ABSTRACT. When the Partition of Unity Method is applied to a discretised integral equation form of the Helmholtz operator, the computational cost is dominated by the evaluation of highly oscillatory integrals over discretisations. This paper presents a new numerical approach that is based on a coordinate transformation to a secondary discretisation that is aligned with an approximation to the curvilinear coordinate in which oscillation is taking place. This transforms a 2D surface integral into an equivalent set of 1D integrals that may be evaluated cheaply yet accurately. A method is proposed for dealing efficiently with difficulties that occurred at the edges of elements in previous work.

1. Introduction. Let $D$ be a domain in $\mathbb{R}^3$, unbounded in the exterior and bounded internally by an obstacle of smooth boundary $\partial D = \Gamma$. We address frequency domain problems of linear wave scattering, with $e^{-i\omega t}$ time-dependence, governed by the Helmholtz equation

$$\left(\Delta + k^2\right) \phi(x) = 0, \quad x \in D$$

in which we seek the potential $\phi : \mathbb{R}^3 \to \mathbb{C}$ and in which the wave number $k$ is defined as $k = 2\pi/\lambda = \omega/c$, $\lambda$ being the wavelength under consideration and $c$ the wave speed. The differential equation (1) is to be solved subject to a boundary condition of the Robin form

$$\nabla \phi(x) \cdot n = \alpha \phi(x) + \beta, \quad x \in \Gamma$$

in which $n$ is the unit normal directed outward from $D$, and therefore into the scattering obstacle.

We assume the obstacle to be impinged by an incident plane wave $\phi^I$, of unit amplitude and propagating in a direction described by the unit vector $\psi = \{(\psi_1, \psi_2, \psi_3) : \psi_1^2 + \psi_2^2 + \psi_3^2 = 1\}$. Conventional treatment of (1) leads to the expression of the problem in combined layer potential form

$$\frac{1}{2} \phi(x_0) + (K\phi)(x_0) - \alpha (S\phi)(x_0) = \phi^I(x_0) + (S\beta)(x_0), \quad x_0 \in \Gamma$$

where

$$(S\phi)(x_0) := \int_{\Gamma} G(x, x_0) \phi(x) d\Gamma(x)$$
and
\[(K\phi)(x_0) := \int_{\Gamma} \frac{\partial G(x, x_0)}{\partial n(x)} \phi(x) d\Gamma(x) \tag{5}\]
are the single and double layer potential operators. \(G\) denotes the Green’s function, which in this case is well known:
\[G(x, x_0) = e^{ikr} \frac{4\pi}{4\pi r} \tag{6}\]
where \(r := |x - x_0|\) is the usual radial coordinate in boundary integral methods.

There are many examples in the literature of the numerical solution of wave propagation problems governed by the above expressions, and solution is common using a discretisation of \(\Gamma\),
\[\Gamma = \bigcup_{e=1}^{E} \Gamma_e, \quad \Gamma_s \cap \Gamma_t = 0, s \neq t \tag{7}\]
with a piecewise polynomial approximation space. It has been the subject of much recent attention that this approach becomes impractical for large \(k\) because of the requirement that the discretisation (7) be sufficiently refined that the model contains a minimum of approximately 10 degrees of freedom per wavelength in each coordinate direction. Bettes [1] provides a review of some methods that aim to overcome or circumvent this limitation, or at least reduce the practical upper bound on frequency for any given computational resource; readers are further directed to the theme issue of Phil. Trans. Royal Soc. London A in which [1] appears for more details of some of the approaches. One class of approaches that shows promise is based on the enrichment of the approximation space by the expansion of \(\phi(x)\) in wave functions, usually plane waves. This is seen in the Ultraweak Variational Formulation of Cessenat and Després [2], for example. Other authors, firstly Abboud et al. [3], write integral equations derived from the expansion of potential as \(\phi(x) = A(x)\phi^f(x) = A(x)e^{ik\psi \cdot x}\), and solve for \(A\). This approach can be particularly effective for convex scatterers of size >> \(\lambda\). Bruno et al. [4] have presented an approach of \(O(1)\) complexity for convex scatterers of dimension up to \(10^6\lambda\). Anand et al. [5] have considered problems involving multiple scattering from a set of obstacles that are required to present a convex face to each other.

