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Numerische Simulation auf massiv parallelen Rechnern

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Stable evaluation of the Jacobians for curved triangles

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Abstract

In the adaptive finite element method, the solution of a p.d.e. is approximated from finer and finer meshes, which are controlled by error estimators. So, starting from a given coarse mesh, some elements are subdivided a couple of times. We investigate the question of avoiding instabilities which limit this process from the fact that nodal coordinates of one element coincide in more and more leading digits. In a previous paper the stable calculation of the Jacobian matrices of the element mapping was given for straight line triangles, quadrilaterals and hexahedrons. Here, we generalize this ideas to linear and quadratic triangles on curved boundaries.

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1 Introduction

In the last two decades the use of adaptive mesh refinement in the finite element solution of partial differential equations is widely recognized as having significant potential for improving the efficiency of the solution process. The development of the adaptive finite element method focused mainly on two ingredients, the error estimators for detecting some elements with large contribution to the H^1–error and the mesh subdivision technique for subdividing these elements. Here, we investigate the question whether a very fine mesh in small parts of the domain as a result of continued subdivisions can terminate this process due to numerical instabilities and how to overcome this difficulty.

The main tool that has to be considered for producing or avoiding numerical instabilities is the calculation of the local Jacobian matrix of the mapping from the master–element onto the real element, as usually done in finite element calculations. From this reason our investigations are valid for each kind of 2nd order partial differential equation. So, we consider only a model problem for numerical experiments.

2 The adaptive strategy

In the adaptive finite element method, we have several error estimators, which mark some of the elements (with large contribution to the overall error) for subdivision. For a overview of known error estimators see [AO00, Verf96] and the references therein. The marked elements are subdivided into smaller parts due to some strategies.

For 2D–calculations and triangular meshes two basic strategies for one triangle are employed: The so called "red" subdivision of a triangle into 4 sub–triangles of equal shape and size (see Fig. 1) and the so called "green" subdivision into 2 parts (see Fig. 2).

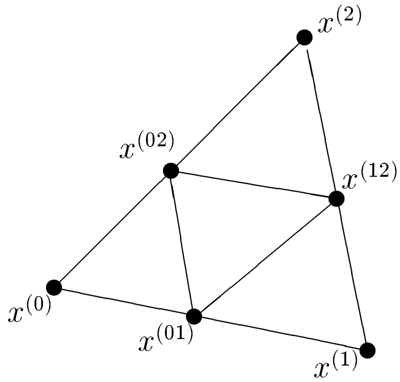

Figure 1: "red"

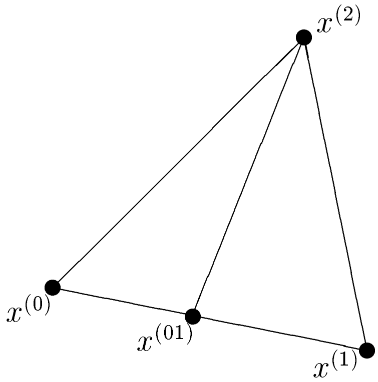

Figure 2: "green"

An important fact for the following considerations is the definition of the vertices of the son–elements. In the triangular case with straight lines the new nodes are calculated first from the formula

$$x^{son} := \frac{1}{2}(x^{father1} + x^{father2})$$

and then used for defining the new sub–edges. If this technique is repeated a couple of times neighboring nodes coincide in more and more leading digits. More precisely, a node x^{son} generated at an L–th level subdivision of some coarse element coincides with its two fathers in about L leading digits (in their binary representation). This means, the coordinates itself are correct until machine accuracy, but differences of neighboring nodes lead to cancellations of about L digits. In classical finite element codes with uniform mesh refinement this fact has played no role, because L has been about 8...10 maximally (the amount of storage and work grows with 4^L in 2D!). In an adaptive regime this is not longer true, we can have L larger then 20 (in small parts of the domain, for instance near singularities). So, differences of nodal coordinates should not be allowed (except at the beginning).

3 Unstable calculation of the Jacobian

Let K denote one of the finite elements of the given mesh. The n nodes of K are

$$x^{(0)},\ \ldots,\ x^{(n-1)} \in \mathbb{R}^2.$$

Here, $n = 3$ or $n = 6$ in the triangular case and usually $n = 4, 8$ or 9 for quadrilaterals. We denote by $\hat{K}$ the master element which is the unit triangle with vertices

$$\hat{x}^{(0)} = (0,0)^T,\ \hat{x}^{(1)} = e_1 := (1,0)^T \text{ and } \hat{x}^{(2)} = e_2 := (0,1)^T$$

or the unit square $[0,1]^2$ (then $\hat{x}^{(3)} = e := (1,1)^T$), resp. Let $\hat{x} = (\hat{x}_1, \hat{x}_2)^T \in \hat{K}$.

