# Extrapolation Expansions for Hanging-Chad-Type Galerkin Integrals with Plane Triangular Elements* 

J. N Lyness<br>Mathematics and Computer Science Division<br>Argonne National Laboratory<br>Argonne, IL 60439, USA<br>and<br>School of Mathematics<br>University of New South Wales<br>Sydney, NSW 2052, Australia


#### Abstract

Applications of three-dimensional Galerkin boundary element methods require the numerical evaluation of many four-dimensional integrals. In this paper we explore the possibility of using extrapolation quadrature. To do so, one needs appropriate error functional expansions. The treatment here is limited to integration over a region $\mathcal{T}_{1} \times \mathcal{T}_{2}$, where $\mathcal{T}_{1}$ and $\mathcal{T}_{2}$ are planar triangular elements in a hanging-chad configuration; that is, they have one vertex in common but are otherwise disjoint. We derive error expansions for product trapezoidal rules valid for integrands having an $\left|r_{12}\right|^{-1}$ factor. This factor gives rise to a weak singularity at the common vertex.


## 1 Introduction

Two-dimensional boundary value problems are set in $\mathbb{R}^{3}$. In a conventional application of the Galerkin method, a (two-dimensional) surface is discretized into a set of (twodimensional) plane triangular elements $\mathcal{T}_{i}$, with $1 \leq i \leq n$. For each pair, say $\mathcal{T}_{1}$ and $\mathcal{T}_{2}$, one must evaluate a four-dimensional integral of the form

$$
\begin{equation*}
I\left(\mathcal{T}_{1} \times \mathcal{T}_{2}\right) F=\iint_{\mathcal{T}_{1}} \iint_{\mathcal{T}_{2}} F\left(\mathbf{t}_{1}, \mathbf{t}_{2}\right) d \mathbf{t}_{1} d \mathbf{t}_{2}, \tag{1.1}
\end{equation*}
$$

where the integrand function is of the form

$$
\begin{equation*}
F\left(\mathbf{t}_{1}, \mathbf{t}_{2}\right)=\left|\mathbf{t}_{2}-\mathbf{t}_{1}\right|^{\gamma} H\left(\mathbf{t}_{1}, \mathbf{t}_{2}\right) . \tag{1.2}
\end{equation*}
$$

Here, $H\left(\mathbf{t}_{1}, \mathbf{t}_{2}\right)$ is a regular function of its arguments, and, in the cases of interest, $\gamma$ is a small negative integer.

[^0]This integral is evaluated for all pairs $\mathcal{T}_{i} \times \mathcal{I}_{j}$, with $1 \leq i \leq j \leq n$. Many standard methods exist for cases in which $\mathcal{T}_{i}$ and $\mathcal{T}_{j}$ are disjoint. For a significant number of pairs however, the closures of these regions have a single vertex in common, or one edge in common, or (when $i=j$ ) they actually coincide. In this paper, we treat the hanging-chad configuration; that is, $\mathcal{T}_{1}$ and $\mathcal{T}_{2}$ have one vertex in common but are otherwise disjoint.

We employ the following notation. $\mathcal{T}(\mathbf{d} ; \mathbf{a}, \mathbf{b})$ stands for a triangle having vertices $\mathbf{d}, \mathbf{d}+\mathbf{a}, \mathbf{d}+\mathbf{b}$; and $\mathcal{R}(\mathbf{d} ; \mathbf{a}, \mathbf{b})$ stands for a parallelogram having vertices $\mathbf{d}, \mathbf{d}+\mathbf{a}, \mathbf{d}+\mathbf{b}, \mathbf{d}+$ $\mathbf{a}+\mathbf{b}$. This is composed of two triangles, namely, $\mathcal{T}(\mathbf{d} ; \mathbf{a}, \mathbf{b})$ and a complementary triangle $\overline{\mathcal{T}}(\mathbf{d} ; \mathbf{a}, \mathbf{b})$ having vertices $\mathbf{d}+\mathbf{a}, \mathbf{d}+\mathbf{b}, \mathbf{d}+\mathbf{a}+\mathbf{b}$. We abbreviate $\mathcal{T}\left(\mathbf{d}_{i} ; \mathbf{a}_{i}, \mathbf{b}_{i}\right)$ by $\mathcal{T}_{i}$.

We denote the standard unit triangle and its complement with respect to the unit square by

$$
\begin{equation*}
\triangle=\mathcal{T}((0,0) ;(1,0),(0,1)), \quad \nabla=\overline{\mathcal{T}}((0,0) ;(1,0),(0,1)) \tag{1.3}
\end{equation*}
$$

respectively.
To effect extrapolation, one needs to define an $m$-copy version of a quadrature rule for this product triangular domain $\mathcal{T}_{1} \times \mathcal{T}_{2}$. In later sections we do so in some generality. In this section, we treat a familiar special case, based on the one-dimensional midpoint trapezoidal rule. For the parallelogram $\mathcal{R}(\mathbf{d} ; \mathbf{a}, \mathbf{b})$, we introduce the product midpoint trapezoidal rule or the cell-center rule,

$$
\begin{equation*}
Q^{[m ; 0,0]}(\mathcal{R}) F=|\mathbf{a} \times \mathbf{b}| \frac{1}{m^{2}} \sum_{j_{1}=1}^{m} \sum_{j_{2}=1}^{m} F\left(\mathbf{d}+\frac{\left(2 j_{1}-1\right) \mathbf{a}+\left(2 j_{2}-1\right) \mathbf{b}}{2 m}\right) \tag{1.4}
\end{equation*}
$$

The corresponding rule for the triangle $\mathcal{T}(\mathbf{a}, \mathbf{b})$ may be obtained from this by omitting function values outside the triangle and applying a factor $1 / 2$ to those on its boundary. We get

$$
\begin{equation*}
Q^{[m ; 0,0]}(\mathcal{T}) F=|\mathbf{a} \times \mathbf{b}| \frac{1}{m^{2}} \sum_{j_{1}=1}^{m} \sum_{j_{2}=1}^{m-j_{1}+1}{ }^{\prime} F\left(\mathbf{d}+\frac{\left(2 j_{1}-1\right) \mathbf{a}+\left(2 j_{2}-1\right) \mathbf{b}}{2 m}\right) \tag{1.5}
\end{equation*}
$$

A single prime on a summation symbol indicates that the final term is assigned a factor $1 / 2$. (A double prime indicates that both the first term and the last term are assigned a factor $1 / 2$.)

