Integrating Composed Singularities using Non-uniform Subdivision and Extrapolation.

Kristoffer Singstad [a] and Terje O. Espelid [b]

[a] *ISI AS, Kanalveien 119, 5059 Bergen, Norway*

[b] *Institutt for informatikk, Universitetet i Bergen, Høyteknologisenteret, 5020 Bergen, Norway*

Abstract

An approach to the computation of approximations to multidimensional integrals over an n-dimensional hyper-rectangular region, when the integrand has a composed singularity, is described. This approach is based on nested applications of a recently published non-uniform subdivision technique of the region of integration. The technique fits well to the sub-division strategy used in many adaptive algorithms. As in the non-composed problems the technique turns out to have good numerical stability properties. A two dimensional experimental code is used to demonstrate the power of this approach.

Key words: Numerical integration, multidimensional quadrature, singular integrands, extrapolation, non-uniform subdivision, homogeneous functions.

1 Introduction

The first paper that addresses the problem of finding the error functional expansion in multidimensional quadrature with a singular integrand function was published in 1976 by Lyness [11]. Knowing such expansions are essential in order to compute such integrals effectively. Since 1976 several related papers have appeared, some giving expansions for different regions and others giving expansions for different types (or combinations) of singular behavior [4–6,10,12–15,17]. These expansions are all based on a *uniform* subdivision of the region and application of the same rule on each subregion.

In two papers Espelid [7,8] describes a new idea applying extrapolation on a sequence of estimates produced through a *non-uniform* subdivision of the initial region. The first of these papers addresses n-dimensional problems having vertex singularities associated with homogeneous functions. In the second

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paper this new approach is extended to include problems with line singularities in 2 dimensions, line or face singularities in 3 dimensions and subregion (line, face , etc.) singularities in n-dimensions. In order to achieve this generalization the region of integration has to be restricted to an n-dimensional hyperrectangle.

In a third paper Espelid and Genz [9] present software based on [1,2,7] which combines an adaptive subdivision strategy with this non-uniform extrapolation idea.

In [7–9] it was necessary to restrict the problem class to integrands with one singularity only. In a recent master thesis Singstad [16] demonstrates how this approach may be applied in a nested way to handle composed singularities in two dimensions. In this paper we will describe the approach for the two dimensional full corner singularity and indicate how this may be extended to an n-dimensional problem with a composed singularity.

This paper is organized as follows: in the next section we present the problem and develop the basic error expansion. Then we describe the subdivision approach and finally we give some examples and concluding remarks. The presentation of ideas in the composed setting is quite similar to those given in [7,8].

2 Homogeneous functions: basic error expansion

A function $f(\mathbf{x})$, where $\mathbf{x} \in R^n$, is said to be homogeneous of degree α (about the origin) if

$$f(\lambda \mathbf{x}) = \lambda^\alpha f(\mathbf{x}) \text{ for } \forall\ \lambda > 0.$$

The notation introduced by Lyness (1976), [11], is useful and we denote such a function $f_\alpha(\mathbf{x})$. This notation implies the following simple rules: $f_\alpha f_\beta$ is of homogeneous of degree $\alpha + \beta$ and $(f_\alpha)^\beta$ is of homogeneous of degree $\alpha\beta$.

In order to simplify the presentation we will restrict ourselves to a full corner singularity in a two-dimensional integration problem over a rectangle. We will assume that the singularities are caused by a homogeneous function about the origin.

An affine transformation may be used to transform the given rectangular region on to the unit square. Any homogeneous function will still be homogeneous after such a transformation and its degree will be invariant. It is well known that any given cubature rule can be transformed as well and its polynomial degree will be invariant too. Choosing the unit square, C_2, as the region of integration represents therefore no restriction

$C_2 : 0 \leq x \leq 1$ and $0 \leq y \leq 1$.

Define

$$I(f) = \int_{C_2} f(x,y)\; dx\; dy = \int_0^1 \int_0^1 f(x,y)\; dx\; dy. \tag{1}$$

We will discuss how to compute numerical estimates to integration problems of type (1), where the function involved, f, is a product of a homogeneous function $f_{\alpha+\beta+\gamma}(x,y) = c_\alpha(x) d_\beta(y) e_\gamma(x,y)$ and a function $g(x,y)$ which is regular in C_2. The function $e_\gamma(x,y)$ is assumed to have a pure point singularity at the origin of C_2 due to the homogeneous property, while both $c_\alpha(x)$ and $d_\beta(y)$ are homogeneous around the origin of degree α and β respectively. Thus we get

$$\begin{cases} f_{\alpha+\beta+\gamma}(\lambda x, \lambda y) = \lambda^{\alpha+\beta+\gamma} f(x,y) \\ g(0,0) \neq 0, \end{cases}$$

Furthermore we assume that the origin is the only point where $c_\alpha(x)$, $d_\beta(y)$ and $e_\gamma(x,y)$ are non-analytic. We give three examples to illustrate the type of singular problems we will be able deal with using the non-uniform approach.

A) A combination of two line singularities, possibly of different strengths, along the axes and a corner singularity at the origin (a full corner problem),

$$\int_{C_2} x^\alpha y^\beta (x+y)^\gamma g(x,y)\; dxdy \text{ with } \alpha, \beta > -1 \text{ and } \alpha + \beta + \gamma > -2.$$

B) It is possible to handle a logarithmic singularities as well, e. g. we may add to the difficulties i example A) say

$$\int_{C_2} x^\alpha y^\beta (x+y)^\gamma \ln r\; g(x,y)\; dxdy \text{ with } \alpha, \beta > -1 \text{ and } \alpha + \beta + \gamma > -2,$$

where $r = \sqrt{x^2 + y^2}$.
C) A corner singularity in C_3 , with $r = \sqrt{x^2 + y^2 + z^2}$, combined with a line and a face singularity

$$\int_{C_3} r^\gamma x^\alpha (x+y)^\beta\; g(x,y,z)\; dxdydz$$

with $\alpha > -1, \alpha + \beta > -2$ and $\alpha + \beta + \gamma > -3$.