For calculating the element stiffness matrix, for post processing after having the approximate solution and for most of the error estimators, we have to consider gradients at points $x \in K$. Here, the usual technique considers the mapping $x(\hat{x}) : \hat{K} \to K$ and calculates gradients from transformations of master–gradients. Let $N_0(\hat{x}) \ldots, N_{n-1}(\hat{x})$ be the n form functions (defined on $\hat{x} \in \hat{K}$). Then, usually on some Gaussian points $\hat{g} \in \hat{K}$ we obtain at first the values:

$$\begin{aligned} N(\hat{g}) &= (N_0(\hat{g}), \ldots, N_{n-1}(\hat{g})) \quad \text{and} \\ \hat{\nabla} N(\hat{g}) &= \left(\hat{\nabla} N_0(\hat{g}), \ldots, \hat{\nabla} N_{n-1}(\hat{g})\right). \end{aligned}$$

Here, $\hat{\nabla} = (\partial/\partial\hat{x}_1, \partial/\partial\hat{x}_2)^T$ means formal differentiation with respect to the master coordinates. The values in $N(\hat{g})$ had $\hat{\nabla} N(\hat{g})$ are given in a stable way, usually these are copies from a fixed list.

From the definition

$$x(\hat{x}) = \sum_{k=0}^{n-1} N_k(\hat{x})\, x^{(k)} \tag{1}$$

of the mapping $\hat{K} \longleftrightarrow K$ we obtain the Jacobian matrix

$$T(\hat{g}) = \hat{\nabla} x^T|_{\hat{g}} = \sum_{k=0}^{n-1} \hat{\nabla} N_k(\hat{g})\,(x^{(k)})^T \tag{2}$$

from a simple matrix–matrix–multiply of $\hat{\nabla} N$ with the nodal coordinates. The values of T seem to be simple short inner products, but are calculated with a serious cancellation of leading digits. Let us consider the most simple triangular case with $n = 3$, then the form functions are

$$N_0(\hat{x}) = 1 - \hat{x}_1 - \hat{x}_2, \quad N_1(\hat{x}) = \hat{x}_1, \quad N_2(\hat{x}) = \hat{x}_2\ . \tag{3}$$

So,

$$\hat{\nabla} N = (-e \,\vdots\, e_1 \,\vdots\, e_2) = \begin{pmatrix} -1 & 1 & 0 \\ -1 & 0 & 1 \end{pmatrix} \tag{4}$$

and

$$T = (x^{(1)} - x^{(0)} \,\vdots\, x^{(2)} - x^{(0)})^T. \tag{5}$$

In the case of 6–node triangles the same is true if the edge mid nodes define straight edges ($x^{(3)} = \frac{1}{2}(x^{(0)} + x^{(1)})$ and so on).

The instability of succeeding calculations results from the use of the inverse of T for instance in:

$$\nabla N_k(g) = T^{-1} \hat{\nabla} N_k(\hat{g}). \tag{6}$$

In [Mey01, Mey03], the stable calculation of these Jacobians was given for linear triangles (”red” or ”green” subdivision) and for quadrilaterals or hexahedrons (in 2D and 3D, resp.). This work was restricted to straight boundaries and will be generalized to curved triangles here.

4 Stable calculation of T for “red” subdivisions of linear triangles on a curved boundary

A stable calculation of T (and especially T^{-1}) is possible, if we avoid these differences of nodal coordinates in (5) for the fine grid elements. This is very easy in the triangular case, if all triangles have straight edges. Then the “red” strategy leads to sub–triangles which are all similar to one of the given coarse mesh triangles. We suppose that T was calculated in a stable way on these coarse mesh triangles, then all Jacobians on all finer triangles are multiples of the Jacobian of its father triangle (for suitable node numbering), which stabilizes this procedure totally.