For the four-dimensional region $\mathcal{T}_{1} \times \mathcal{T}_{2}$ we take the straightforward product rule based on double application of (1.5). Thus

$$
\begin{aligned}
& Q^{[m ; 0,0,0,0]}\left(\mathcal{T}_{1} \times \mathcal{T}_{2}\right) F=\left|\mathbf{a}_{1} \times \mathbf{b}_{1}\right|\left|\mathbf{a}_{2} \times \mathbf{b}_{2}\right| \frac{1}{m^{4}} \\
& \quad \sum_{j_{1}=1}^{m} \sum_{j_{2}=1}^{m-j_{1}+1} \\
& \sum_{j_{3}=1}^{m} \sum_{j_{4}=1}^{m-j_{3}+1}{ }^{\prime} F\left(\mathbf{d}_{1}+\frac{\left(2 j_{1}-1\right) \mathbf{a}_{1}+\left(2 j_{2}-1\right) \mathbf{b}_{1}}{2 m}, \mathbf{d}_{2}+\frac{\left(2 j_{3}-1\right) \mathbf{a}_{2}+\left(2 j_{4}-1\right) \mathbf{b}_{2}}{2 m} . \oint\right)
\end{aligned}
$$

To fix ideas, we remark that, when the integrand function is regular and the domain is $\mathcal{R}_{1} \times \mathcal{R}_{2}$ the error expansion is the four-dimensional product of a simple modification of the classical Euler Maclaurin summation formula. This is:

Theorem 1.1 When $\Phi$, together with all partial derivatives of order $p-1$ or less are integrable and those of order $p$ are absolutely integrable over $\mathcal{R}_{1} \times \mathcal{R}_{2}$, then

$$
\begin{equation*}
Q^{[m ; 0,0,0,0]}\left(\mathcal{R}_{1} \times \mathcal{R}_{2}\right) \Phi-I\left(\mathcal{R}_{1} \times \mathcal{R}_{2}\right) \Phi=\sum_{\substack{s=1 \\ \text { s even }}}^{p} \frac{B_{s}}{m^{s}}+R_{p}(m), \tag{1.7}
\end{equation*}
$$

where $B_{s}$ is independent of $m$ and $R_{p}(m)=o\left(m^{-p}\right)$ as $m$ becomes infinite.
Integral representations for $B_{s}$ and for $R_{p}(m)$ are available.
As part of the development, in Section 4 we shall establish a result corresponding to this for the domain $\mathcal{T}_{1} \times \mathcal{T}_{2}$. However, expansion (1.7) is valid only for integrand functions that are regular over $\mathcal{R}_{1} \times \mathcal{R}_{2}$. When $\mathcal{T}_{1}$ and $\mathcal{T}_{2}$ are in the hanging-chad configuration, the integrand function has a singularity, and a different expansion is required. We shall establish the theory using the following definition.

Definition 1.2 $\mathcal{T}_{1}$ and $\mathcal{T}_{2}$ are in hanging-chad configuration when $\mathbf{d}_{1}=\mathbf{d}_{2}=\mathbf{0}$ and $\mathcal{T}_{1}$ is otherwise disjoint from $\mathcal{T}_{2}$

It will appear that no loss in generality is incurred. Other hanging-chad configurations can be transformed to this one without compromising the expansion. (This is discussed in the final paragraph of Section 4.)

The purpose of this paper is to determine expansions for integrands (1.2) when the elements are in the hanging-chad configuration. A special case of our principal result, derived in Section 5, is the following.

Theorem 1.3 Let $\mathcal{T}_{1}$ and $\mathcal{T}_{2}$ be in the hanging-chad configuration; let $F$ be of form (1.2) with $\gamma=-1$ and with $H$ regular in $\mathcal{T}_{1} \times \mathcal{T}_{2}$. Then

$$
\begin{equation*}
Q^{[m ; 0,0,0,0]}\left(\mathcal{T}_{1} \times \mathcal{T}_{2}\right) F-I\left(\mathcal{T}_{1} \times \mathcal{T}_{2}\right) F \sim \sum_{s=2} \frac{A_{s}}{m^{s}}+\sum_{t=4} \frac{C_{t} \log m}{m^{t}} \tag{1.8}
\end{equation*}
$$

where $A_{s}$ and $C_{t}$ are independent of $m$ and $C_{t}=0$ for all odd $t$.
Other variant results are also derived. These include the corresponding result for more general rules, such as (3.3) below and for values of $\gamma$ other than -1 .

In Section 2 we scale each problem to that of integrating a linearly transformed function over the unit hypercube $[0,1]^{4}$, or over $\Delta x \triangle$. In Section 3 we list several already available error expansions for homogeneous and pseudohomogeneous integrand function and exploit these to establish the variant of Theorem 1.3 for $\left(\mathcal{R}_{1} \times \mathcal{R}_{2}\right)$. In Section 4, the corresponding theory for triangles is presented. In Section 5 we establish Theorem 5.2 of which Theorem 1.3 is a special case; and we draw attention to some more general results.

## 2 Scaling to Unit Hypercube

It is convenient to scale these problems from $\mathcal{R}_{1} \times \mathcal{R}_{2}$ to the unit hypercube $[0,1]^{4}$. In the new system, the integrand function appears to be more complicated. But the change facilitates the exploitation of already known expansions collected together in Section 3.

In this paper, when the integration domain is the unit hypercube, the specification $\left([0,1]^{N}\right)$ is suppressed.

