the integral to be computed, i.e, coarse where we detect “smooth behaviour” and fine in “difficult places”.

§2. An elementary simple rule

Let K be the initial spherical triangle and $\mathbf{v}_1,\ \mathbf{v}_2,\ \mathbf{v}_3 \in \mathbb{R}^3$ be its three vertices. Let

$$\widehat{K} := \{(s,t)\,|\,0 \le s, t, s+t \le 1\}$$

be the plane reference triangle and let $\mathbf{f} : \widehat{K} \to \mathbb{R}^3$ be given by

$$\mathbf{f}(s,t) := \mathbf{v}_1 + t(\mathbf{v}_2 - \mathbf{v}_1) + s(\mathbf{v}_3 - \mathbf{v}_1).$$

It is clear that $\mathbf{f}$ maps $\widehat{K}$ onto K_*, the plane triangle in $\mathbb{R}^3$ with vertices $\mathbf{v}_1,\ \mathbf{v}_2,\ \mathbf{v}_3$.

When those vertices belong to the same open hemisphere of S_2, the function $\mathbf{g} : \widehat{K} \to S_2$

$$\mathbf{g}(s,t) := \frac{\mathbf{f}(s,t)}{|\mathbf{f}(s,t)|}$$

is a parameterization of the spherical triangle K. If $\sigma(s,t) := |\partial_s\mathbf{g} \times \partial_t\mathbf{g}|(s,t)$ represents the

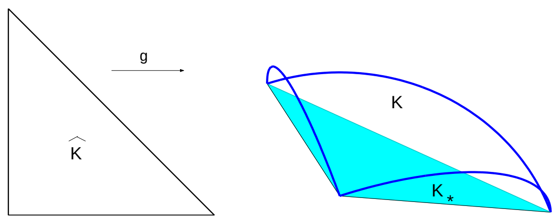

Figure 1: Mapping the reference triangle $\widehat{K}$ onto the spherical triangle K.

area element, being

$$\partial_t\mathbf{g} = \frac{1}{|\mathbf{f}|}\,(\mathbf{v}_2 - \mathbf{v}_1) - \frac{\mathbf{f}\cdot(\mathbf{v}_2 - \mathbf{v}_1)}{|\mathbf{f}|^3}\,\mathbf{f},$$
$$\partial_s\mathbf{g} = \frac{1}{|\mathbf{f}|}\,(\mathbf{v}_3 - \mathbf{v}_1) - \frac{\mathbf{f}\cdot(\mathbf{v}_3 - \mathbf{v}_1)}{|\mathbf{f}|^3}\,\mathbf{f},$$

then we can write

$$\int_K \psi = \int_{\widehat{K}} (\psi \circ \mathbf{g})\,\sigma \tag{2}$$

and use a quadrature rule on $\widehat{K}$ to approximate the integral.

In the plane we can opt for different rules. We select the simplest, the barycentre (centroid) rule. Therefore, if we denote $\widehat{\mathbf{b}} := (1/3, 1/3)$ the barycentre of the reference triangle, we have

$$\int_{\widehat{K}} \phi \approx \frac{1}{2}\phi(\widehat{\mathbf{b}}).$$

Employing the parameterization $\mathbf{g}$ and applying this formula to (2) we obtain

$$\int_K \psi \approx \frac{1}{2}\psi(\mathbf{g}(\widehat{\mathbf{b}}))\,\sigma(\widehat{\mathbf{b}}).$$

On the other hand, $\mathbf{g}$ maps the barycentre $\widehat{\mathbf{b}}$ to the intersection point of three medians on the spherical triangle that we denote

$$\mathbf{b} := \mathbf{g}(\widehat{\mathbf{b}}).$$

We thus define *the barycentre rule on a spherical triangle* to approximate the integral (2) as

$$I_0(\psi, K) := \omega_K \, \psi(\mathbf{b}) \tag{3}$$

with weight

$$\omega_K := \sigma(\widehat{\mathbf{b}})/2.$$

It is important to remark that, although the two-dimensional barycentre formula has degree of precision 1, i.e, it is exact for polynomials of degree up to 1, this basic rule I_0 is not consistent since it does not integrate exactly even for constant functions.