For this purpose we save the four values of T additionally to the data structure for storing the element. During the “red” subdivision of an element K we calculate the 4 Jacobians of the son elements from T. Let $x^{(0)}, x^{(1)}, x^{(2)}$ the vertices of K, then the 4 sons have to be defined as (see Fig. 1)

$$\begin{array}{llll} K_1: & x^{(0)} & x^{(01)} & x^{(02)} \\ K_2: & x^{(01)} & x^{(1)} & x^{(12)} \\ K_3: & x^{(02)} & x^{(12)} & x^{(2)} \\ K_4: & x^{(12)} & x^{(02)} & x^{(01)} \end{array}$$

Following [Mey01, Mey03] the Jacobians are $\frac{1}{2}T$ (for K_1, K_2, K_3) and $-\frac{1}{2}T$ (for K_4), which is totally free of rounding errors.

Now, let us consider a curved boundary, which is approximated on each triangle as a straight line. Then (see Fig. 3), the Jacobians of the son elements are no simple multiples of T.

Let $x^{(01)} = (x^{(0)} + x^{(1)})/2$ and $x^{(02)} = (x^{(0)} + x^{(2)})/2$, but let $x^{(12)}$ the node on the curved boundary, so $x^{(12)} \neq \tilde{x}^{(12)} := (x^{(1)} + x^{(2)})/2$. If we suppose that a vector d has been calculated in a stable manner, such that $x^{(12)}$ is defined as $x^{(12)} = \tilde{x}^{(12)} + d$, then the Jacobians of the son elements are stable given from $T^T = (x^{(1)} - x^{(0)} \vdots x^{(2)} - x^{(0)})$ and d :

$$\begin{aligned}
T_1^T &= (x^{(01)} - x^{(0)} \vdots x^{(02)} - x^{(0)}) = \tfrac{1}{2}T^T \,, \\
T_2^T &= (x^{(1)} - x^{(01)} \vdots x^{(12)} - x^{(01)}) = \\
&= (x^{(1)} - x^{(01)} \vdots \tilde{x}^{(12)} - x^{(01)} + d) = \tfrac{1}{2}T^T + (0 \vdots d) \,, \\
T_3^T &= (x^{(12)} - x^{(02)} \vdots x^{(2)} - x^{(02)}) = \tfrac{1}{2}T^T + (d \vdots 0) \quad \text{and} \\
T_4^T &= (x^{(02)} - x^{(12)} \vdots x^{(01)} - x^{(12)}) = -\tfrac{1}{2}T^T - (d \vdots d)
\end{aligned}$$

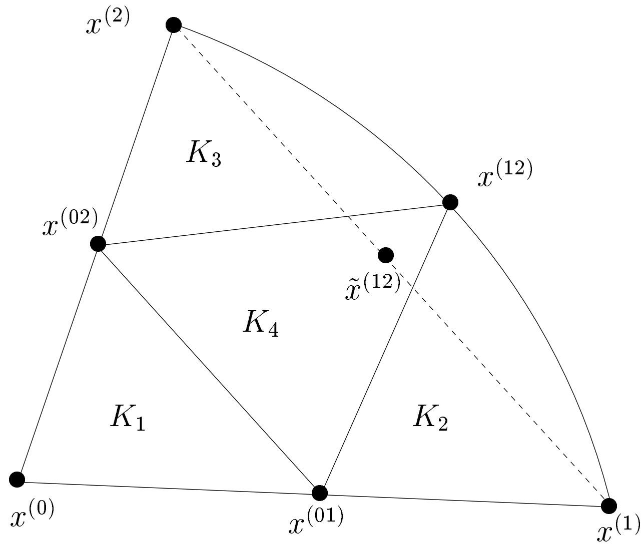

Figure 3:“red” subdivision of a triangle on a curved boundary

The formulas for defining the Jacobians T_i of the son elements K_i are stable (rounding error on last digits only) if we are able to compute the vector d in a stable manner. This is shown in Chapter 7 for circular boundaries.