The transformation

$$
\begin{equation*}
\left(\mathbf{t}_{1}, \mathbf{t}_{2}\right)=\left(\mathbf{d}_{1}+x_{1} \mathbf{a}_{1}+y_{1} \mathbf{b}_{1} ; \mathbf{d}_{2}+x_{2} \mathbf{a}_{2}+y_{2} \mathbf{b}_{2}\right) \tag{2.1}
\end{equation*}
$$

applied to (1.1) gives

$$
\begin{align*}
I\left(\mathcal{R}_{1} \times \mathcal{R}_{2}\right) F & =\iint_{\mathcal{R}_{1}} \iint_{\mathcal{R}_{2}} F\left(\mathbf{t}_{1} ; \mathbf{t}_{2}\right) d \mathbf{t}_{1}, d \mathbf{t}_{2} \\
& =\left|\mathbf{a}_{1} \times \mathbf{b}_{1}\right|\left|\mathbf{a}_{2} \times \mathbf{b}_{2}\right| \iiint \int_{[0,1]^{4}} f\left(x_{1}, y_{1} ; x_{1}, y_{2}\right) d x_{1} d y_{1} d x_{2} d y_{2} \tag{2.2}
\end{align*}
$$

where $f$ is simply

$$
\begin{equation*}
f\left(x_{1}, y_{1} ; x_{2}, y_{2}\right)=F\left(\mathbf{d}_{1}+x_{1} \mathbf{a}_{1}+y_{1} \mathbf{b}_{1} ; \mathbf{d}_{2}+x_{2} \mathbf{a}_{2}+y_{2} \mathbf{b}_{2}\right) \tag{2.3}
\end{equation*}
$$

The same change of variables, applied to the quadrature rule in (1.6), gives immediately

$$
\begin{align*}
Q^{[m ; 0,0,0,0]}\left(\mathcal{R}_{1} \times \mathcal{R}_{2}\right) F= & \left|\mathbf{a}_{1} \times \mathbf{b}_{1}\right|\left|\mathbf{a}_{2} \times \mathbf{b}_{2}\right| \frac{1}{m^{4}} \\
& \sum_{j_{1}=1}^{m} \sum_{j_{2}=1}^{m} \sum_{j_{3}=1}^{m} \sum_{j_{4}=1}^{m} f\left(\frac{2 j_{1}-1}{2 m}, \frac{2 j_{2}-1}{2 m}, \frac{2 j_{3}-1}{2 m}, \frac{2 j_{4}-1}{2 m}\right) \\
= & \left|\mathbf{a}_{1} \times \mathbf{b}_{1}\right|\left|\mathbf{a}_{2} \times \mathbf{b}_{2}\right| Q^{[m ; 0,0,0,0]} f \tag{2.4}
\end{align*}
$$

It follows from (2.2) and (2.4) that

$$
\begin{equation*}
Q^{[m ; 0,0,0,0]}\left(\mathcal{R}_{1} \times \mathcal{R}_{2}\right) F-I\left(\mathcal{R}_{1} \times \mathcal{R}_{2}\right) F=\left|\mathbf{a}_{1} \times \mathbf{b}_{1}\right|\left|\mathbf{a}_{2} \times \mathbf{b}_{2}\right|\left(Q^{[m ; 0,0,0,0]} f-I f\right) \tag{2.5}
\end{equation*}
$$

Precisely the same transformation applied to an integral over $\mathcal{T}_{1} \times \mathcal{T}_{2}$ scales the problem in an analogous way to one over $\triangle \times \triangle$, where $\triangle=\mathcal{T}((1,0),(0,1))$ is the conventional standard triangle. Corresponding to (2.5) we have

$$
\begin{align*}
Q^{[m ; 0,0,0,0]}\left(\mathcal{T}_{1} \times \mathcal{T}_{2}\right) F- & I\left(\mathcal{T}_{1} \times \mathcal{T}_{2}\right) F=\left|\mathbf{a}_{1} \times \mathbf{b}_{1}\right|\left|\mathbf{a}_{2} \times \mathbf{b}_{2}\right| \\
& \left(Q^{[m ; 0,0,0,0]}(\triangle \times \triangle) f-I(\triangle \times \triangle) f\right) \tag{2.6}
\end{align*}
$$

It follows that we may limit our detailed investigation to the unit hypercube $[0,1]^{4}$ or to $\triangle \times \triangle$ and the modified integrand function $f$. Once an expansion for the final factor in (2.5) and (2.6). is available, one of precisely the same form applies to the left hand side of these equations.

In our problem, applying transformation (2.1) to $F$ in (1.1), we find

$$
\begin{equation*}
f\left(x_{1}, y_{1} ; x_{2}, y_{2}\right)=\left|r_{12}\right|^{\gamma} h\left(x_{1}, y_{1} ; x_{2}, y_{2}\right) \tag{2.7}
\end{equation*}
$$

with

$$
\begin{equation*}
\left|r_{12}\left(x_{1}, y_{1} ; x_{2}, y_{2}\right)\right|=\left|\mathbf{d}_{1}+x_{1} \mathbf{a}_{1}+y_{1} \mathbf{b}_{1}-\mathbf{d}_{2}-x_{2} \mathbf{a}_{2}-y_{2} \mathbf{b}_{2}\right| \tag{2.8}
\end{equation*}
$$

and

$$
\begin{equation*}
h\left(x_{1}, y_{1} ; x_{2}, y_{2}\right)=H\left(\mathbf{d}_{1}+x_{1} \mathbf{a}_{1}+y_{1} \mathbf{b}_{1} ; \mathbf{d}_{2}+x_{2} \mathbf{a}_{2}+y_{2} \mathbf{b}_{2}\right) \tag{2.9}
\end{equation*}
$$

## 3 Error Expansions for the Region $\mathcal{R}_{1} \times \mathcal{R}_{2}$.

In this section we treat completely a simpler hanging-chad problem. This is the variant of problem (1.1) obtained when triangular elements are replaced by parallelograms. The error expansion is in fact an immediate application of Theorem 3.5, which was established in Lyness [Ly76]. This result is of moderate interest in its own right, but it is exploited later to obtain the corresponding result for triangular elements. This section is concerned mainly with establishing the notation needed to express the result.

Let $Q_{N}$ be any $N$-dimensional quadrature rule operator for $[0,1]^{N}$ of the form

$$
\begin{equation*}
Q_{N} \psi=\sum_{i=1}^{\nu} w_{i} \psi\left(\mathbf{t}^{i}\right), \tag{3.1}
\end{equation*}
$$

that integrates the unit function $\psi(\mathbf{x})=1$ correctly to 1 . Let $Q_{N}^{[m]}$ stand for the $m$-copy version. This is constructed by partitioning $[0,1]^{N}$ into $m^{N}$ equal hypercubes and applying the same appropriately scaled version of $Q$ to each. Thus

$$
\begin{equation*}
Q_{N}^{[m]} \psi=\frac{1}{m^{N}} \sum_{i=1}^{\nu} w_{i} \sum_{j_{1}=0}^{m-1} \sum_{j_{2}=0}^{m-1} \ldots . \sum_{j_{N}=0}^{m-1} \psi\left(\frac{\mathbf{t}^{i}+\mathbf{j}}{m}\right) . \tag{3.2}
\end{equation*}
$$

As is conventional, we express this as a weighted sum of the $m$-copy versions of offset trapezoidal rules defined as follows.