§3. Compound integrate rules

Let $\mathbf{m}_1$, $\mathbf{m}_2$ and $\mathbf{m}_3$ be the midpoints of the sides of the spherical triangle K, which can be computed as

$$\mathbf{m}_1 = \frac{1}{|\mathbf{v}_2 + \mathbf{v}_3|}(\mathbf{v}_2 + \mathbf{v}_3), \quad \mathbf{m}_2 = \frac{1}{|\mathbf{v}_1 + \mathbf{v}_3|}(\mathbf{v}_1 + \mathbf{v}_3), \quad \mathbf{m}_3 = \frac{1}{|\mathbf{v}_1 + \mathbf{v}_2|}(\mathbf{v}_1 + \mathbf{v}_2).$$

We refine this triangle by the simple procedure of connecting the midpoints of the three sides with geodesic arc and building four smaller spherical triangles denoted by K_j, $j = 1, \ldots, 4$ with vertices

$$\{\mathbf{v}_1, \mathbf{m}_2, \mathbf{m}_3\}, \qquad \{\mathbf{v}_2, \mathbf{m}_3, \mathbf{m}_1\}, \qquad \{\mathbf{v}_3, \mathbf{m}_1, \mathbf{m}_2\}, \qquad \{\mathbf{m}_1, \mathbf{m}_2, \mathbf{m}_3\}$$

(see Figure 2).

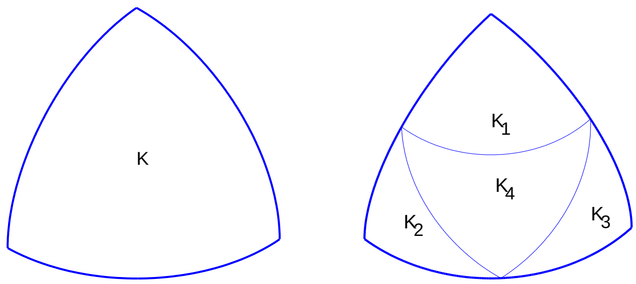

Figure 2: Subdiving the spherical triangle in four

If we consider this refinement of K and if we apply the simple barycentre rule I_0 on each subtriangle, we can define

$$I_1(\psi, K) := \sum_{j=1}^{4} I_0(\psi, K_j) \approx \int_K \psi. \tag{4}$$

In fact, generalizing this idea, we can construct a sequence of approximations

$$\begin{aligned} I_2(\psi, K) &:= \sum_{j=1}^{4} I_1(\psi, K_j), \\ &\vdots \\ I_N(\psi, K) &:= \sum_{j=1}^{4} I_{N-1}(\psi, K_j). \end{aligned}$$

Subdividing each new triangle K_j, $j = 1, \dots, 4$ into four smaller ones by the same procedure, we obtain a triangulation with 16 elements. If we consider this triangulation of K and we sum the approximations obtained with the simple rule I_0 on each these triangles, the result is the same that we directly apply the compound rule I_2 on K.

In general, we can subdivide K repeatedly over and over again, N times in all. Like this, we generate an almost uniform triangulation of the original triangle K with 4^N elements that we denote by $\mathcal{T}_N$. In this case,

$$I_N(\psi, K) = \sum_{T \in \mathcal{T}_N} I_0(\psi, T). \tag{5}$$

This kind of subdivision appears originally in [3] and provides triangles with very regular shapes and almost uniform areas. This subdivision can be iterated to generate a kind of non–smooth spherical barycentric coordinates (see [3] and [1]) which have some very interesting properties. There is a much simpler option, based on simply transferring a uniform triangulation of $\widehat{K}$ onto K by the mapping $\mathbf{g}$. This alternative way of triangulating K gives much wider triangles in the interior and very small ones near the vertices and is, therefore, not very well suited for almost-uniform approximation.

We base our exposition simply on the barycenter rule although many of the ideas could be transferred to more complicated rules on triangles (see [2] and [4]).