Following the uniform strategy, analyzed by Lyness and others, we may subdivide the original square in m^2 equal squares and then use the same rule Q over all these squares. Denoting the compound rule $Q^{(m)}$ we get, Sidi (1983) [15] and Lyness and de Doncker-Kapenga (1987) [13] and Verlinden and Haegemans (1993) [17]

$$Q^{(m)}(f) \sim I(f) + \sum_{\ell \geq 0} \frac{A_\ell + B_\ell \log m}{m^{\alpha+\beta+\gamma+2+\ell}} + \sum_{\ell \geq 0} \frac{C_\ell + D_\ell \log m}{m^{\alpha+1+\ell}} + \sum_{\ell \geq 0} \frac{E_\ell + F_\ell \log m}{m^{\beta+1+\ell}} + \sum_{\ell \geq 1} \frac{G_\ell}{m^\ell}. \tag{2}$$

For many integrals, some of the coefficients in (2) vanish e.g., the D-coefficients vanish if α is non-integer or if a special rule Q is used; some of the G-coefficients may vanish depending on the degree of precision and symmetry of Q. Finally, concatenation of terms in the series may occur if two or more m-exponents become equal. Based on (2) we may now compute $Q^{(m)}$ for different values of m and then use extrapolation to improve these approximations. This approach does not need information about where the line singularities are, however there are serious drawbacks due to the amount of work and the numerical stability with this method, [10].

We will, in what follows, present an alternative approach following [7,8]. This approach is based on a *non-uniform* subdivision of the region of integration combined with extrapolation. The non-uniform strategy, used in a nested way in our problem, makes it possible to treat the difficulties differently in the different directions of integration.

In our two-dimensional problem we know (a) that both variables are involved in the singularity, (b) the position of the vertex where the function is singular (the origin in this presentation) and (c) the three parameters α, β and γ. Define the square $C_2(h) = [0,h]^2$, with $h \leq 1$. Define

$$I_{C_2(h)}(f) = \int_0^h \int_0^h f(x,y)\; dxdy. \tag{3}$$

Assume that (x,y) is a point in C_2. Next we expand $g(x,y)$ in a Taylor series around the origin with p basic terms and a remainder term r

$$g(x,y) = g(0,0) + (x\frac{\partial}{\partial x} + y\frac{\partial}{\partial y})g(0,0) + \frac{1}{2}(x\frac{\partial}{\partial x} + y\frac{\partial}{\partial y})^2 g(0,0) + \ldots + \frac{1}{(p-1)!}(x\frac{\partial}{\partial x} + y\frac{\partial}{\partial y})^{p-1} g(0,0) + r.$$

This expression may be multiplied by $f_{\alpha+\beta+\gamma}(x,y)$ and then we may integrate over $C_2(h)$. New integration variables $x = h\,u$ and $y = h\,v$ moves all integrals to C_2 and gives

$$I_{C_2(h)}(f_{\alpha+\beta+\gamma}g) \ = c_0\ h^{\alpha+\beta+\gamma+2} + \sum_{\ell=1}^{p-1} c_\ell\ h^{\alpha+\beta+\gamma+2+\ell} + O(h^{\alpha+\beta+\gamma+2+p}), \quad (4)$$

with

$$\begin{cases} c_0 = \int_{C_2} f_{\alpha+\beta+\gamma}(x,y)g(0,0)\ dx\ dy, \\ c_\ell = \frac{1}{\ell!}\int_{C_2} f_{\alpha+\beta+\gamma}(x,y)(x\frac{\partial}{\partial x} + y\frac{\partial}{\partial y})^\ell g(0,0)\ dx\ dy, \quad \ell = 1,2,\ldots p-1. \end{cases}$$

The fact that the term ℓ involves functions which are of homogeneous degree $\alpha+\beta+\gamma+\ell$ in C_2 about the origin has been used.

Given a fixed cubature rule Q on a rectangle, R, using L evaluation points

$$Q_R(f) = \sum_{i=1}^{L} w_i\ f(x_i, y_i).$$

If $\sum_{i=1}^{L} w_i$ equals the area of rectangle R then the rule Q has degree of precision at least 0. The evaluation points (x_i, y_i) are assumed to be translated to R. The rule may be applied on f over $C_2(h)$ giving

$$Q_{C_2(h)}(f_{\alpha+\beta+\gamma}g) = b_0\ h^{\alpha+\beta+\gamma+2} + \sum_{\ell=1}^{p-1} b_\ell\ h^{\alpha+\beta+\gamma+2+\ell} + O(h^{\alpha+\beta+\gamma+2+p}), \quad (5)$$

where

$$\begin{cases} b_0 = Q_{C_2}(f_{\alpha+\beta+\gamma}(x,y)g(0,0), \\ b_\ell = \frac{1}{\ell!}Q_{C_2}(f_{\alpha+\beta+\gamma}(x,y)(x\frac{\partial}{\partial x} + y\frac{\partial}{\partial y})^\ell g(0,0)), \\ \ell = 1,2,\ldots p-1. \end{cases}$$

The term ℓ involves functions which are of homogeneous degree $\alpha+\beta+\gamma+\ell$ in C_2 and applying Q over $C_2(h)$ is a simple h-scaling of C_2 in the two variables. This implies that the area and the weights w_ℓ must be scaled by a h^2 factor. (4) and (5) give the error expansion

$$\begin{aligned} E_2(h) &= |Q_{C_2(h)}(f_{\alpha+\beta+\gamma}g) - I_{C_2(h)}(f_{\alpha+\beta+\gamma}g)| \\ &= \sum_{\ell=0}^{p-1} a_\ell\ h^{\alpha+\beta+\gamma+2+\ell} + O(h^{\alpha+\beta+\gamma+2+p}), \end{aligned} \quad (6)$$

with

$$a_\ell = b_\ell - c_\ell,\ \ell = 0,1,\ldots,p-1.$$

b_ℓ is the numerical estimate produced by the rule Q of the integral c_ℓ and the functions involved will become smoother with increasing values of ℓ. Therefore it is reasonable to expect $|a_\ell| >> |a_{\ell+1}|$, at least as long as $\alpha + \beta + \gamma + 2 + \ell \leq \text{degree}(Q)$.

The extrapolation scheme will, just as in [7,8], be based the error expansion (6). In fact, we assume that the error given in (6) will be the major error source in the estimate of $I(f)$. The error contribution from the rest of the original region C_2 has to be handled too, being aware of the two line singularities present. We will handle these problems with the same technique and finally show how the error in each subregion will influence the extrapolation process and the final global estimate of $I(f)$.