5 Stable calculation of T for quadratic triangles on a curved boundary

Obviously, the boundary approximation is much better in using 6-node quadratic triangles. That is, we use the nodes $x^{(0)}, x^{(1)}, x^{(2)}$ (vertices) and $x^{(01)} = x^{(3)}, x^{(02)} = x^{(4)}$ and $x^{(12)} = x^{(5)}$ (edge nodes) for defining the shape of the quadratic element K and have the mapping (1) with the quadratic form functions $N_i(\hat{x}) \quad (i = 0, ..., 5)$. Then $T(\hat{x})$ is a function of $\hat{x} \in \hat{K}$, but it depends on T and d only. So, under the assumptions above we have a stable formula for $T(\hat{x})$ as well:

Lemma 1: With $q(\hat{x}) = (\hat{x}_2, \hat{x}_1)^T$, $d = x^{(12)} - \tilde{x}^{(12)}$ and $T^T = (x^{(1)} - x^{(0)} \vdots x^{(2)} - x^{(0)})$ we have

$$T(\hat{x}) = T + 4\, q(\hat{x})\, d^T \tag{7}$$

Proof: If all three edge nodes are exact side mid-nodes (i.e. $x^{(12)} = \tilde{x}^{(12)}$) then from direct calculation in (2) we have $T(\hat{x}) = T$ (constant w.r.t. $\hat{x}$). Using $x^{(5)} = x^{(12)} = \tilde{x}^{(12)} + d$ in (2) we obtain

$$T(\hat{x}) = T + \hat{\nabla} N_5(\hat{x})\, d^T$$

which is the desired result ($N_5(\hat{x}) = 4\hat{x}_1\hat{x}_2$).

The subdivision of this element K into the 4 son elements as in Fig.3 leads to a stable calculation of the Jacobians of K_i from combining the results of the previous section with the above lemma:

The son elements K_1 and K_4 have no curved edge anymore, hence

$$T_1 = \tfrac{1}{2}T \qquad \text{and} \qquad T_4 = -\tfrac{1}{2}T - (d \vdots d)^T$$

as in the linear case. The definition of the other two elements requires first the definition of the new nodes on the curved boundary, by giving the vectors d_2 and d_3 in a stable manner:
Here, in K_2 the 6th node is defined by $\frac{1}{2}(x^{(1)} + x^{(12)}) + d_2$ and in K_3 as $\frac{1}{2}(x^{(2)} + x^{(12)}) + d_3$. This leads to

$$T_2(\hat{x}) = \frac{1}{2}T + (0 \vdots d)^T + 4\, q(\hat{x})\, d_2^T$$

and

$$T_3(\hat{x}) = \frac{1}{2}T + (d \vdots 0)^T + 4\, q(\hat{x})\, d_3^T \ .$$

6 The case of "green" subdivisions

For "green" subdivisions the same calculations as in the previous chapters lead to stable formulas for the Jacobians T_1 and T_2 for the son triangles. In case (a) (see Fig. 4) the curved boundary is not the subdivision edge, then the rules of [Mey01, Mey03] remain valid:

$$T_1^T = (x^{(2)} - x^{(0)} \vdots x^{(01)} - x^{(0)}) = T^T \begin{pmatrix} 0 & 1/2 \\ 1 & 0 \end{pmatrix}$$

$$T_2^T = (x^{(2)} - x^{(1)} \vdots x^{(01)} - x^{(1)}) = T^T \begin{pmatrix} -1 & -1/2 \\ 1 & 0 \end{pmatrix},$$

if the son elements are defined as

$$\begin{array}{llll} K_1: & x^{(0)} & x^{(2)} & x^{(01)} \\ K_2: & x^{(1)} & x^{(2)} & x^{(01)} . \end{array}$$

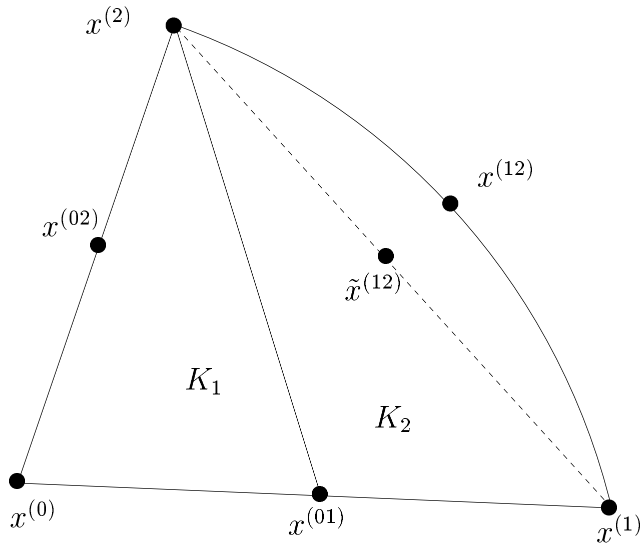

Figure 4:“green” subdivision of a triangle on a curved boundary, case (a)