Definition 3.1 Let $\sigma_{i} \in[-1,1]$ and $\tau_{i}=\left(\sigma_{i}+1\right) / 2$. Then

$$
\begin{equation*}
Q_{N}^{\left[m ; \sigma_{1}, \sigma_{2} \ldots \sigma_{N}\right]} \psi=\frac{1}{m^{N}} \sum_{j_{1}=0}^{m-1} \sum_{j_{2}=0}^{m-1} \ldots \sum_{j_{N}=0}^{m-1} \psi\left(\frac{j_{1}+\tau_{1}}{m}, \frac{j_{2}+\tau_{2}}{m}, \ldots, \frac{j_{N}+\tau_{N}}{m}\right) . \tag{3.3}
\end{equation*}
$$

It is conventional to determine error functional expansions for this offset trapezoidal rule. The corresponding expansion for the general rule (3.2) is simply a weighted sum of individual expansions for offset trapezoidal rules. The cell-center rule, (2.4), is a special case of (3.3) with $N=4, \sigma_{i}=0$, and $\tau_{i}=1 / 2$.

Another standard rule is a symmetrical endpoint rule, that is the $N$-product of a trapezoidal rule

$$
\begin{equation*}
Q^{[m ; \pm 1]} \psi=\frac{1}{m}\left(\frac{1}{2} \psi(0)+\sum_{j=1}^{m-1} \psi(j / m)+\frac{1}{2} \psi(0)\right):=\frac{1}{m}\left(\sum_{j=1}^{m-1}{ }^{\prime \prime} \psi(j / m) \psi(0)\right) . \tag{3.4}
\end{equation*}
$$

The somewhat unusual superscript $\pm 1$ indicates that this is an average of rules, namely,

$$
\begin{equation*}
Q^{[m ; \pm 1]} \psi=\frac{1}{2}\left(Q^{[m ;-1]} \psi+Q^{[m ; 1]} \psi\right) . \tag{3.5}
\end{equation*}
$$

We denote the $N$-dimensional version of this rule by

$$
\begin{equation*}
Q_{N}^{[m ; \pm 1, \pm 1, \ldots, \pm 1]} \psi=\frac{1}{m^{N}} \sum_{j_{1}=0}^{m} " \sum_{j_{2}=0}^{m} " \ldots \sum_{j_{N}=0}^{m} " \psi\left(\frac{j_{1}}{m}, \frac{j_{2}}{m}, \ldots, \frac{j_{N}}{m}\right) . \tag{3.6}
\end{equation*}
$$

This is akso known as the cell-vertex rule. Here, as is conventional, a double prime attached to a summation symbol indicates that the first and the last terms are to halved. A symbol $\pm 1$ occuring in the superscript indicates that one is to take the average of two expressions, one having +1 and the other having -1 in the same position. This rule is then the average of $2^{N}$ different offset rules.

A standard classical result that may be applied to all rules mentioned above is the following theorem.

Theorem 3.2 When $\psi(\mathbf{x})$ and its derivatives of order $p-1$ and less are integrable and those of order $p$ are absolutely integrable in $[0,1]^{N}$,

$$
\begin{equation*}
Q_{N}^{[m]} \psi=I \psi+\sum_{s=1}^{p} \frac{B_{s}}{m^{s}}+o\left(m^{-p}\right) \tag{3.7}
\end{equation*}
$$

where $B_{s}$ is independent of $m$.
This is an $N$-dimensional version of the standard Euler Maclaurin expansion. When $Q_{N}^{[m]}$ is symmetric, $B_{s}=0$ for all odd $s$. Simple integral representations are known for $B_{s}$. For example, for the two-dimensional offset trapezoidal rule (3.3) above, we have,

$$
\begin{equation*}
B_{s}=\sum_{q=0}^{s} \frac{B_{q}\left(\tau_{1}\right)}{q!} \frac{B_{s-q}\left(\tau_{2}\right)}{(s-q)!} \int_{0}^{1} \int_{0}^{1} \psi^{(q, s-q)}\left(t_{1}, t_{2}\right) d t_{1} d t_{2} \tag{3.8}
\end{equation*}
$$

where $B_{q}(x)$ is the Bernoulli polynomial of degree $q$.
When the integrand function has a singularity in $[0,1]^{N},(3.7)$ is generally not valid. However, an expansion is known for integrand functions that are homogeneous of specified degree about the origin and are $C^{\infty}[0,1]^{N} \backslash(\mathbf{0})$.

Definition 3.3 $f(\mathbf{x})$ is homogeneous about the origin of degree $\lambda$ if $f(\lambda \mathbf{x})=\lambda f(\mathbf{x})$ for all $\lambda>0$ and $|\mathbf{x}|>0$.

For example, in two dimensions, let $A \neq 0$ and $B$ be constants. Then functions such as

$$
\begin{equation*}
\left(A x^{2}+B y^{2}\right)^{\lambda / 2},(A x+B y)^{\lambda},\left(x y^{2}\right)^{\lambda / 3} \tag{3.9}
\end{equation*}
$$

are homogeneous of degree $\lambda$ about the origin.

Definition 3.4 $f(\mathbf{x})$ is termed pseudohomogeneous of degree $\lambda$ about the origin if it may be expressed in the form $f(\mathbf{x})=f_{\lambda}(\mathbf{x}) h(\mathbf{x})$, where $f_{\lambda}(\mathbf{x})$ is homogeneous of degree $\lambda$ about the origin and $h(\mathbf{x})$ is analytic in a neighborhood of the origin.

A regular function $h$ is pseudohomogeneous of integer degree 0 or higher. In two dimensions the function (using conventional notation with $g$ and $h$ regular)

$$
r^{\alpha} g(r) h(x, y) \Theta(\theta)
$$

is pseudohomogeneous of degree $\alpha$. In the sequel, we shall omit the phrase "about the origin" and require that $H\left(t_{1}, t_{2}\right)$ be regular in $\mathcal{R}_{1} \times \mathcal{R}_{2}$, that is, that $h\left(x_{1}, y_{1}, x_{2}, y_{2}\right)$ be regular in $[0,1]^{4}$.