3 The Series with Tail-correction Approach

We will now use the error expansion developed in the previous section combined with the series with tail-correction approach presented in [8]. Let us, through an adaptive procedure, repeatedly cut out squares $C_2(h_i)$, with $h_i = 1/2^i$, for $i = 0, 1, 2, \ldots, k$. Define

$$\begin{cases} I_i = I_{C_2(h_i)}(f_{\alpha+\beta+\gamma}g), \; i = 0, 1, 2, \ldots, k, \\ Q_i = Q_{C_2(h_i)}(f_{\alpha+\beta+\gamma}g), \; i = 0, 1, 2, \ldots, k, \\ U_i = I_{i-1} - I_i, \; i = 1, 2, \ldots, k, \\ S_k = \sum_{i=1}^k U_i, \; \hat{S}_k = \sum_{i=1}^k \hat{U}_i, \end{cases} \tag{7}$$

where $\hat{U}_i$ and Q_i are approximations to U_i and I_i respectively. The sequence $U_1, U_2, \ldots$ are by definition (7) integrals over a sequence of subregions, $L_2(h) = [0, 2h] \times [h, 2h] \cup [h, 2h] \times [0, h]$ for a given value of h. I_0 is the original integral. In Figure 1 we illustrate the subregion sequences in 2 dimensions:

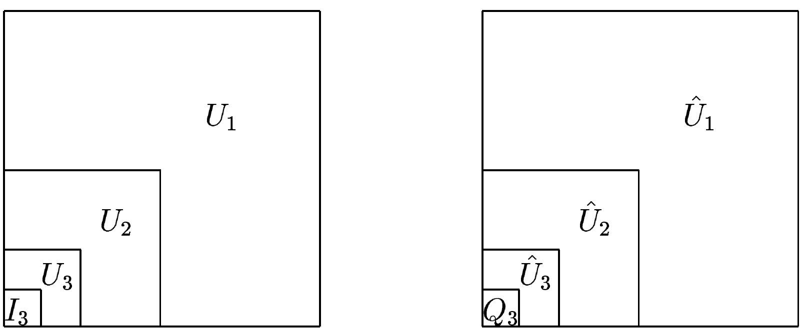

Fig. 1. Corner singularity:(a) U and I-sequences, (b) $\hat{U}$ and Q-sequences

The definition of U_i gives $S_k = I_0 - I_k$. S_k may be viewed as an approximation to I_0 with error $-I_k$. Observe that we have to approximate U_i, e. g.: in order to apply the basic cubature rule we have to divide the U-region into two rectangles. Due to accuracy requirement we may even have to subdivide further. Following [8] we may improve the approximation $\hat{S}_k$ by adding the tail Q_k defining

$$T_{i0} = Q_i + \sum_{\ell=1}^{i} \hat{U}_\ell, \; i = 0, 1, 2, \ldots, k.$$

T_{i0} is an approximation to I_0 and we have according to (6)

$$T_{i0} - I_0 = \sum_{\ell=1}^{i} E_{\hat{U}_\ell} + \sum_{\ell=0}^{p-1} a_\ell h_i^{\alpha+\beta+\gamma+2+\ell} + O(h_i^{\alpha+\beta+\gamma+2+p}), \tag{8}$$

where $E_{\hat{U}_\ell} = \hat{U}_\ell - U_\ell$. Richardson extrapolation may be used on (8) to eliminate the k first terms in the sum of h-powers. Let

$$n_1 = 2^{\alpha+\beta+\gamma+2} - 1, \; n_{j+1} = 2n_j + 1, \; j = 1, 2, 3, \ldots,$$

and

$$T_{ij} = T_{i,j-1} + (T_{i,j-1} - T_{i-1,j-1})/n_j, i = 1, 2, \ldots, k, \; j = 1, 2, 3, \ldots, i. \tag{9}$$

Putting the T_{ij} in a standard extrapolation tableau

$$\begin{array}{llll} T_{00} & & & \\ T_{10} & T_{11} & & \\ \vdots & \vdots & \ddots & \\ T_{k0} & T_{k1} & \cdots & T_{kk} \end{array}$$

gives after j extrapolation steps in row k

$$T_{kj} = I_0 + \sum_{\ell=j}^{p-1} a_\ell^{(j)} h_k^{\alpha+\beta+\gamma+2+\ell} + O(h_k^{\alpha+\beta+\gamma+2+p}) + \sum_{\ell=1}^{k} (1 - \beta_{k+1-\ell,j}) E_{\hat{U}_\ell}. \tag{10}$$

We refer the reader to [8] for more details about these $\beta-$coefficients. The important point to be made is that these coefficients may be computed and make it possible to keep track of the effect of not knowing each U_ℓ exactly. We can through this expression control the effect of these errors on the extrapolation process and compute a better approximation to at least one these U_ℓs whenever needed.

Computing these $\hat{U}$-terms, in view of the fact that we have line-singularities present in the problem, is a task that needs extra attention.

4 Computing the $\hat{U}$-terms

Define $R(h) = [0,h] \times [h,2h]$ and $S(h) = [h,2h] \times [0,2h]$ then $L(h) = R(h) \cup S(h)$. A typical U-term is given as an integral over an L-shaped region depending on the parameter h and may be written as follows

$$\begin{cases} V = \int_{R(h)} (f_{\alpha+\beta+\gamma} g) dxdy \\ W = \int_{S(h)} (f_{\alpha+\beta+\gamma} g) dxdy \\ U = V + W \end{cases} \tag{11}$$

The computational difficulties associated with V and W are similar: both integrals have a line-singularity along one of the sides and such problems can be dealt with using the ideas in [7]. We have indicated how to do this in $R(h)$ creating a sequence $V_1, V_2, ...$ which are integrals over regions as indicated in Figure 2.

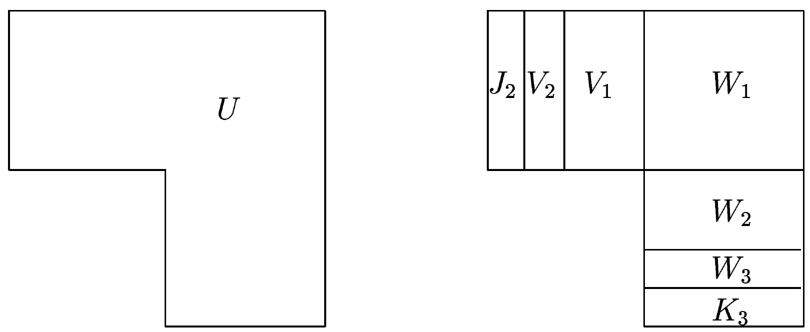

Fig. 2. The U-region $L(h)$, subdivided in V- and W-regions.