The extension of this idea to a basis containing multiple plane waves was introduced in an integral equation context by de la Bourdonnaye [6, 7] under the name ‘microlocal discretisation’. Around the same time, the Partition of Unity Method (PUM) was introduced by Melenk & Babuška [8] as a general approach in which \textit{a priori} knowledge of the solution space may be used to enrich an approximation. This has since been adopted using both finite element methods (FEM) [9, 10] and boundary element methods (BEM) [11] in a number of works in wave scattering, demonstrating a significant reduction in error in comparison to the conventional polynomial approximation space. Notably, Perrey-Debain et al. [12] show that the required number of degrees of freedom can be reduced
to approximately one quarter of those required in conventional BEM in each coordinate direction. When adopted for wave problems, the PUM presents the multiple plane wave expansion for the potential, in an element containing $J$ nodes, as

$$\phi(x) = \sum_{j=1}^{J} N_j(x) \sum_{m=1}^{M} A_{jm} e^{ikd_{jm} \cdot x}$$  \hfill (8)

where the terms $N_j(x)$ are the traditional Lagrange polynomial shape functions, and $A_{jm} \in \mathbb{C}$ and unit vectors $d_{jm} \in \mathbb{R}^3$ describe the amplitudes and directions respectively of the $M$ plane waves in the basis. In 2D the directions are usually uniformly distributed around the unit circle, i.e.

$$d_{jm} = (\cos \theta_{jm}, \sin \theta_{jm}), \quad \theta_{jm} = \frac{2\pi(m-1)}{M}.$$  \hfill (9)

Apart from the few special cases that are analogous to the platonic solids, i.e. $M = 4, 6, 8, 12, 20$, there are no analytical solutions leading to uniform distribution of directions around the unit sphere in 3D for arbitrary $M$. However, there are various practical methods of achieving a quasi-uniform distribution.

Collocating (3) at a sufficient number of boundary points and CHIEF points (Schenck [13]) yields the matrix system

$$Aa = (W + K)a = b,$$  \hfill (10)

where the vector $a$ contains the plane wave amplitudes. The sparse matrix $W$ may be interpreted as the plane wave interpolation matrix for the potential, and matrix $K$ is dense, arising from the evaluation of the boundary integrals. Following solution of this system, which is usually overdetermined when using the CHIEF method, the potential field can be quickly recovered using (8). It is also noted that we present here the direct collocation BIE using CHIEF points to address the non-uniqueness of the solution at the eigenfrequencies of the associated interior problem. Other formulations using the Burton & Miller [14] approach (also called the Combined Field Integral Equation, or CFIE) and/or Galerkin BIE are also admissible and appear in the literature, e.g. Bériot et al. [15].

It should be noted that plane wave enriched boundary elements are applicable to general, non-convex scatterers. However, the reductions in error and in the required number of degrees of freedom that accrue by use of the PUM for wave problems come at the cost of the requirement to evaluate some highly oscillatory integrals of the general form

$$I = \int_{-1}^{+1} \int_{-1}^{+1} f(\xi, \eta) e^{ikg(\xi, \eta)} d\xi d\eta$$  \hfill (11)

where $f(\xi, \eta)$ is slowly varying and large $k$ implies many wavelengths in $(\xi, \eta) \in [-1, 1]^2$. In the wave boundary element (i.e. PU-BEM) literature to date, these
boundary integrals have been evaluated using Gauss-Legendre quadrature, but this is well known to be inefficient for integrating trigonometric functions, and very large numbers of Gauss point evaluations are required, dominating the run-time. Care needs to be taken to evaluate integrals accurately because of the much-reported ill-conditioning that accompanies a plane wave basis.