§4. Analysis of the error

For the construction of I_N we have basically used three facts: the parameterization of any spherical triangle from $\widehat{K}$, the two-dimensional barycentre rule and the subdivision of K to generate the triangulation. Out of those characteristics, we can think that the compound rule in the space I_N is equivalent to applying some composite quadrature rule on the reference triangle, and thus, we could try to analyse the asymptotic behaviour in a similar way as in (see [5] for compound rules on $\widehat{K}$ and their full asymptotic behaviour). Things are however somewhat more complicated. If we use the inverse of $\mathbf{g} : \widehat{K} \to K$ to map the compound integration rule onto $\widehat{K}$ we obtain a non–uniform partition of $\widehat{K}$ and a full asymptotic analysis (including a posteriori error estimates) does not follow from simple arguments. Our approach for a full theoretical justification of the arguments we are going to expose here will be that of mapping the barycenters of a uniform triangulation of $\widehat{K}$ to the quadrature nodes of the rule I_N via a continuous piecewise smooth function and put the stress on studying this sequence of mappings from $\widehat{K}$ onto K.

Let N be the number of times that we have refined the original triangle K, that is, we have subdivided each side into 2^N pieces. We denote

$$h := 2^{-N}.$$

It can be seen that [1]

$$h \approx \mathrm{diam}(T), \qquad \forall T \in \mathcal{T}_N, \tag{6}$$

and that the area of each triangle T is also equivalent to h^2.

Theorem 1. *For ψ smooth enough*

$$\left| I_N(\psi, K) - \int_K \psi \right| \leq C(\psi, K)\, h^2.$$

Proof. The proof follows from standard arguments of two–dimensional quadrature rules and bounds on the subdivision procedure similar to those that serve to prove (6). The quantity $C(\psi, K)$ is shown to depend on derivatives of ψ up to order two. □

It is our belief that the bound of the error can be made very sharp and that we can obtain a beginning of an asymptotic expansion of the error, such as the following one.

Conjecture 2. *For ψ smooth enough*

$$I_N(\psi, K) - \int_K \psi = h^2 C(\psi, K) + \mathcal{O}(h^4).$$

We now give some numerical evidence of this and refer to [1] for analysis. If this conjecture holds true, we have

$$I_N(\psi, K_j) - \int_{K_j} \psi = \frac{h^2}{4} C(\psi, K_j) + \mathcal{O}(h^4), \qquad j = 1, \ldots, 4.$$

Then,

$$\sum_{j=1}^{4} I_N(\psi, K_j) - \int_K \psi = \frac{h^2}{4} \sum_{j=1}^{4} C(\psi, K_j) + \mathcal{O}(h^4)$$

with

$$\sum_{j=1}^{4} C(\psi, K_j) \approx C(\psi, K).$$

Therefore,

$$\begin{aligned} I_N(\psi, K) - \textstyle\int_K \psi &= h^2 C(\psi, K) + \mathcal{O}(h^4), \\ I_{N+1}(\psi, K) - \textstyle\int_K \psi &= \frac{h^2}{4} C(\psi, K) + \mathcal{O}(h^4) \end{aligned}$$

and we would observe an increase of the order of convergence using Richardson extrapolation, i.e,

$$\left[\frac{4}{3} I_{N+1}(\psi, K) - \frac{1}{3} I_N(\psi, K) \right] - \int_K \psi = \mathcal{O}(h^4). \tag{7}$$

Assuming the existence of more terms in the error expansion of Conjecture 2, we can consider $(4/3) I_{N+1} - (1/3) I_N$ as quadrature rule and use again Richardson extrapolation to obtain

$$\frac{16}{15} \left[\frac{4}{3} I_{N+2} - \frac{1}{3} I_{N+1} \right] - \frac{1}{15} \left[\frac{4}{3} I_{N+1} - \frac{1}{3} I_N \right] - \int_K \psi = \mathcal{O}(h^6). \tag{8}$$

The following examples show some numerical evidence of these facts. In the first example, we are going to approximate the area of one octant of S_2. In the second, we integrate $\psi(x, y, z) = yz$ on the spherical triangle with vertices $(1, 0, 0),\ (1/\sqrt{2}, 1/\sqrt{2}, 0),$ and $(0, 0, 1)$. In both cases, the errors expected with each rule are: order 2 for (5), order 4 for (7) and order 6 for (8).