Defining $R_i = [0, h/2^i] \times [h, 2h]$, $i = 0, 1, \ldots$ and $\tilde{h}_i = h/2^i$ then we may define T_{i0}^{α} as the tail approximation to J_0 giving the expansion

$$T_{i0}^{\alpha} - J_0 = \sum_{\ell=1}^{i} E_{\hat{V}_\ell} + \sum_{\ell=0}^{p-1} \tilde{a}_\ell \tilde{h}_i^{\alpha+1+\ell} + O(\tilde{h}_i^{\alpha+1+p}), \tag{12}$$

where $E_{\hat{V}_\ell} = \hat{V}_\ell - V_\ell$. By standard linear extrapolation we may use (12) to eliminate the k first terms in the sum of h-powers. Thus we reduce the effect of the singularity along the y-axis with strength α through this extrapolation process and finally we compute a good approximation of V, possibly through an adaptive handling of the V_i terms. This procedure has to be followed for all $R(h)$ regions produced through the approximation of the U-terms used in the series with tail correction toward the corner singularity.

Similarly we may approximate W: the $S(h)$ region has a line singularity along the x-axis of strength β and by repeatedly halving the region toward the x-axis we produce estimates $\hat{W}_1, \hat{W}_2, \ldots$ and tail estimates $Q_0^\beta, Q_1^\beta \ldots$ to be used in the extrapolation process. Defining $\bar{h}_j = 2h/2^j$ we may define T_{j0}^β as the tail approximation to K_0 giving the expansion

$$T_{j0}^\beta - K_0 = \sum_{\ell=1}^{j} E_{\hat{W}_\ell} + \sum_{\ell=0}^{p-1} \bar{a}_\ell \bar{h}_j^{\beta+1+\ell} + O(\bar{h}_j^{\beta+1+p}), \tag{13}$$

where $E_{\hat{W}_\ell} = \hat{W}_\ell - W_\ell$.

We observe that there will be a number of extrapolation tableaus: having k U-terms in the tableau for the corner singularity then each U-term will need two tableaus, α and β, giving a total of $2k+1$ extrapolation tableaus. All tableaus may have different sizes in order to be extrapolation-adaptive. An alternative procedure would be to force all such local tableaus to have the same length and thus reduce the number of such tableaus to one along each axis. This way one would loose the extrapolation-adaptive property, but save on the number of extrapolation tableaus one has to handle. In addition there are a number of subregions associated with say V_i and W_j that might need further subdivision in an adaptive strategy.

5 A global adaptive algorithm

In order to describe the algorithmic structure we need, in addition to the weights and coordinates of the basic rule for a rectangle, Q_R, a way to compute an error bound, $B_R \geq |E_R|$, where E_R is the true error we get by applying this rule to the a given rectangle and function $f(x, y)$. Furthermore we need to estimate the pure extrapolation errors, say $X_{T_{kk}}$, associated with diagonal elements in the extrapolation tableaus. We will not discuss how to compute the error bounds B_R and $X_{T_{kk}}$ in this paper and refer the interested reader instead to [1,2,9]. Finally we have to combine all these errors in order to estimate the global error. Based on (12) and (13) and local extrapolation giving expressions similar to (10), we get the following two estimates over region $R(h)$ and $S(h)$

respectively, associated with the term m in the U sequence

$$\begin{cases} B_V^{m,i} = \sum_{\ell=1}^{i} |1-\tilde{\beta}_{i+1-\ell,i}| B_{\hat{V}_\ell}^m \\ B_W^{m,j} = \sum_{\ell=1}^{j} |1-\bar{\beta}_{j+1-\ell,j}| B_{\hat{W}_\ell}^m \\ E_{T_{ii}^{m,\alpha}} = X_{T_{ii}^{m,\alpha}} + B_V^{m,i} \\ E_{T_{jj}^{m,\beta}} = X_{T_{jj}^{m,\beta}} + B_W^{m,j} \end{cases} \tag{14}$$

We have used different indices i and j in order to indicate that the number of extrapolation levels may differ. Furthermore the indices i and j depend on the index m (a fact that we suppress in the notation). $T_{ii}^{m,\alpha}$ and $T_{jj}^{m,\beta}$ are the two integral estimates over $R(h)$ and $S(h)$ respectively, associated with U-term number m. $B_{\hat{V}_\ell}^m$ are the sum of all error-bounds over all subregions that may have been used in the subregion-adaptive strategy for the basic region that the term refers to, and similarly for $B_{\hat{W}_\ell}^m$. Now, $\hat{U}_\ell$ and the overall error may be written

$$\begin{cases} \hat{U}_\ell = T_{ii}^{\ell,\alpha} + T_{jj}^{\ell,\beta} \\ B_{\hat{U}_\ell} = E_{T_{ii}^{\ell,\alpha}} + E_{T_{jj}^{\ell,\beta}} \\ Y_k = \sum_{\ell=1}^{k} |1-\beta_{k+1-\ell,k}| B_{\hat{U}_\ell} \\ E_{T_{kk}} = X_{T_{kk}} + Y_k \end{cases} \tag{15}$$

Y_k represents the worst case extrapolation effect on the error-bounds for each U-term.

A Globally Adaptive Cubature Algorithm

Initialize: Given the original rectangle, the basic rule, α, β and γ;

Compute Q_k, Q_k^α and Q_k^β for $k = 0$ and 1,

$\hat{V}_1^1$ and $\hat{W}_1^1$ and error-bounds $B_{\hat{V}_1^1}$ and $B_{\hat{W}_1^1}$;

Initialize the non-singular subregion collection;

Extrapolation: compute $T_{1,1}^{1,\alpha}$, $T_{1,1}^{1,\beta}$ and the local error estimates;

Compute $\hat{U}_1$ and the local error $E_{\hat{U}_1}$;

Put $k = 1$, compute $T_{k,k}$ and the global error estimate $E_{T_{k,k}}$;

Control: **while** $E_{T_{k,k}} >$ tolerance **do**

if $X_{T_{k,k}} > Y_k$ **then**

Global step Take a new global extrapolation step:

Put $h = h/2$, $k = k+1$, compute Q_k, $Q_\ell^{k,\alpha}$, $Q_\ell^{k,\beta}$, $\ell = 0, 1$,