There has been recent activity in developing procedures for evaluating oscillatory integrals of this character. Ortiz & Sanchez [16] accelerated 2D integrations in the Partition of Unity Finite Element Method (PU-FEM) by treating the integral in a rotated coordinate system. Bettess et al. [17] introduced an efficient semi-analytical scheme for PU-FEM that has been extended recently by Honnor et al. [18]. This, and other similar schemes, proceed by writing the integrand as the divergence of some subsidiary function, and using the divergence theorem to transform the integral to one over a boundary contour. However, this is not directly applicable to the Partition of Unity Boundary Element Method (PU-BEM) because the presence of the Green’s function prevents the writing of the subsidiary function. It is also found that, in addition to possible difficulties with singular boundary integrals, the asymptotic method presented by Iserles & Norsett [19] becomes impractical for these integrands because of the very lengthy expressions that emerge for the coefficients and slow convergence. In this paper we present an alternative, efficient integration scheme for PU-BEM for wave problems. The scheme is an adaptation of that presented recently by Honnor & Trevelyan [20] for enhanced computational efficiency. In Section 2 we present the integrand under consideration and the scheme of [20], which has been published only in conference proceedings. This scheme is enhanced with a new adaptation in Section 3. In Section 4 we present some notes on implementation. In Section 5 we illustrate the scheme for both flat and curved triangular element cases, showing the errors and computational efficiency, and we close with some concluding remarks in Section 6.

2. Integration scheme. Substitution of the PUM expansion (8) and the Green’s function (6) into the single and double layer potential operators (4) and (5) leads to the required boundary integral over boundary element $\Gamma_e$.

$$I_e = \frac{1}{4\pi} \int_{\Gamma_e} \frac{\mu(x)e^{ikr(x)}}{\mu(x)} \sum_{j=1}^{J} N_j(x) \sum_{m=1}^{M} e^{ikd_{jm}^{-2}} \, d\Gamma(x)$$  \hspace{1cm} (12)$$

where

$$\mu(x) = \begin{cases} r^{-1}(x) & \text{for single layer potential} \\ (ikr^{-1}(x) - r^{-2}(x)) \frac{\partial r(x)}{\partial n(x)} & \text{for double layer potential} \end{cases}$$ \hspace{1cm} (13)$$

and in which the amplitudes $A_{jm}$ have been removed to appear instead as unknowns in the vector $a$. This paper specifically refers to cases in which $x_0 \notin \Gamma_e$; however, we believe the adaptation of the scheme to the singular boundary integrals should be straightforward. Taking each term in the double summation independently, and denoting each by $I_{e,jm}$, the evaluation of $I_e$ reduces to the
summation of a number of integrals of the form
\[ I_{ejm} = \int_{\Gamma_e} \frac{\mu(x)e^{ikr(x)}}{4\pi} N_j(x)e^{ikdjm \cdot x} d\Gamma(x). \]  
(14)