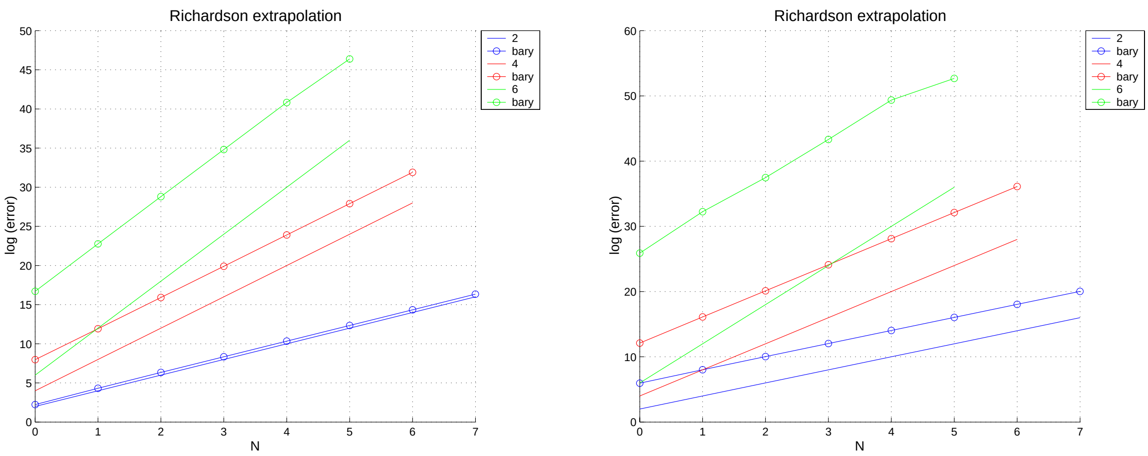

Figure 3: Behaviour of the errors with the rules (5), (7) and (8) in Examples # 1 and # 2, respectively

N / # extrap	0	1	2	0	1	2
0	2.13(-1)	3.99(-3)	9.34(-6)	1.61(-2)	2.26(-4)	1.60(-8)
1	5.04(-2)	2.58(-4)	1.40(-7)	3.87(-3)	1.41(-5)	1.96(-10)
2	1.24(-2)	1.63(-5)	2.13(-9)	9.56(-4)	8.81(-7)	5.24(-12)
3	3.08(-3)	1.02(-6)	3.31(-11)	2.38(-4)	5.50(-8)	9.13(-14)
4	7.71(-4)	6.38(-8)	5.15(-13)	5.95(-5)	3.44(-9)	1.39(-15)
5	1.92(-4)	3.98(-9)	1.09(-14)	1.49(-5)	2.15(-10)	1.39(-16)
6	4.82(-5)	2.49(-10)		3.72(-6)	1.34(-11)	
7	1.20(-5)			9.30(-7)		

Table 1: Errors with the rules (5), (7) and (8) in Examples # 1 and # 2, respectively. Notice that Richardson extrapolation not only improves the order of the method (accelerates its convergence) but also reduces errors significantly.

We also show some experiment based upon the three-vertices formula as basic rule, i.e.,

$$I_0(\psi, K) := \frac{1}{6}\sum_{i=1}^{3} \sigma(\widehat{\mathbf{v}}_\mathbf{i})\, \psi(g(\widehat{\mathbf{v}}_\mathbf{i}))$$

with $\widehat{\mathbf{v}}_\mathbf{i}$ the vertices of reference triangle $\widehat{K}$. This is the two-dimensional equivalent to one-dimensional trapezoidal rule. It has the same order as the barycenter rule adapted to the sphere. Results on Examples # 1 and # 2 are show in table 2.

In figure 4, we show together the results for both the barycenter and the three-vertices rules on Examples # 1 and # 2. As happens with the original plane rules, the midpoint one has a better performance.

N / # extrap	0	1	2	0	1	2
0	4.67(-1)	2.98(-2)	3.74(-4)	3.83(-2)	1.80(-3)	1.34(-5)
1	1.39(-1)	2.21(-3)	6.76(-6)	1.09(-2)	1.25(-4)	2.25(-7)
2	3.64(-2)	1.45(-4)	1.10(-7)	2.82(-3)	8.02(-6)	3.57(-9)
3	9.22(-3)	9.14(-6)	1.73(-9)	7.12(-4)	5.05(-7)	5.60(-11)
4	2.31(-3)	5.73(-7)	2.70(-11)	1.78(-4)	3.16(-8)	8.77(-13)
5	5.78(-4)	3.58(-8)	4.25(-13)	4.46(-5)	1.98(-9)	1.32(-14)
6	1.45(-4)	2.24(-9)		1.12(-5)	1.24(-10)	
7	3.61(-5)			2.79(-6)		