$\hat{V}_1^{k,\alpha}$, $\hat{W}_1^{k,\beta}$ and $\hat{U}_k = T_{1,1}^{k,\alpha} + T_{1,1}^{k,\beta}$;

Compute a new global estimate $T_{k,k}$ and error $E_{T_{k,k}}$;

Update the non-singular subregion collection with two new regions;

else

Pick the term $\hat{U}_\ell$ with the biggest local error, say $E_{\hat{U}_m}$;

if $E_{T_{i,i}^{m,\alpha}} > E_{T_{j,j}^{m,\beta}}$ **then**

α-step **if** $X_{T_{i,i}^{m,\alpha}} > B_V^{m,i}$ **then**

Take a new local extrapolation step in the V-region: $i = i+1$;

Update the non-singular subregion collection: one new region;

Update the global estimate and error-bound;

else

adaptive Pick the term $\hat{V}_\ell^m$ with the biggest local error, say $E_{\hat{V}_n^m}$;

step $\hat{V}_n^m$ is associated with a collection of subregions;

Find the subregion, r, with greatest error bound; Cut r in two

halves r_1 and r_2: compute Q_{r_1} and Q_{r_2} and the error-bounds;

Let r_1 and r_2 replace r in the non-singular subregion collection;

Update the local and global estimates and error-bounds;

end if

else

β-step Do the same procedure for β (W-terms) as for the α-singularity;

end if

end if

end while

6 Numerical stability: dimension 2

A cubature rule, say $Q_R(f) = \sum_{i=1}^{L} w_i f(x_i, y_i)$, over a region R is just a linear combination function values from this region. We associate a condition number with such a cubature rule, say

$$\tau_Q = \sum_{i=1}^{L} |w_i| / |\sum_{i=1}^{L} w_i|.$$

Assuming that the degree of precision for this rule is at least 0 then $\sum_{i=1}^{L} w_i = A$, where A is the area (volume) of the region R. The product $A\,\tau_Q$ is then the maximum growth-factor on the errors in the function values when applying this rule. Furthermore we note that if $w_i > 0, \forall i$, then $\tau_Q = 1$. Suppose now that a rule Q_3, applied to a region R_3, is a linear combination of two rules Q_1 and Q_2 (regions R_1 and R_2 respectively)

$$Q_3(f) = \gamma_1 Q_1(f) + \gamma_2 Q_2(f),$$

and that all three rules have degree of precision at least 0. If the cubature rules Q_1 and Q_2 are assumed to be independent (no common evaluation point) then we have the following simple computational rule for the condition numbers

$$\tau_3 = |\gamma_1| \tau_1 A_1 / A_3 + |\gamma_2| \tau_2 A_2 / A_3. \tag{16}$$

The area ratios are the relative sizes of the regions R_1 and R_2 compared to the size of the region R_3. In [8] we observed that T_{kk} can be written

$$T_{kk} = \sum_{m=1}^{k} \gamma_m^{(k)} \hat{U}_m + \sum_{m=0}^{k} \delta_m^{(k)} Q_m,$$

where the coefficients $\gamma_m^{(k)}$ and $\delta_m^{(k)}$ will depend on the value of $\alpha + \beta + \gamma + 2$. Since the terms $\hat{U}_m$ in this approach are the results of extrapolation we find

$$\begin{aligned} T_{kk} &= \textstyle\sum_{m=1}^{k} \gamma_m^{(k)} (T_{ii}^{m,\alpha} + T_{jj}^{m,\beta}) + \sum_{m=0}^{k} \delta_m^{(k)} Q_m \\ &= \textstyle\sum_{m=1}^{k} \gamma_m^{(k)} [\sum_{\ell=1}^{i} \tilde{\delta}_\ell^{(i)} Q_\ell^{m,\alpha} + \sum_{\ell=1}^{i} \tilde{\gamma}_\ell^{(i)} \hat{V}_\ell^{(m)} + \sum_{\ell=1}^{j} \bar{\delta}_\ell^{(j)} Q_\ell^{m,\beta} \\ &\quad \textstyle + \sum_{\ell=1}^{j} \bar{\gamma}_\ell^{(j)} \hat{W}_\ell^{(m)}] + \sum_{m=0}^{k} \delta_m^{(k)} Q_m. \end{aligned}$$

In order to simplify the notation we have suppressed the fact that the indices i and j both, in general, will depend on m. Since $Q_\ell^{m,\alpha}, Q_\ell^{m,\beta}, \hat{V}_\ell^{(m)}, \hat{W}_\ell^{(m)}$ and Q_m are cubatures based on different evaluation points, all with condition number 1, we can write the condition number for the cubature rule T_{kk} using the rule

(16) as follows

$$\begin{array}{l}\kappa^{(k)} = \sum_{m=1}^{k} 4^{-m}|\gamma_m^{(k)}|\ [\ \sum_{\ell=0}^{i_m}|\tilde{\delta}_\ell^{(i_m)}|2^{-\ell} + \sum_{\ell=1}^{i_m}|\tilde{\gamma}_\ell^{(i_m)}|2^{-\ell} + \\ 2(\sum_{\ell=0}^{j_m}|\bar{\delta}_\ell^{(j_m)}|2^{-\ell} + \sum_{\ell=1}^{j_m}|\bar{\gamma}_\ell^{(j_m)}|2^{-\ell})] + \sum_{m=0}^{k}|\delta_m^{(k)}|4^{-m}.\end{array} \tag{17}$$

Observe that the areas associated with the estimates $Q_\ell^{m,\alpha}, Q_\ell^{m,\beta}, \hat{V}_\ell^{(m)}, \hat{W}_\ell^{(m)}$ and Q_m, relative to the area of C_2, enter this expression. Note that this expression involves many parameters and some of these (e. g. the number of necessary extrapolation steps in a subproblem) we know only after all the extrapolation steps are finished. In order to evaluate this approach it is of interest to compute the worst case condition number and to illustrate how the condition numbers vary with the number of extrapolation steps, both on a local and global level. Therefore we have computed the condition number $\kappa^{(k)}$, using (17), for different values of $i = j$ (independent of m) and k in Table 1

Table 1
κ-table: $\alpha = \beta = \gamma = -1/2$ and $i = j$

i/k	1	2	3	4	7	10
1	18.19	10.22	10.61	7.65	5.87	5.83
2	20.99	11.57	12.30	8.97	6.97	6.92
3	19.40	10.80	11.34	8.21	6.34	6.30
4	14.76	8.58	8.54	6.02	4.52	4.49
7	7.24	4.96	3.99	2.47	1.57	1.55
10	6.01	4.37	3.24	1.88	1.09	1.07

Observe that the worst case condition number, 20.99, is associated with one global extrapolation step and two local steps (note: the maximum is the same if we allow i and j to be different and in addition vary with m). Taking several steps in both the local and global situation reduces the condition number below this maximum ; e. g. at least 4 steps both locally and globally implies a condition number less than or equal to 6.02.