We also introduce the usual parameterisation of a finite/boundary element, i.e.
\[ \Gamma_e = \{ \gamma_e(\xi, \eta) : (\xi, \eta) \in [-1,1]^2 \} \]  
(15)
where \( \gamma_e : \mathbb{R}^2 \to \mathbb{R}^3 \), so that the integral may be further rewritten as
\[ I_{ejm} = \int_{-1}^{+1} \int_{-1}^{+1} \frac{\mu(x(\xi, \eta))}{4\pi} N_j(x(\xi, \eta))e^{ikgjm(x(\xi, \eta))} J_0(\xi, \eta) d\xi d\eta, \]  
(16)
Here, \( J_0(\xi, \eta) \) is the Jacobian of the coordinate transformation, and
\[ g_{jm}(x(\xi, \eta)) := r(x) + d_{jm} \cdot x. \]  
(17)
This integral has been evaluated using high order quadrature in the PU-BEM literature to date. However, for the new scheme we now subdivide the element \( \Gamma_e \) into non-overlapping three- and four-sided patches
\[ \Gamma_e = \bigcup_{q=1}^{Q} \Gamma_{eq}, \quad \Gamma_{es} \cap \Gamma_{et} = 0, s \neq t \]  
(18)
such that the boundaries between adjacent subdivisions lie on contours describing \( g_{jm}(x) = const \) (denoted the minor directions) and on a set of lines formed orthogonally to these contours, such that these (major) lines lie in the direction of increasing \( g_{jm}(x) \). An example is presented in Figure 1. Without loss of generality, the figure considers the case of a flat, rectangular element bounded by points \((x, y, z) = (1,0,0), (0,1,0), (0,1,2) \) and \((1,0,2) \), with the collocation point lying at \((1,0.7,0) \) and the plane wave direction \( d_{jm} = (0,0,1) \). A moderately small wave number \( k = 40 \) is considered for clarity of presentation. Figure 1(a) shows contours of the real part of the integrand in (16), considering \( \mu(x) \) for the double layer potential, displayed on axes of the planar parameterisation \((\xi, \eta) \). Figure 1(b) shows the sets of major and minor lines generated using \( g_{jm}(x) \) for this particular case, and Figure 1(c) shows a set of quadratic subdivisions generated from the orthogonal set of major and minor lines. In Figure 1(c) circles are used to mark the points defining the quadratic geometry of the subdivisions; it should be remembered that these points are not nodes in the normal BEM/FEM sense and that no degrees of freedom are associated with these points. We reserve discussion of Figure 1(d) until the last paragraph in this section.

In subdividing \( \Gamma_e \) according to (18) we introduce for each quadratic subdivision a local parameterisation for each basis wave direction, \( m \), using
\[ \Gamma_{eq} = \{ \gamma_{eq}(\xi_{eqm}, \eta_{eqm}) : (\xi_{eqm}, \eta_{eqm}) \in [-1,1]^2 \} \]  
(19)
Figure 1: Flat rectangular element: (a) Real part of integrand (b) Major and minor contours (minor contours follow the wave crests in the integrand) (c) Quadratic subdivisions (d) Shaded subdivisions requiring augmentation
where \( \gamma_{eq} : \mathbb{R}^2 \rightarrow \mathbb{R}^3 \), such that the coordinate \( \eta_{eqm} \) lies in the direction in which the integrand is oscillatory. The parameterisation is independent of the node \( j \). For clarity of presentation we henceforth denote by \((\xi', \eta')\) the coordinates \((\xi_{eqm}, \eta_{eqm})\), and their implicit dependence on \((e, q, m)\) shall be assumed. Further, the implicit dependence \( x := x(\xi', \eta') \) shall be assumed. The evaluation of \( I_e \) reduces now to the summation over all subdivisions of a number of integrals of the form

\[
I_{eqjmn} = \int_{-1}^{+1} \int_{-1}^{+1} \mu(x) \frac{N_j(x) e^{ikg_{jmn}(x)}}{4\pi} J_1(\xi', \eta') d\xi' d\eta'.
\] (20)

A new Jacobian \( J_1 \) is introduced for the mapping \( \gamma_{eq} \). Readers will notice that the integrand is approximately non-oscillatory in the direction \( \xi' \), and so a low order quadrature may be used in this direction. This is the essence of the new scheme. In practice, the integrand exhibits a small oscillation in this direction for the reasons of (i) the quadratic approximation to the minor contour, and (ii) the effect of the terms other than the exponential term in (20). Honnor & Trevelyan [20] found that 8th order quadrature is sufficient in the \( \xi' \) direction over each subdivision in order that the errors be of the same order as the high order quadrature scheme of [12]. It is noted that the method shares conceptual similarities with the 2D PU-FEM approach of Ortiz & Sanchez [16], but extended to handle the curvature in the required local coordinate of integration that results from both the inclusion of the Green’s function in the integrand and the possibility of curved 3D scatterer surfaces.