The definitions and results given above were mainly introduced and expanded in [Ly76], where the following theorem is established.

Theorem 3.5 Let $\gamma>-N$; let $f(\mathbf{x})$ be pseudohomogeneous of degree $\gamma$ and be regular in $\left([0,1]^{N}\right) / \mathbf{0}$. Then, so long as $Q_{N}^{[m]}$ does not involve an indeterminate function value at the origin,

$$
\begin{equation*}
Q_{N}^{[m]} f \sim I f+\sum_{t=0} \frac{A_{\gamma+N+t}+C_{\gamma+N+t} \log m}{m^{\gamma+N+t}}+\sum_{s=1} \frac{B_{s}}{m^{s}}, \tag{3.10}
\end{equation*}
$$

where the coefficients are independent of $m$ and $C_{\gamma+N+t}=0$, unless $\gamma+N$ is an integer.
When $Q_{N}^{[m]}$ is a symmetric rule, as is (1.4) above, we have

$$
\begin{equation*}
B_{s}=C_{s}=0 \text { for all odd } s \tag{3.11}
\end{equation*}
$$

Note that (3.11) does not apply to the coefficients $A_{s}$. When $f(\mathbf{x})$ is homogeneous, rather than pseudohomogeneous, expansion (3.10) retains only the first term in the $t$ summation. The generalization to pseudohomogeneous functions then follows using a Maclaurin expansion of $h(\mathbf{x})$.

In cases where $f(\mathbf{x})$ is indeterminate at the origin, the offending function value at the origin may be ignored (i.e., set to zero) so long as a term $A_{N} / m^{N}$ is included in the expansion.

We now apply this theorem to $f$ in (2.7) in the case that $\mathcal{R}_{1}$ and $\mathcal{R}_{2}$ are in hangingchad configuration. When we set $\mathbf{d}_{1}=\mathbf{d}_{1}=\mathbf{0}$, the four-dimensional function $\left|r_{12}\right|^{\gamma}$ in (2.8) becomes homogeneous of degree $\gamma$. Since $\mathcal{R}_{1}$ and $\mathcal{R}_{2}$ have no common point other than the origin, it follows that $f$ has no singularity other than at the origin. Thus $f$ satisfies the hypotheses of Theorem 3.5 with $N=4$. Carrying out the scaling in (2.6), we find the following theorem.

Theorem 3.6 Let $\mathcal{R}_{1}$ and $\mathcal{R}_{2}$ be in hanging-chad configuration; let $F$ be of form (1.2) with $\gamma>-4$ and with $H$ regular in $\mathcal{R}_{1} \times \mathcal{R}_{2}$. Then

$$
\begin{equation*}
Q^{[m]}\left(\mathcal{R}_{1} \times \mathcal{R}_{2}\right) F-I\left(\mathcal{R}_{1} \times \mathcal{R}_{2}\right) F \sim \sum_{s=1} \frac{B_{s}}{m^{s}}+\sum_{t=4} \frac{A_{\gamma+t}+C_{\gamma+t} \log m}{m^{\gamma+t}} \tag{3.12}
\end{equation*}
$$

where $A_{t}, B_{s}$, and $C_{t}$ are independent of $m$ and $C_{t}=0$ unless $t$ is an integer.

It is instructive to compare this result with (1.8) above. This result is much simpler to prove because the region is $\mathcal{R}_{1} \times \mathcal{R}_{2}$. However, the expansion is of precisely the same form. In (1.8), $\gamma=-1$; and the rule $Q$ is symmetric, giving $B_{s}=C_{s}=0$ for odd $s$.

## 4 Error Expansions for Triangular Regions

The rest of this paper is devoted to extending this result to the case where the elements are triangles. Many of the results have a similar form but are significantly more difficult to establish.

In this section, we define trapezoidal type rules for the triangle. Then, in Theorem 4.1, we remind the reader of the form of the Euler Maclaurin expansion for the standard unit triangle $\triangle$ (see (1.3)). This is used in Section 5 to obtain the corresponding expansion for the four-dimensional region $\Delta \times \triangle$.

In general, the offset trapezoidal rule for the triangle $\triangle$ coincides with the corresponding offset trapezoidal rule for $[0,1]^{2}$, except that function values outside $\triangle$ are replaced by zero. When the rule requires no abscissas on the boundary $x+y=1$, this is unambiguous. When there are abscissas on a boundary, a definition of the form (4.3) to be given below becomes necessary.

In simple cases, an appropriate definition is intuitive. For example, we have already defined a rule operator (1.5) above for a cell-center rule applied to a triangle. A corresponding modification of the cell-vertex rule to the triangle $\triangle$ might well take the form

$$
\begin{equation*}
Q^{[m ; \pm 1, \pm 1]}(\triangle) \psi=\frac{1}{m^{2}} \sum_{j_{1}=0}^{m} \prime^{m-j_{1}} \sum_{j_{2}=0}^{\prime \prime} \psi\left(\frac{j_{1}}{m}, \frac{j_{2}}{m}\right) . \tag{4.1}
\end{equation*}
$$

This assigns weight $1 / m^{2}$ to all interior abscissas and weight $1 / 2 m^{2}$ to all abscissas on an edge but not at a vertex. It somewhat arbitrarily assigns weights $1 / 4 m^{2}, 0,1 / 4 m^{2}$ to the vertices $(0,0),(1,0)$, and $(0,1)$, respectively. The corresponding rule for the complementary triangle is

$$
\begin{equation*}
Q^{[m ; \pm 1, \pm 1]}(\nabla) \psi=\frac{1}{m^{2}} \sum_{j_{1}=0}^{m} " \sum_{j_{2}=m-j_{1}}^{m} " \psi\left(\frac{j_{1}}{m}, \frac{j_{2}}{m}\right) \tag{4.2}
\end{equation*}
$$

We shall see below that it is quite permissible to use several other modifications of the product trapezoidal rule for the square.

In most applications we know of, either the cell-center rule (1.5) or the rule (4.1) is employed, and the definitions above suffice. The reader may, if he wishes, advance directly to Theorem 4.1 below. In the interests of completeness, however, we present the full theory, as it applies to the triangle; for the modification of the general offset rule (3.3) for a simplex, a less casual definition is required.

The reader will have noticed that a measure of arbitrariness is introduced when one comes to assign the weight to be applied at abscissas on the common boundary of $\Delta$ and $\nabla$. To deal with this, we introduce weight factors $\theta(\mathbf{t})$.