The extrapolation procedure is remarkably stable and increasing the number of extrapolation steps has a positive effect on the methods stability. This comes from the fact that the extrapolations are based on approximations over successively reduced areas. Note that this good stability is in contrast to the stability properties of extrapolation based on uniform subdivision of the integration area [8,10]. We will demonstrate the effect of this difference on practical problems.

The technique described may easily be extended to handle integration of logarithmic singularities in addition to these algebraic singularities. How to do this is demonstrated and analyzed in [7,8,16]. Adding logarithmic singularities has a negative effect on the stability properties, but the nice feature of improved stability through many extrapolation steps is retained. We refer the interested reader to [7,8,16].

7 Numerical stability: dimension $s \geq 2$

In this section we will develop a general recursive expression for the condition number associated with an s-dimensional singularity. The numbers of parameters in this approach is strongly increasing with dimension and it seems as useful insight to compute sharp upper bounds for the condition numbers.

Let us start by looking at how the analysis in the previous section can be written in a recursive way and use this to compute a sharp upper bound. In [7] the condition number, τ, associated to this type of extrapolation process, when there is one singularity only of dimension, say s, was computed. Assuming that $s+\alpha = 1/2$ the following table for this condition number can be found in [7]

Table 2
τ-table for $s+\alpha = 1/2$.

s/k	1	2	3	4	7	10
1	5.83	6.92	6.30	4.49	1.55	1.07
2	5.83	4.28	3.13	1.80	1.02	1.00
3	5.83	2.96	2.15	1.24	1.00	1.00
4	5.83	2.30	1.81	1.09	1.00	1.00
5	5.83	1.97	1.67	1.04	1.00	1.00

Let us introduce the local conditions numbers, $\tau_1^{(i)}$ and $\tau_2^{(j)}$, associated with the local extrapolation processes towards one and two-dimensional non-composed singularities respectively, [8], and let furthermore $\kappa_2^{(k)}$ denote the condition number associated with the extrapolation processes for a composed singularity of dimension 2. Then (17) may be written

$$\kappa_2^{(k)} = \sum_{m=1}^{k} 4^{-m}|\gamma_m^{(k)}|[\tau_1^{(i_m)}+2\tau_1^{(j_m)}]+\sum_{m=0}^{k}|\delta_m^{(k)}|4^{-m} \leq \tau_2^{(k)}[\tau_1^{(i)}+2\tau_1^{(j)}]/3, \quad (18)$$

where the indices i, j represent the worst case local condition numbers. Now,

$\tau_1^{(i_m)}$ and $\tau_1^{(j_m)}$ are related to the line singularities , associated with α and β respectively, while $\tau_2^{(k)}$ is connected to a corner singularity, dimension 2, associated with $\alpha + \beta + \gamma$. Thus we see that the case $\alpha = \beta = \gamma = -1/2$ implies that

$$\kappa_2^{(k)} \leq \max_i \tau_1^{(i)} \max_k \tau_2^{(k)} \approx 6.92 \times 5.83 \approx 40.34$$

We observe that the upper bound 40.34, found as a product of condition numbers (which may be a useful rule of thumb in a more complex setting), is a considerable overestimate of the true condition number 20.99 in this case. The reason for this overestimate is that the condition number has two parts: one part comes from the U-terms (the series approach) and the other part comes from the Q-terms (the tail correction). When k is less than 4 then the Q-effect is dominating in our example. As k increases the effect of the Q-terms vanish: e. g. using four steps both locally and globally gives: $4.49 * 1.8 = 8.08 > 6.02$ and with 7 steps: $1.55 * 1.02 = 1.58 > 1.57$. As we see, the product estimate is fairly good when the number of steps are at least 4 in this case.

Now if we split the numbers in Table 2 in the series part, $\phi_s^{(k)}$, and a tail correction part, $\psi_s^{(k)}$, with $\tau_s^{(k)} = \phi_s^{(k)} + \psi_s^{(k)}$, we find the following two tables

Table 3
ϕ-table for $s + \alpha = 1/2$

s/k	1	2	3	4	7	10
1	1.71	1.48	1.82	1.60	1.10	1.01
2	2.56	1.23	1.55	1.21	1.00	1.00
3	2.99	0.86	1.38	1.06	1.00	1.00
4	3.20	0.61	1.32	1.01	1.00	1.00
5	3.31	0.47	1.30	0.99	1.00	1.00

Table 4
ψ-table for $s + \alpha = 1/2$

s/k	1	2	3	4	7	10
1	4.12	5.44	4.47	2.89	0.45	0.06
2	3.27	3.05	1.58	0.59	0.01	0.00
3	2.84	2.10	0.77	0.18	0.00	0.00
4	2.63	1.69	0.49	0.08	0.00	0.00
5	2.52	1.50	0.38	0.05	0.00	0.00

Using this new notation, splitting the condition number, we rewrite (18)

$$\begin{aligned}
\kappa_2^{(k)} &= \textstyle\sum_{m=1}^{k} 3 \times 4^{-m} |\gamma_m^{(k)}| [\tau_1^{(i_m)} + 2\tau_1^{(j_m)}]/3 + \sum_{m=0}^{k} |\delta_m^{(k)}| 4^{-m} \\
&\leq \max_m(\tau_1^{(i_m)}, \tau_1^{(j_m)}) \phi_2^{(k)} + \psi_2^{(k)} \\
&\leq \max_m(\tau_1^{(i_m)}, \tau_1^{(j_m)}) \max_k \phi_2^{(k)} + \max_k \psi_2^{(k)} \\
&\approx 6.92 \times 2.56 + 3.27 \approx 20.99
\end{aligned} \tag{19}$$

We observe that the upper bound becomes sharp in this case ($\alpha = \beta = \gamma = -1/2$).