The scheme may be further enhanced by the use of the method of steepest descent (Bender & Orszag [21]) for the evaluation of oscillatory integrals. This approach may be applied numerically as described by Huybrechs & Vandewalle [22] and has been applied to 2D PU-BEM boundary integrals by Trevelyan et al. [23]. It may be feasible to apply the method of numerical steepest descent to the bidimensional integrals (20) arising in 3D PU-BEM. A simpler, yet efficient, scheme is proposed, as described in the following paragraphs, in which 1D steepest descent integrals are used in conjunction with the element subdivision approach.

The boundary integral (20) contains the product of a slowly varying function that we shall denote \( f(\xi', \eta') \), and the oscillatory function, \( e^{ikg(x)} \). We now consider evaluating this integral over a subdivision \( \Gamma_{eq} \) using quadrature in one direction only, viz.

\[
I_{eqjmn} = \int_{-1}^{+1} \int_{-1}^{+1} f(\xi', \eta') e^{ikg(x)} d\xi' d\eta'
\] (21)

\[
\simeq \sum_{l=1}^{L} w_l \int_{-1}^{+1} f(\xi_l, \eta') e^{ikg(x)} d\eta'
\] (22)

where \( \xi_l \) and \( w_l \) are the \( L^{th} \) order Gauss-Legendre abscissae and weights respectively. Each of the integrals in the summation in (22) may be considered using the method of numerical steepest descent. Here, the integral over the
real interval $\eta' \in [-1, 1]$ is replaced by an equivalent integral over a path in the complex plane $h$. The path originates at $h = -1 + 0i$ and is found to go to infinity before returning to close at $h = +1 + 0i$, thus preserving the limits of the integral in (22). The path taken is the locus of points satisfying

$$g(h) = g(x(\eta')) + ip$$  \hfill (23)

where $p \in \mathbb{R}$ becomes the variable over which we integrate. This path is chosen since substitution of (23) into (22) yields

$$I_{eqjm} = \sum_{l=1}^{L} w_l e^{ikg(x(\eta'))} \int_0^\infty f(p)e^{-kp} \frac{\partial g}{\partial p} dp|_{\Gamma_{a-c}} - \sum_{l=1}^{L} w_l e^{ikg(x(\eta'))} \int_0^\infty f(p)e^{-kp} \frac{\partial g}{\partial p} dp|_{\Gamma_{b-d}}$$  \hfill (24)

in which $\Gamma_{a-c}$ and $\Gamma_{b-d}$ are the integration paths, which are shown in typical form in Figure 2. Thus the integral becomes one of a non-oscillatory (indeed, exponentially decaying) function in the scalar $p$, and may be evaluated efficiently using Gauss-Laguerre quadrature. Over the path $\Gamma_{a-c}$ we take $\eta' = -1$, and over the path $\Gamma_{b-d}$ we take $\eta' = 1$. The paths may readily be found iteratively using, for example, Newton Raphson to find coordinates in $h$ satisfying (23) for the values of $p$ at the Gauss-Laguerre quadrature abscissae. The path $\Gamma_{c-d}$, which readers might suspect is needed to complete a closed contour of integration, has been omitted from the integral statement since it occurs at $p = \infty$, and the integral over $\Gamma_{c-d}$ vanishes as a result of the term $e^{-kp}$ in the integrand. For the most part, the integrals over the paths $\Gamma_{a-c}$ and $\Gamma_{b-d}$ may be evaluated accurately using an $8^{th}$ order Gauss-Laguerre quadrature, in a similar fashion to that shown by Trevelyan et al. [23] for 2D PU-BEM integrals. However, differentiation of (23) shows that

$$\frac{\partial h}{\partial p} = i \left( \frac{\partial g}{\partial h} \right)^{-1}$$  \hfill (25)