The offset trapezoidal rule for $\triangle$ (corresponding to (3.3) for $[0,1]^{2}$ ) is of the form

$$
\begin{equation*}
Q_{2}^{\left[m ; \sigma_{1}, \sigma_{2}\right]}(\triangle) \psi=\frac{1}{m^{2}} \sum_{j_{1}=0}^{m-1} \sum_{j_{2}=0}^{m-1} \theta\left(\frac{j_{1}+\tau_{1}}{m}, \frac{j_{2}+\tau_{2}}{m}\right) \psi\left(\frac{j_{1}+\tau_{1}}{m}, \frac{j_{2}+\tau_{2}}{m}\right) . \tag{4.3}
\end{equation*}
$$

Naturally, when inventing a rule, one may assign weights as one pleases. But in order to retain the error expansion in a form suitable for extrapolation, the function $\theta(\mathbf{t})$ has to be
assigned in accordance with the following guidelines. We denote the vertices $(0,0),(1,0)$, and $(0,1)$ by $V_{0}, V_{1}$, and $V_{2}$, respectively. We denote by $V_{i, j}$ the edge between $V_{i}$ and $V_{j}$ but not including $V_{i}$ and $V_{j}$ and by $V_{123}$ the interior of $\triangle$. We assign six parameters $\theta^{i, j}$ and $\theta^{i}$, and set:
(i) $\quad \theta(\mathbf{t})=\theta_{I}=\theta^{1,2,3}=1 \quad \mathbf{t} \in V_{123}$
(ii) $\quad \theta(\mathbf{t})=\theta^{i, j} \quad \mathbf{t} \in V_{i, j}$
(iii) $\theta(\mathbf{t})=\theta^{i} \quad \mathbf{t}=V_{i}$
(iv) $\theta(\mathbf{t})=0 \quad$ otherwise.

The convergence of $Q^{[m]}(\triangle) \psi$ to $I(\triangle) \psi$ is guaranteed by assignments (i) and (iv). The choice of the remaining six parameters is arbitrary. However, to retain an even expansion, one must set $\theta^{i, j}=1 / 2$, as is done in both examples (1.5) and (4.1). The assignment of $\theta^{i}$ affects only the coefficient $B_{2}$ in the error expansion; if extrapolation is used, it has no effect on the final result because the term $B_{2} / m^{2}$ is eliminated.

We note that an offset trapezoidal rule for the complementary triangle $\nabla$ may be defined by

$$
\begin{equation*}
Q_{2}^{\left[m ; \sigma_{1}, \sigma_{2}\right]}(\nabla) \psi=\frac{1}{m^{2}} \sum_{j_{1}=0}^{m-1} \sum_{j_{2}=0}^{m-1} \bar{\theta}\left(\frac{j_{1}+\tau_{1}}{m}, \frac{j_{2}+\tau_{2}}{m}\right) \psi\left(\frac{j_{1}+\tau_{1}}{m}, \frac{j_{2}+\tau_{2}}{m}\right) . \tag{4.4}
\end{equation*}
$$

with $\bar{\theta}(\mathbf{t})=1-\theta(\mathbf{t})$. This ensures that

$$
\begin{equation*}
Q_{2}^{\left[m ; \sigma_{1}, \sigma_{2}\right]}\left([0,1]^{2}\right) \psi=Q_{2}^{\left[m ; \sigma_{1}, \sigma_{2}\right]}(\triangle) \psi+Q_{2}^{\left[m ; \sigma_{1}, \sigma_{2}\right]}(\nabla) \psi \tag{4.5}
\end{equation*}
$$

The situation with regard to higher-dimensional simplices $S_{N}$ can become quite complicated. The full theory for $S_{N}$ but restricted to product end point trapezoidal rules $\left(\sigma_{j}= \pm 1\right)$ is presented in [LyGe80]. The coefficients $B_{s}$ in the Euler Maclaurin expansion (4.6) depend on the values assigned to $\theta^{(\mathbf{k})}$. These may be chosen to ensure that this expansion is even in character and to improve the polynomial degree of precision of the extrapolate. Some of these questions are taken up in [LyPu73] and [Ly78].

Theorem 4.1 When $\psi(\mathbf{x})$ and its derivatives of order $p-1$ and less are integrable and those of order $p$ are absolutely integrable in $[0,1]^{2}$,

$$
\begin{equation*}
Q_{2}^{\left[m ; \sigma_{1}, \sigma_{2}\right]}(\triangle) \psi=I(\triangle) \psi+\sum_{s=1}^{p} \frac{B_{s}}{m^{s}}+o\left(m^{-p}\right) . \tag{4.6}
\end{equation*}
$$

Expressions for the coefficients $B_{s}$ are available. These include

$$
\begin{aligned}
B_{s}= & \sum_{q=0}^{s} \frac{\bar{B}_{q}\left(\tau_{1}\right)}{q!} \frac{\bar{B}_{s-q}\left(\tau_{2}+\tau_{1}\right)}{(s-q)!} \int_{0}^{1} \psi^{(q, s-q-1)}(t, 1-t) d t \\
& -\frac{\bar{B}_{q}\left(\tau_{1}\right)}{q!} \frac{\bar{B}_{s-q}\left(\tau_{2}\right)}{(s-q)!} \int_{0}^{1} \psi^{(q, s-q-1)}(t, 0) d t,
\end{aligned}
$$

valid when $\theta^{12}=\theta^{20}=\theta^{01}=1 / 2$ and $\theta^{0}, \theta^{1}, \theta^{2}=1 / 4,0,1 / 4$. Here, $B_{q}(x)$ is the Bernouli polynomial of degree $q$, and $\bar{B}_{q}(x)$ is the corresponding Bernoulli function, which coincides with $B_{q}(x)$ for $x \in(0,1)$ and is periodic with period 1 . Note that $\bar{B}_{q}(0)=\bar{B}_{q}(1)=B_{q}(0)=$ $B_{q}(1)$ for all $q$ except $q=1$. For this special case we have $\bar{B}_{1}(0)=\bar{B}_{1}(1)=0$ while $B_{1}(0)=-B_{1}(1)=-1 / 2$.