In case (b) (see Fig. 5) the curved edge (again the first edge $(x^{(0)}, x^{(1)})$) is subdivided creating the two curved son triangles

$$\begin{array}{llll} K_1: & x^{(0)} & x^{(2)} & x^{(01)} \\ K_2: & x^{(1)} & x^{(2)} & x^{(01)} . \end{array}$$

Then these formulas require the correction

$$\begin{aligned} T_1^T &= (x^{(2)} - x^{(0)} \vdots x^{(01)} - x^{(0)}) = \\ &= (x^{(2)} - x^{(0)} \vdots \tilde{x}^{(01)} - x^{(0)} + d) = T^T \begin{pmatrix} 0 & 1/2 \\ 1 & 0 \end{pmatrix} + \Big(0 \vdots d\Big) \\ T_2^T &= (x^{(2)} - x^{(1)} \vdots x^{(01)} - x^{(1)}) = T^T \begin{pmatrix} -1 & -1/2 \\ 1 & 0 \end{pmatrix} + \Big(0 \vdots d\Big) . \end{aligned}$$

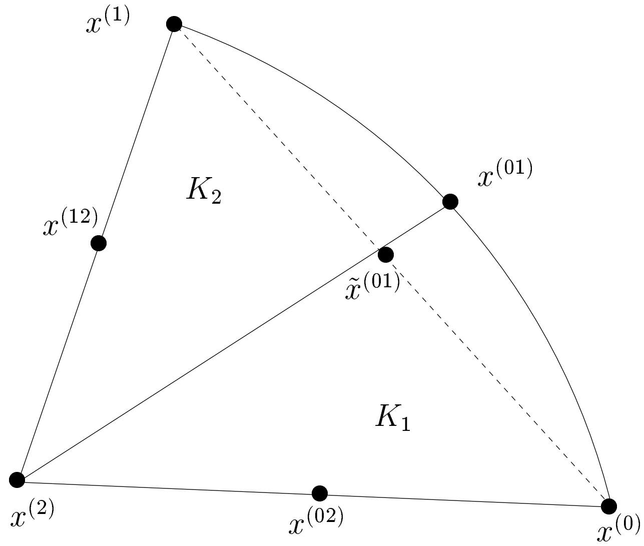

Figure 5:“green” subdivision of a triangle on a curved boundary, case (b)

In case of quadratic 6-node triangles these formulas are improved as in Chapter 5.

7 The stable calculation of the difference vector d for circular arcs

From the previous chapters, we found the necessity to have a formula for the stable calculation of the vector $d = x^{(12)} - \tilde{x}^{(12)}$ for a given curved boundary Γ (according to Fig.3 or Fig.4),

$$\tilde{x}^{(12)} = \frac{1}{2}(x^{(1)} + x^{(2)}) \ , \quad x^{(12)} \in \Gamma.$$

Here, we consider the most important special case of Γ being a circular arc. For defining Γ we assume that the midpoint m and the radius ρ are fixed (from $x^{(1)} \in \Gamma$ or $x^{(2)} \in \Gamma$ the radius could be obtained from $\|x^{(1)} - m\|$ as well, but m has to be given as extra information on Γ). Let the node $x^{(12)} \in \Gamma$ be defined as mid-node between $x^{(1)}$ and $x^{(2)}$ w.r.t. the arc length. Additionally, as shown in the previous chapters, we suppose that

$$T^T = (x^{(1)} - x^{(0)} \vdots x^{(2)} - x^{(0)}) \tag{8}$$

has been given in a stable manner. Then the vector $x^{(2)} - x^{(1)}$ is defined from the difference of the columns of T^T without cancellation of leading digits, because both columns can be small, but never near to collinear.
Now, d will be calculated by stable formulas from $\xi = \|x^{(2)} - x^{(1)}\|$ and $(\tilde{x}^{(12)} - m)$:

Lemma 2: The desired vector d and the node $x^{(12)} = \tilde{x}^{(12)} + d$ are calculated by the stable formulas:

$$d = \frac{\tilde{x}^{(12)} - m}{\|\tilde{x}^{(12)} - m\|} \cdot \delta \tag{9}$$

with

$$\delta = \frac{(\xi/2)^2}{\rho + \sqrt{\rho^2 - (\xi/2)^2}} \tag{10}$$

Proof: The midpoint of the circle m is "far away" from the points $x^{(1)}, x^{(2)}$ and $\tilde{x}^{(12)}$. Hence, the direction of d, the vector $\tilde{x}^{(12)} - m$, is obtained without dangerous cancellation of leading digits. The length $\delta = \|d\|$ follows from Pythagoras in the triangle $(m, x^{(1)}, \tilde{x}^{(12)})$:

$$(\rho - \delta)^2 + (\xi/2)^2 = \rho^2$$

which yields the stable formula (10) for δ.