and the steepest descent integrals become singular when $\partial g/\partial h$ vanishes. As has been found in 2D [23], we further find that in 3D some cases require special treatment if $|\partial g/\partial h|$ falls below a certain threshold at the start and/or end of the path. This treatment involves a change of coordinate

$$p = y^u$$  \hfill (26)

so that the integrals over the steepest descent paths become transformed to the form

$$\int_0^\infty f(y^u)e^{-k y^u} i \left( \frac{\partial g}{\partial h} \right)^{-1} y y^{-1} dy$$  \hfill (27)

which may be evaluated by Gauss-Legendre quadrature since the presence of $y^{-1}$ in the numerator cancels the singularity. This approach is also required for cases involving stationary points (i.e. points at which $\partial g/\partial h = 0$) in the
real interval. In principle, \( u = 2 \) should be sufficient to cancel the singularity at \( p = y = 0 \), but numerical experiments have shown that these integrals are best evaluated using \( u = 4 \) and taking 64 Gauss points in the truncated interval \( y \in (0, (4.5\lambda)^2) \). For cases in which the value of \( |\partial g/\partial h| \) at the element ends becomes very small (numerical tests suggest a threshold of \( 10^{-3} \)), the method of steepest descent fails and our algorithm reverts to high order quadrature along the real axis.

Use of the method of steepest descent requires care over the presence of stationary points/singularities in the integrand in the region of the complex plane \( h \) contained within the contour of integration. The situation is ameliorated somewhat by the observed behaviour that typically \( p \to \infty \) quickly with \( 3(h) \), particularly at high wave number \( k \), and so the contour of integration encloses a comparatively small region, but a robust implementation will require detailed consideration of these cases. Moreover, it has been found in 2D PU-BEM using this approach that care is also required in respect of a branch cut in the square root function which is implicitly present in the Euclidean distance \( r \) \([24]\). It is important that the appropriate branch be followed in order to satisfy the requirements of Cauchy's integral theorem. The full analysis of the points raised in this paragraph is a subject for further research in 3D PU-BEM.

As a final remark, and one that introduces the new adaptation of this scheme, we return to Figure 1(d), which depicts with shading some subdivisions around the periphery of the element for which the low order scheme is inadmissible, since the \( \xi' \) direction for these subdivisions does not coincide with lines of constant \( g_{jm}(x) \). Honnor & Trevelyan \([20]\) reverted here to a high order quadrature, incurring a similar computational cost to the scheme of \([12]\), but found that, small though these peripheral subdivisions may be, they dominated the number of computations and the complexity. It is the treatment of these subdivisions that is the focus of the following section.

3. **Augmented subdivisions.** The integration scheme presented in section 2 may not be directly applied to some subdivisions around the periphery of the element. Examples are illustrated by shading in Fig. 1(d). Cases requiring further consideration for this reason include the following:
1. three-sided subdivisions, in the corners of the element, in which no edge of the subdivision is a contour \( g_{jm}(x) = \text{const.} \).

2. four-sided subdivisions which do not contain a pair of opposite edges, both of which are contours \( g_{jm}(x) = \text{const.} \).

3. subdivisions with greater than four edges.

A simple approach to the problem of integrating in these cases is provided by augmenting them to include regions outside the parent element \( \Gamma_e \). Let \( \Gamma_{et} \) be a member of the set of such subdivisions, and let us append to \( \Gamma_{et} \) a fictitious portion of parameterised boundary, denoted \( \Gamma_{et}^+ \), over the entirety of which \( (\xi, \eta) \notin [-1, 1]^2 \). We may then evaluate the integral of a smooth function \( (f(x) : x \in \Gamma_{et} \cup \Gamma_{et}^+) \) over \( \Gamma_{et} \) using

\[
\int_{\Gamma_{et}} f(x) d\Gamma = \int_{\Gamma_{et} \cup \Gamma_{et}^+} f(x) d\Gamma - \int_{\Gamma_{et}^+} f(x) d\Gamma, \quad x \in \Gamma_{et} \cup \Gamma_{et}^+.
\] (28)