We conclude this section by noting that the effect of carrying out an affine transformation which takes $\triangle$ into itself, but changes the rule can be duplicated by simply altering parameters $\sigma_{i}$ appropriately. For example the rules $Q^{[m ; 0,0]}(\triangle)$ and $Q^{[m ; \pm 1,0]}(\triangle)$ are related to each other by an affine transformation. Any result obtained for general $\sigma_{i}$ applies to both. Because of this, the restriction in definition 1.2 to $\mathbf{d}_{1}=\mathbf{d}_{2}$ has no overall effect. When the contact point is different, for example $\mathbf{d}_{2}=\mathbf{d}_{1}+\mathbf{a}_{1}$, we may reexpress one of the rules so that these contact points coincide simply by altering the parameters $\sigma_{i}$. This is worth noting because, in the absence of singularities, many properties of a rule are unaltered by an affine transformation. When there is a singularity, the affine transformation relocates any singularity, in many cases voiding the required result.

## 5 Error Expansions for the Region $\mathcal{T}_{1} \times \mathcal{T}_{2}$.

The original problem involves integrations over a product region $\mathcal{T}_{1} \times \mathcal{T}_{2}$; after scaling this becomes a product region $\Delta \times \triangle$. We shall require the Euler Maclaurin expansion for a region $\Delta \times \triangle$. Note that, in the literature, this and other expansions are available for the $N$-dimensional simplex $S_{N}$, namely, $x_{i}>0$ for $i=1,2, \ldots, N ; \sum_{i=1}^{N} x_{i}<1$. We have stated above the result for the triangle, namely $S_{N}$ with $N=2$. We are seeking the corresponding result for the region $\triangle \times \triangle$, namely, $x_{i}>0 i=1,2,3,4 ; x_{1}+x_{2}<0 ; x_{3}+x_{4}<0$. Exploiting the fact that this is a product region we write

$$
\begin{equation*}
Q_{x_{1}, x_{2}, x_{3}, x_{4}}^{\left[m ; \sigma_{1}, \sigma_{2}, \sigma_{3}, \sigma_{4}\right]}(\triangle \times \triangle) f\left(x_{1}, x_{2}, x_{3}, x_{4}\right)=Q_{x_{1}, x_{2}}^{\left[m ; \sigma_{1}, \sigma_{2}\right]}(\triangle) \psi\left(x_{1}, x_{2}\right) \tag{5.1}
\end{equation*}
$$

where

$$
\begin{equation*}
\psi\left(x_{1}, x_{2}\right)=Q_{x_{3}, x_{4}}^{\left[m ; \sigma_{3}, \sigma_{4}\right]}(\triangle) f\left(x_{1}, x_{2}, x_{3}, x_{4}\right) \tag{5.2}
\end{equation*}
$$

In the inner quadrature rule sum, $x_{1}$ and $x_{2}$ are simply incidental parameters.
We may apply expansion (4.6) to the right-hand side of (5.2) to obtain an expression for $\psi$ involving coefficients $B_{s^{\prime}}$ as defined in (4.7) but having $x_{1}, x_{2}$ as an incidental parameter. The derivation of Theorem 5.1 is straightforward. It rests on the facts that $Q$ involves only a finite number of terms; the sum of a finite number of terms, each of order $m^{-p}$, is also of order $m^{-p}$; and in (4.7) the dependence on $\psi\left(t_{1}, t_{2}\right)$ is linear.

Theorem 5.1 When $\psi(\mathbf{x})$ and its derivatives of order $p-1$ and less are integrable and those of order $p$ are absolutely integrable in $[0,1]^{4}$,

$$
\begin{equation*}
Q^{\left[m ; \sigma_{1}, \sigma_{2}, \sigma_{3}, \sigma_{4}\right]}(\triangle \times \triangle) \psi=I(\triangle \times \triangle) \psi+\sum_{s=1}^{p} \frac{B_{s}}{m^{s}}+o\left(m^{-p}\right) \tag{5.3}
\end{equation*}
$$

where $B_{s}$ is independent of $m$.

This result is technically new. It is important not to confuse it with the corresponding result for the four-dimensional simplex. Theorem 5.1 refers to the product of two independent triangular elements; and it plays a key role in establishing the corresponding result, Theorem 5.2, for two triangular elements having one vertex in common.

We are now in a position to establish the error expansion for the hanging-chad configuration when both elements are triangles. This is the generalization of Theorem 3.6 to $\mathcal{T}_{1} \times \mathcal{T}_{2}$. We note the following geometric identity.

$$
\begin{equation*}
Q^{[m]}\left(\mathcal{R}_{1} \times \mathcal{R}_{2}\right) \psi=Q^{[m]}\left(\mathcal{T}_{1} \times \mathcal{T}_{2}\right) \psi+Q^{[m]}\left(\overline{\mathcal{T}}_{1} \times \mathcal{T}_{2}\right) \psi+Q^{[m]}\left(\mathcal{T}_{1} \times \overline{\mathcal{T}}_{2}\right) \psi+Q^{[m]}\left(\overline{\mathcal{T}}_{1} \times \overline{\mathcal{T}}_{1}\right) \psi \tag{5.4}
\end{equation*}
$$

We consider the case in which $\mathcal{R}_{1}$ and $\mathcal{R}_{2}$ are in the hanging-chad configuration. It follows immediately that $\mathcal{T}_{1}$ and $\mathcal{T}_{2}$ are also in the hanging-chad configuration. However, the final three terms on the right refer to pairs of triangles that are disjoint. Thus, the standard Euler Maclaurin expansion (5.3) may be applied to each. These three expansions involve only terms $I \psi$ and $B_{s} / m^{s} s=1,2, \ldots$. They may be combined. An expansion for the term on the left is simply (3.12) mentioned above. Thus (5.4) may be used to obtain an expansion for the first term on the right. We find the following.

Theorem 5.2 Let $\mathcal{T}_{1}$ and $\mathcal{T}_{2}$ be in the hanging-chad configuration; let $F$ be of form (1.2) with $\gamma>-4$ and with $H$ regular in $\mathcal{T}_{1} \times \mathcal{T}_{2}$. Then

$$
\begin{equation*}
Q^{\left[m ; \sigma_{1}, \sigma_{2}, \sigma_{3}, \sigma_{4}\right]}\left(\mathcal{T}_{1} \times \mathcal{T}_{2}\right) F-I\left(\mathcal{T}_{1} \times \mathcal{T}_{2}\right) F \sim \sum_{s=1} \frac{B_{s}}{m^{s}}+\sum_{t=4} \frac{A_{\gamma+t}+C_{\gamma+t} \log m}{m^{\gamma+t}} \tag{5.5}
\end{equation*}
$$

where $A_{t}, B_{s}$, and $C_{t}$ are independent of $m$ and $C_{t}=0$ unless $t$ is an integer.
A restriction that $H$ be regular in $\left(\mathcal{R}_{1} \times \mathcal{R}_{2}\right)$ comes in because Theorem 3.6 is used in the proof. In fact, using an elementary continuation process, this restriction can be replaced by the one stated in the theorem.