8 Numerical Results

For demonstrating the above results, we consider the following model diffusion problem

$$\begin{cases} -\Delta u = 0 & \text{in} & \Omega & \\ u = 0 & \text{on} & \Gamma_{D,1} & \text{(left boundary)} \\ u = 1 & \text{on} & \Gamma_{D,2} & \text{(right boundary)} \\ \frac{\partial u}{\partial n} = 0 & \text{on} & \Gamma_N & \text{(the rest)} \end{cases}$$

within a domain with two circular curves meeting in a re-entrant corner (see in Fig.6 the mesh after some mesh refinement steps).

From the re–entrant corner with $270°$ interior angle, we have a serious singularity at this point, hence the mesh refinement has to be done near this point.This requires subdivisions of curved triangles in each of the adaptive refinement steps. We have used the same error estimator as in [Mey01, Mey03]. Each subdivision of a straight line triangle defines the Jacobians of its sons directly as in [Mey01, Mey03]. Then the error decrease is limited up to about 15 000 unknowns as seen in Fig. 8 from increasing instabilities on the Jacobians of the curved triangles.

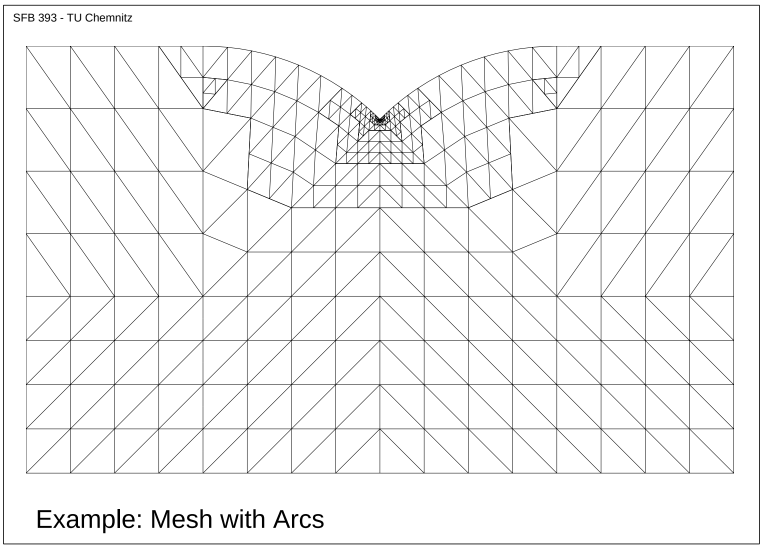

Figure 6: Mesh after some refinement

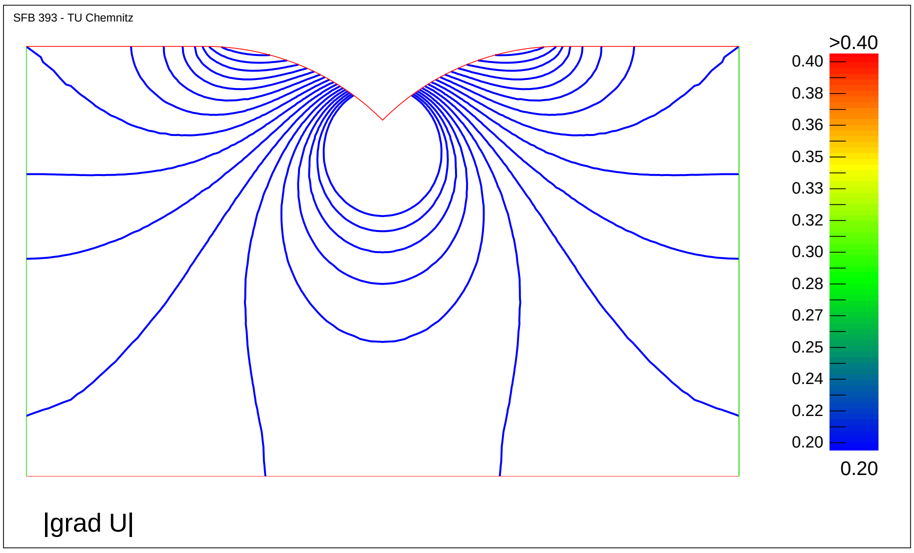

Figure 7: Isolines of $|\nabla u|$