The augmentation must be performed in such a manner as to allow the use of the scheme presented in Section 2 for both integrals in (28), but this is always possible. A typical situation is illustrated in Fig. 3, which shows a case in which the low order scheme is not directly applicable because the top edge of \( \Gamma_{et} \) is formed by the edge \( \eta = 1 \) of the parent element, and is not aligned with the behaviour of \( g_{jm}(x) \). Here, the augmentation \( \Gamma_{et}^+ \) is shown above the subdivision and is bounded by a new contour of equal \( g_{jm}(x) \). Note that, as for all triangular regions containing one edge defined by a contour \( g_{jm}(x) = \text{const.} \), the region \( \Gamma_{et}^+ \) may be considered using a local \((\xi', \eta')\) coordinate system in which \( \xi' = 0 \) passes through both the mid-point of the contour \( g_{jm}(x) = \text{const.} \) and the corner opposite that contour. Thus, both integrals in (28) may be considered now using the low order scheme, with or without the enhancement of numerical steepest descent. It is, of course, necessary for the augmentation \( \Gamma_{et}^+ \) to be defined geometrically using the same parameterisations as the parent element; it is independent of the geometry of the scatterer outside \( \Gamma_e \). Equivalent schemes may also be devised in which subdivisions \( \Gamma_{et} \) are further subdivided internally.

![Figure 3: Augmented subdivision \( \Gamma_{et}^+ \) defined outside the parent element](image-url)
The quadrilateral element considered in Figure 1 may be treated using augmented subdivisions as shown in Figure 4, so that all integrals may now be evaluated using low order quadrature in one direction. Details of the implementation of the algorithm are presented in Section 4. However, at this stage it is remarked that the contours of $g_{jm}(x)$ and the set of lines orthogonal to these contours are found numerically, and that the computational cost of this operation is very small in comparison with that of the low order quadrature.

![Figure 4: Augmented subdivisions for quadrilateral element example from Figure 1](image)

4. Implementation. Let us assume for the sake of simplicity that each of the $E$ elements in the model has the same number of nodes, $J$, and that the PUM expansion for the potential (8) is written so that all nodes have the same set of a total of $M$ plane wave basis functions. Let us also assume we have a total of $Z$ nodes, requiring us to collocate at a total of $P$ points, where $P \geq MZ$ is required for solution of (10). Note that the $P$ collocation points include a set distributed over the elements in addition to the extra collocation points prescribed inside the scatterer for the CHIEF method [11].

A total of $n_lPEJM$ integrals of the form (16) are required to be evaluated independently, where $n_l$ is the number of single and double layer potential operators remaining in the BIE following application of boundary conditions. The process of generating the subdivision of parent element $\Gamma_e$ into curved quadratic patches $\Gamma_{eq}$ is based on the behaviour of the function $g_{jm}$, which is identical for both single and double layer potentials, and is independent of the particular node being taken for the shape function term. Thus a total of $PEM$ element subdivisions of the form (18) are required for the new scheme.

The authors’ implementation of the subdivision process includes the following steps:

1. evaluate $\min(g_{jm})$ along each edge of the element $\Gamma_e$ to be subdivided.
2. for each minimum point found in step 1, determine the direction of the contour \( g_{jm} = \text{const.} \) If the contour is directed into the element, initiate a minor contour line \( g_{jm} = \text{const.} \).

3. advance the minor contour in steps (we use steps of size sufficient to cross the element in 300 steps), at each step locating iteratively a new point on the contour.

4. locate 7 equally spaced contour start locations along each edge of \( \Gamma_e \).

5. for each start location, if:
   
   (a) there is no previously defined contour that ends in the close vicinity of the start location, and
   
   (b) the angle between the direction of \( g_{jm} = \text{const.} \) and \( \partial \Gamma_e \) exceeds a threshold (we use 20°)

   generate a minor contour \( g_{jm} = \text{const.} \) from this start location that will follow the curved \( \xi' \) coordinate.