In Section 2 we gave a 3 dimensional problem, C), with a composed corner singularity, a composed line singularity and finally a face singularity. In the global problem we focus on the corner singularity of dimension 3. Each U-term in this approach is an integral with a composed singularity (line + face). Assume that this integral is evaluated over 7 subcubes (of equal volume). Only three of these subcubes have singularities: one has a composed singularity and two have face singularities. The other four cubes we assume to deal with using adaptive integration with condition number 1 per cube. This gives the following expression (assuming that we use i steps for all U-terms)

$$\begin{aligned}
\kappa_3^{(k)} &= \textstyle\sum_{m=1}^{k} 7 \times 8^{-m} |\gamma_m^{(k)}| [4 + 2\tau_1^{(j)} + \kappa_2^{(i)}]/7 + \sum_{m=0}^{k} |\delta_m^{(k)}| 8^{-m} \\
&= \phi_3^{(k)} [4 + 2\tau_1^{(j)} + \kappa_2^{(i)}]/7 + \psi_3^{(k)}
\end{aligned} \tag{20}$$

where $\kappa_2^{(i)}$, assuming j steps for all U-terms, can be written

$$\begin{aligned}
\kappa_2^{(i)} &= \textstyle\sum_{m=1}^{i} 3 \times 4^{-m} |\gamma_m^{(i)}| [2 + \tau_1^{(j)}]/3 + \sum_{m=0}^{i} |\delta_m^{(i)}| 4^{-m} \\
&= \phi_2^{(k)} [2 + \tau_1^{(j)}]/3 + \psi_2^{(k)}
\end{aligned} \tag{21}$$

Note that the 2 dimensional problem only has one 1-dimensional singularity which differs from the problem discussed in the previous section. Now we can use these two expression and the tables 2, 3 and 4 to find that example C) with $\alpha = -1/2$ and $\beta = \gamma = -1$ gives

$$\begin{aligned}
&\kappa_2^{(i)} \leq 2.56 \times [2 + 6.92]/3 + 3.27 \approx 10.88, \text{and} \\
&\kappa_3^{(k)} \leq 2.99 \times [4 + 2 \times 6.92 + 10.88]/7 + 2.84 \approx 15.10
\end{aligned}$$

These two upper bounds are true even if the indices i and/or j varies with the U-terms. We observe a good stability property.

Note that the 3-dimensional problem may be much more difficult: it may involve a corner singularity, three line singularities and three face singularities.

These singularities form a dependency tree: in the root we have the corner singularity (γ), three branches from the root to the three line singularities (β_n) and two branches from each of these nodes to two of the three face singularities (α_n, the leaves). This observation gives the following relations

$$\begin{aligned}\kappa_3^{(k)} &\leq \max_\ell\{\phi_3^{(\ell)}[1 + 3\max_{\text{face}}[\max_j \tau_1^{(j)}] + \\ &\quad 3\max_{\text{line}}[\max_i \kappa_2^{(i)}]]/7 + \psi_3^{(\ell)}\} \\ \kappa_2^{(i)} &\leq \max_\ell\{\phi_2^{(\ell)}[1 + 2\max_{\text{face}}[\max_j \tau_1^{(j)}]]/3 + \psi_2^{(\ell)}\}\end{aligned} \tag{22}$$

Assuming: $\alpha_1 = \alpha_2 = \alpha_3 = \beta_1 = \beta_2 = \beta_3 = -1/2$ and $\gamma = 1/2$ we can use tables 2, 3 and 4 in this case too giving a worst case

$$\begin{aligned}\kappa_2^{(i)} &\leq 2.56(1 + 2 \times 6.92)/3 + 3.27 \approx 15.93, \text{ and} \\ \kappa_3^{(k)} &\leq 2.99(1 + 3 \times 6.92 + 3 \times 15.93)/7 + 2.84 \approx 32.55\end{aligned}$$

Comment: note that instead of 20.99 we got 15.93 due to a subdivision of $R(h)$ in 3 regions of equal size (in contrast to Figure 2): one regular and two regions with a face singularity. This strategy implies more work but slightly better stability.

We observe that there is a recursive procedure involved in general; given a singularity of dimension s we may compute the condition number if we know the condition numbers associated to the algorithm applied to each of the produced subregions, all of lower singular dimension than s. Let Ω_s be the set of all subregions, produced in the recursive step, to this singular point numbered $1, 2, \ldots, 2^s - 1$. Let k be the number of global extrapolation steps, i_m the number of extrapolation steps in each subregion (the strength of the singularity (if present at all) in each subregion may vary too)

$$\kappa_s^{(k)} = \phi_s^{(k)}[\sum_{m=1}^{2^s-1} \kappa_{s_m}^{(i_m)}]/(2^s - 1) + \psi_s^{(k)}, \tag{23}$$

with, $0 \leq s_m < s$, $\kappa_1^{(i)} = \tau_1^{(i)}$ for $\forall i$ and $\kappa_0^{(j)} = 1$ for $\forall j$.

This recursive computation of the condition numbers demonstrates how to organize the computation of such integrals as well. We need to know the dependency tree for the singularities and to organize the algorithm accordingly.

8 Numerical Examples

In this section we will demonstrate on one example in 2 dimensions, how efficient this approach may be. We will for this illustrative purpose apply the highest degree basic rule Q (degree 13, 65 function evaluations) implemented in DCUHRE [2] (Berntsen et. al.) and furthermore subdivide the rectangles which does not contain the singularity in an adaptive manner following this code. The code used in this experiment is named, Q2DADEX, and is an experimental code developed by Singstad in his master thesis implementing the algorithm described in Section 5.

In our example we look at a problem with a corner singularity in C_2, line singularities along the two axes combined with a peak at the center of the square.

$$\int_{C_2} \frac{x^{-1/5}y^{-1/3}(x^2+y^2)^{-1/2}}{(x-.5)^2+(y-.5)^2+.01}dxdy \approx 32.63961049\ldots \qquad (24)$$

The algebraic singularities in this example are: $\alpha = -1/5, \beta = -1/3$ and $\gamma = -1$.