We have plotted the value of the error estimator over the degrees of freedom for three different mesh refinement strategies. These are (see [Mey01, Mey03]) the Bänsch strategy ("Bg"), a strategy with red and green subdivisions mixed ("rg") and using only red subdivisions together with hanging nodes ("hn",as in the mesh in Fig. 6). We used 6–node quadratic triangles on the tests. The instabilities occurred in each of the strategies with different effects, such as zero determinant of a Jacobian and stop (vertical line in Fig. 8) or absurd error growth and coarsening as seen in Fig. 8.

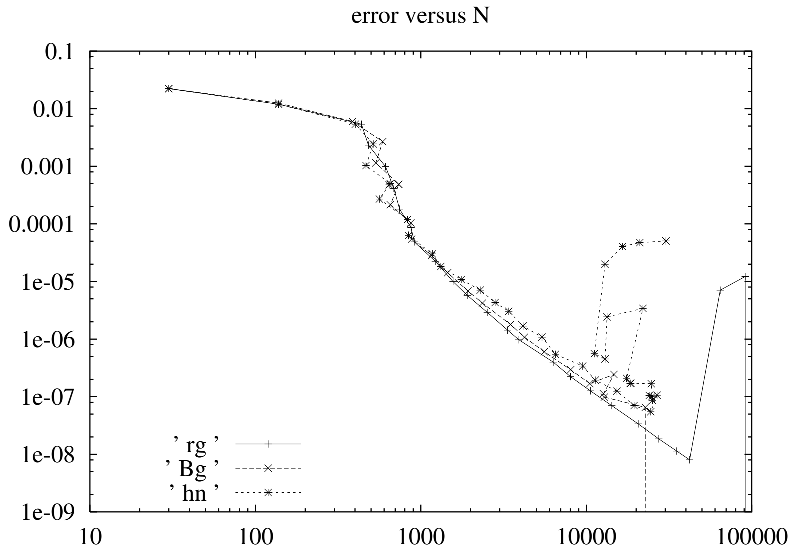

Figure 8: Error decrease without stable Jacobians on the curved boundary

Using additionally the formulas of the previous chapters on the curved triangles the expected behavior of the error development is reestablished as seen in Fig. 9.

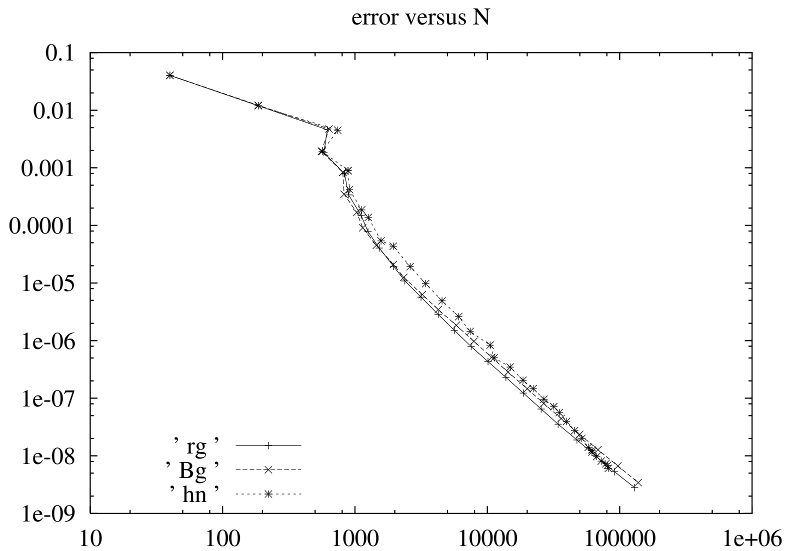

Figure 9: Error decrease with stable Jacobians on the curved boundary

9 Conclusion

The classical element routines in finite element codes can lead to break downs if they are used in an adaptive regime. The reason is the possibly unstable calculation of the Jacobian matrices due to serious cancellations of leading digits of nodal coordinates. We avoid a restricted accuracy of the method, by calculating stable Jacobian matrices on the coarse mesh. These are inherited to finer elements during the subdivision. This is easily done on straight line triangles but requires more information and work on curved boundaries. Here, we presented a way out for circular arcs.

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