As in the constituent results on which (5.5) is based, we have the condition that $B_{s}=C_{s}=0$ for odd $s$ when the rule is symmetric.

## 6 Concluding Remarks

The results in this paper represent a contribution in the area of extrapolation quadrature. In one dimension the extrapolation approach (e.g., Romberg integration) is rarely competitive with Gaussian quadrature. However, there are applications in multidimensional quadrature where it is without question more efficient. These are generally categorized by a finite linearly bounded region of integration, with an integrand having an algebraic or logarithmic singularity of known character along a boundary.

Earlier results in this area include the Euler Maclaurin asymptotic expansion for the simplex (with regular integrand) [LyPu73],[Ly78] and the corresponding expansions for the hypercube and for the Simplex when the integrand has algebraic radial singularity [Ly76], [Ly76a]. More recent contributions involve Hadamard Finite Part integrals, [Mo94], [MoLy98] Sidi transformations [Si93], and Jacobian-free integration over curved surfaces. For the hypercube $[0,1]^{N}$, Verlinden has developed an umbrella approach based on Mellin

Transforms for constructing error functional expansions [Ve93],[VeHa93]. And this has been extended to the calculation of two-dimensional Hadamard finite part integrals [LyMo05].

The present paper is the second in a sequence devoted to applying extrapolation to the four-dimensional integrals occurring in the Galerkin method for two-dimensional boundary value problems. In the first, [Ly05], a prototype integral is treated. This is $I\left(\mathcal{R}_{1} \times \mathcal{R}_{2}\right) F$ with $F=\left|r_{12}\right|^{-1}$, and with both $\mathcal{R}_{1}$ and $\mathcal{R}_{2}$ being the same unit square. A somewhat special proof was constructed to establish an error expansion of the same nature as, but different from (5.5) and limited to the midpoint rule $Q^{[m ; 0,0,0,0]}$. Numerical results obtained using the extrapolation were presented. For example a standard extrapolation procedure obtained four-figure accuracy using 1,000 function values and eight-figure accuracy using 25,000 function values. (Indeterminate function values were ignored, i.e., replaced by zero.) The reader should bear in mind that this prototype example is a very special case indeed. It is one for which the result is known in analytic form. And our relatively simple proof cannot readily be extended to offset trapezoidal rules or even to the case in which $\mathcal{R}$ is replaced by a rectangle.

On the other hand, the present paper is thorough. It treats all hanging-chad configurations involving triangular or rectangular elements. It allows a complete choice of trapezoidal-type product rules, including offset rules and, by extension, even copy-versions of Gaussian rules. And it allows the $\left|r_{12}\right|^{\gamma}$ singularity for all $\gamma>-4$. (For lower values of $\gamma$ the integral does not exist in the conventional sense.)

Preliminary results indicate that that expansions of this general type apply also to the (open book) configuration in which the elements have an edge in common.

## References

[Ly78] J. N. Lyness Quadrature over a Simplex: Parts 1 and 2. SIAM J. Numer. Anal. 15, 122-133 and 870-887, 1978.
[Ly76] J. N. Lyness, An Error Functional Expansion for N-dimensional Quadrature with an Integrand Function Singular at a Point, Math. Comp. 30, 1-23, 1976.
[Ly76a] J. N. Lyness, Applications of Extrapolation Techniques to Multidimensional Quadrature of Some Integrand Functions with a Singularity, J. Comput. Phys. 20, 346-364, 1976.
[Ly05] J. N. Lyness, A Prototype Four-Dimensional Galerkin-Type Integral, Publ. RIMS, Kyoto Univ. 41, 843-851, 2005. See also Preprint ANL/MCS-P1196-0604, Mathematics and Computer Science Division, Argonne National Laboratory, June 2004.
[LyGe80] J. N. Lyness and A. C. Genz, On Simplex Trapezoidal Rule Families, SIAM J. Num. Anal. 17, 126-147, 1980.
[LyMo05] J. N. Lyness and G. Monegato, Asymptotic Expansions for two-dimensional hypersingular integrals, Numer. Math. 100, 293-329, 2005.
[LyPu73] J. N. Lyness and K. K. Puri, The Euler Maclaurin Expansion for the Simplex, Math. Comp. 27, 273-293, 1973.
[Mo94] G. Monegato, Numerical Evaluation of Hypersingular Integrals, JCAM 50, 9-31, 1994.
[MoLy98] G. Monegato and J. N. Lyness, The Euler-Maclaurin Expansion and Finite-Part Integrals, Numer. Math. 81, 273-291, 1998.
[Si93] A. Sidi, A new variable transformation for numerical integration, in Numerical Integration, Vol 4, eds. H Bräss and B Hämmerlin (Birkhäuser, Basel, 1993) pp 359-373.
[Ve93] P. Verlinden, Cubature Formulas and Asymptotic Expansions, Ph.D. thesis, Katholieke Universiteit Leuven, 1993.
[VeHa93] P. Verlinden and A. Haegemans, An Error Expansion for Cubature with an Integrand with Homogeneous Boundary Singularities, Numer. Math. 65, 383-406, 1993.

The submitted manuscript has been created by the University of Chicago as Operator of Argonne National Laboratory ("Argonne") under Contract W-31-109-ENG-38 with the U.S. Department of Energy. The U.S. Government retains for itself, and others acting on its behalf, a paid-up, nonexclusive, irrevocable worldwide license in said article to reproduce, prepare derivative works, distribute copies to the public, and perform publicly and display publicly, by or on behalf of the Government.


[^0]:    *This work was supported in part by the Mathematical, Information, and Computational Sciences Division subprogram of the Office of Advanced Scientific Computing Research, Office of Science, U.S. Department of Energy, under Contract W-31-109-Eng-38. This is 20 May 2005 version.