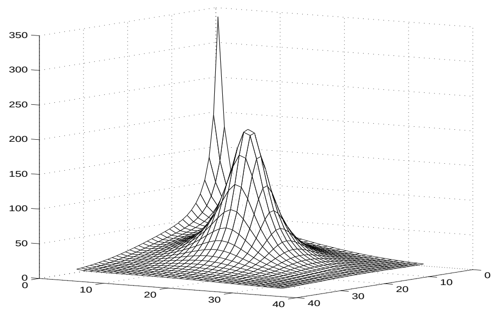

Fig. 3. Plot of the integrand in (24)

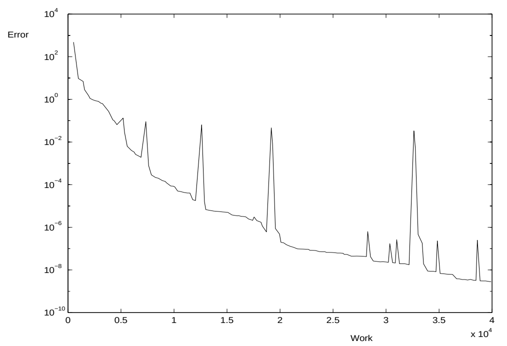

Fig. 4. The relative error versus the number of function evaluations (nfe) applying Q2DADEX on (24).

Note that the drops in accuracy, Figure 4, are connected to new local or global extrapolation steps: then the new regions need subdivision and extrapolation in order to regain the quality of the previous estimates. The stability of the scheme is demonstrated through the fact that the routine is able to steadily improve the estimate of the integral, no sign of degeneration is observed.

Table 5
Q2DADEX behavior when applied to (24)

Global subdivision:	$\hat{U}_1$	$\hat{U}_2$	$\hat{U}_3$	$\hat{U}_4$	$\hat{U}_5$	$\hat{U}_6$	$\hat{U}_7$	$\hat{U}_8$	$\hat{U}_9$
Established after # nfe	520	975	1430	3835	5200	7345	12610	19175	32630
# Subdivisions towards									
the x-axis:	9	8	5	5	5	5	5	5	5
# Subdivisions towards									
the y-axis:	8	4	4	4	4	4	4	4	4
Regular subdivisions:	194	60	24	24	15	15	15	15	15

Having achieved the requested accuracy 10^{-10} we have: 1 region with a composed singularity, 18 regions with a line singularity and 377 regular subregions. Totally the code had to make 179 adaptive decisions between the three options: (1) new global extrapolation step , (2) new local extrapolation step or (3) subdivide a regular region. Note that much work has been spent on estimating $\hat{U}_1$ and $\hat{U}_2$ due to the peak in the center of the square. Furthermore all regions associated with $\hat{U}_j, j = 5, 6, 7, 8, 9$ have been subdivided in a similar manner (4 and 5 extrapolation steps for V and W respectively).

Now we want to illustrate the difference between this non-uniform approach and a code, ADLEV, [3]. ADLEV is based on a uniform subdivision strategy, a harmonic sequence of subdivisions and the Levin d-transform. The code is based on triangles and offers cubature rules of degree 1, 4, 6, 8 and 11. We were unable to get the code to work using the degree 11 rule and have therefore chosen the degree 8 rule in all experiments. In addition to (24) we use the following two problems in our experiment

$$\begin{aligned}&\textstyle\int_{C_2} x^{-1/5}y^{-1/7}(x+y)^{-1/9}\log(x)\log(y)\log(x+y)\exp(2x+y)\;dxdy\\ &\approx -4.\;58488\;6940\ldots,\end{aligned} \tag{25}$$

with algebraic singularities $\alpha = -1/5$, $\beta = -1/7$ and $\gamma = -1/9$. The logarithmic singularities have order 1 along both axes and at the origin the total order is 3.

$$\int_{C_2} x^{-1/9}y^{-2/3}(\log(x))^2 \exp(x+y)\cos(20x)\; dxdy \approx 4.\,19602\,02\ldots, \qquad (26)$$

with algebraic singularities $\alpha = -1/9$, $\beta = -2/3$ and $\gamma = 0$. The logarithmic singularity has order 2 along the y-axis implying order two at the origin as well.

Table 6
The number of function evaluations used by Q2DADEX and ADLEV ADLEV: degree 8 basic rule; Q2DADEX: degree 9 basic rule. The symbol '-' indicates that the routine was unable to produce a satisfactory result

Relative tolerance	Q2DADEX on (24)	ADLEV on (24)	Q2DADEX on (25)	ADLEV on (25)	Q2DADEX on (26)	ADLEV on (26)
10^{-1}	2 178	2 640	990	960	2 343	2 336
10^{-2}	4 455	3 616	1 881	960	3 267	7 040
10^{-3}	6 369	8 000	2 508	2 320	5 973	8 976
10^{-4}	9 702	13 600	3 300	8 576	8 580	72 992
10^{-5}	15 840	-	5 214	21 536	14 817	131 536
10^{-6}	21 813	-	14 124	77 696	43 263	326 304
10^{-7}	38 511	-	25 179	362 768	63 888	-
10^{-8}	56 562	-	46 530	-	133 023	-
10^{-9}	115 038	-	98 472	-	208 032	-

Table 6 demonstrates that the non-uniform strategy and extrapolation is a more stable approach than the uniform strategy and extrapolation. We observe Q2DADEX's ability to give steadily better results while increasing the accuracy request, while ADLEV in all three cases gets into trouble mainly due to stability problems. Both codes will perform better using a higher degree rule when asking for high accuracy. However, qualitatively the performance will be basicly the same as the one demonstrated through Table 6 for these two strategies with this change.

Q2DADEX requires more information about the integrand than does ADLEV. Furthermore Q2DADEX uses Richardson extrapolation while ADLEV uses Levin's d-transform. We consider the fact that a harmonic sequence is chosen (in order to reduce the work) to be the main source to the stability problems. A geometrical sequence implies a more stable strategy while the work load becomes unacceptable taking many extrapolation steps. On the other hand it is reasonable to assume that ADLEV is more efficient than Q2DADEX when low accuracy is required due to the overhead associated with the extrapolation-adaptive strategy in the latter.

9 Conclusions

The power of this non-uniform technique on composed singularities is clearly demonstrated through these examples. We observe that the technique is very stable. Asking for high accuracy implies that it pays to choose a high degree basic rule. Extrapolation is, as we have seen, the key to the success of both the uniform and non-uniform approaches. It is of course possible to use some non-linear extrapolation on the sequence produced through the non-uniform approach too. The non-uniform approach fits well with the general strategy one finds in adaptive codes. Therefore it is reasonable to expect good performance on problems where adaptivity is important as in (24).

Finally we feel that the non-uniform strategy has a potential to handle composed singularities in more that 2 dimensions. The dependency tree for the singularity is obviously important information and we consider recursive programming in combination with the dependency tree to be a good approach in order to develop a general n-dimensional code.

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