Table 2: Errors with the rules (5), (7) and (8) in Examples # 1 and # 2, respectively when we take the three-vertices formula as I_0

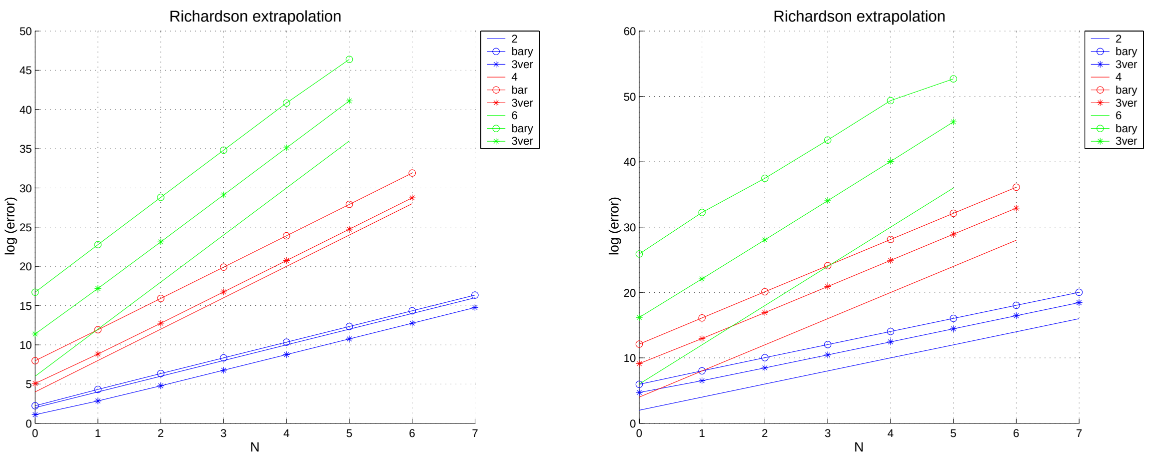

Figure 4: Comparison of the errors using the three vertices and barycentre formulas as basic rules in (5), (7) and (8) in Examples # 1 and # 2, respectively

§5. Adaptive method

The beginning of an asymptotic series relies heavily on the definition of $h = 2^{-N}$, where N is the number of times we have subdivided the original triangle. If we work with K_1, K_2, K_3, K_4, it will happen that

$$\sum_{j=1}^{4} C(\psi, K_j) \approx C(\psi, K)$$

so we will be able to begin at refined levels taking the same point of reference (the large initial triangle). We can then cancel the term $\int_K \psi$ in the 'asymptotic expansion' and take

$$E(\psi, K) := \frac{4}{3}\left[I_1(\psi, K) - I_0(\psi, K)\right] \approx C(\psi, K)$$

as a posteriori estimate of the error that has been committed on each triangle.

This allows to design an adaptive compound rule to approximate (2) which be resumed in this code:

begin with a trivial triangulation of the polygon
for $n = 1$: maxNumRefinements
  for $K \in$ Triangulation
    compute $I_0(K), I_1(K), E(K)$ (a)
  end
  if $|\sum_K E(K)| <$ Tol $|\sum_K I_0(K)|$ stop
  decide which triangles concentrate more error (b)
  for $K \in$ List_Of_Triangles_To_Refine
    compute midpoints of the sides
    add 4 new triangles and delete K
  end
end

Remark 1. The computations in (a) can be reduced to the newly created triangles. If carefully done, we can even avoid computing $I_0(K)$, by using information of $I_1(K)$ at the finer level.

Remark 2. In (b) we can use the following criterion

$$|E(K)| > \frac{\gamma}{\#\text{Triang}} \sum_T |E(T)|$$

for some parameter $\gamma \geq 1$. Some other criteria can be used by following widely employed methods in FEM literature and in one–dimensional adaptive quadrature.

We have programmed this quadrature formula using MATLAB and applied it to two new examples, which have an peak in some points. In Example #3 we consider

$$\psi(x, y, z) = \frac{1}{x^2 + y^2 + (z - 1.2)^2}$$

and we choice $\gamma = 1.5$ and Tol=10^{-3}. Example #4 corresponds to

$$\psi(x, y, z) = \frac{1}{(x - 0.4)^2 + (y - 0.4)^2 + (z - 0.4)^2} + \frac{1}{x^2 + y^2 + (z - 0.8)^2}$$

and we take the same tolerance but $\gamma = 1$. The integration domain is the first octant in both cases.

The following figures show the adaptive triangulations obtained with the proposed rule taking the barycenter formula as I_0. It can be observed that the results agree with could be expected a priori. In the figures we have drawn the plane triangles subtended by the spherical ones, so a crack can be seen when the refining level of adjacent triangles is different.

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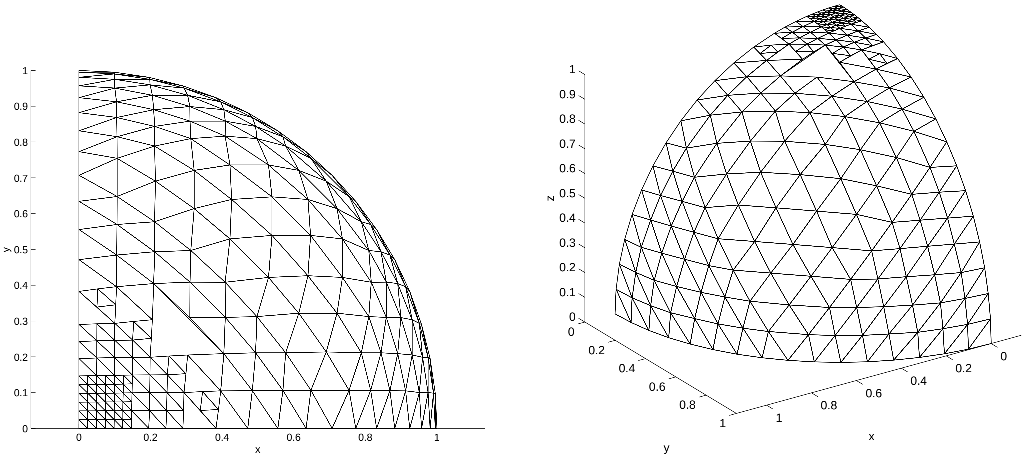

Figure 5: Two different views of adaptive polyhedric triangulation for the Example #3

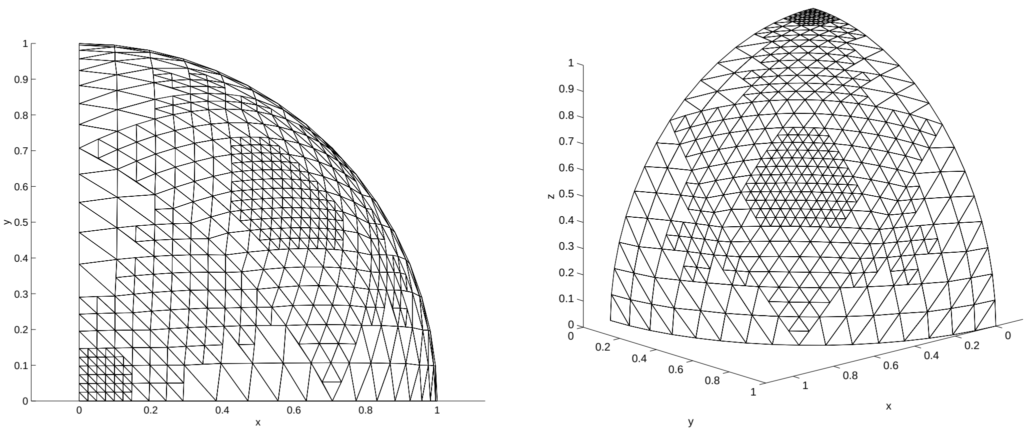

Figure 6: Two different views of adaptive polyhedric triangulation for the Example #4

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Natalia Boal and Francisco-Javier Sayas
Departamento de Matemática Aplicada
Universidad de Zaragoza
Centro Politécnico Superior
María de Luna, 3 - 50018 Zaragoza, Spain
`nboal@unizar.es` and `jsayas@unizar.es`