6. determine start points for the major contours that will follow the curved \( \eta' \) coordinate. These are taken to be:
   
   (a) any points found in step 1 from which minor contours are generated in step 2
   
   (b) equally spaced locations along the longest minor contour

7. from each of these start points, generate the major contours in steps, locating each new point iteratively to ensure the incremental portion of line remains perpendicular to \( g_{jm} = \text{const.} \).

8. subdivide further, in a similar fashion, if the curvature of \( g_{jm} \) causes the size of any subdivision to exceed a threshold value.

9. merge the ends of major and minor contours where they are closer together than some tolerance (we use 0.05 in (\( \xi, \eta \))) at the element edges. This is performed by moving the end of the major contour

10. locate points on each subdivision that will define the quadratic approximation to its geometry

11. identify subdivisions around the periphery of the element that require augmentation, and define the augmentation \( \Gamma_{et}^+ \) for each in a similar fashion to the above.

The numerical values for certain parameters, as used in steps 3, 4, 5 and 9 have been developed empirically. We note that there are cases in which the integrand in (16) exhibits a stationary point at \( (\xi_s, \eta_s) \in [-1, 1]^2 \), which lends a characteristic ‘bulls-eye’ appearance to contours of the integrand. In these cases the subdivision algorithm will fail and we revert to conventional quadrature.
Enhancement of the above algorithm to handle these cases is a subject for further research.

Numerical tests have shown that Gauss-Legendre quadrature using 8 points is sufficient in the non-oscillatory direction $\xi'$ over each subdivision, this giving errors of the same order as high order quadrature used in [12]. However, the quadrature order is increased to 12 points in this direction for elements considered in the augmentation process. If Gauss-Legendre quadrature is used in the oscillatory direction $\eta'$, i.e. the method of steepest descent is not used, we use a number of quadrature points sufficient to provide an average spacing of $\lambda/30$ when mapped back to the parent element $\Gamma_e$.

5. Numerical examples. The scheme presented in Sections 2 and 3 is applied in this Section to two cases: a flat triangular element and a curved triangular element.

**Flat element.** We consider the three-noded, flat triangular element bounded by vertices at $(x, y, z) = (1,0,0)$, $(0,1,0)$ and $(1,0,2)$. The collocation point lies at $(x, y, z) = (-1.0, 0.7, -0.6)$ and the plane wave considered is $d_{jm} = (-1, 0, 0)$. We take the wave number to be $k = 125, 250, 500, 1000$, so that the element spans approximately $40\lambda, 80\lambda, 160\lambda, 320\lambda$. The shape function $N_j$ is used for the node at the lower left corner as illustrated in figure 5, which depicts the element in $(\xi, \eta)$ space. The quadratic subdivisions for this case are shown in the figure. The augmented subdivisions $\Gamma^+_{et}$, required around the periphery of the element in this case, are clearly to be seen.

![Figure 5: Quadratic subdivisions for flat triangle, showing augmented subdivisions](image)

Table 1 shows the number of integration points required by the scheme, with and without the use of numerical steepest descent (nsd), and the relative error.
Table 1: Number of Gauss points (NGP) and relative error  $\varepsilon$ for for flat triangular element

<table>
<thead>
<tr>
<th>$k$</th>
<th>High order</th>
<th>New scheme</th>
<th>New scheme (nsd)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>NGP</td>
<td>$\varepsilon$</td>
<td>NGP</td>
</tr>
<tr>
<td>125</td>
<td>1 603 083</td>
<td>1.38 x 10$^{-12}$</td>
<td>61 576</td>
</tr>
<tr>
<td>250</td>
<td>6 412 332</td>
<td>2.92 x 10$^{-12}$</td>
<td>123 104</td>
</tr>
<tr>
<td>500</td>
<td>25 649 328</td>
<td>1.23 x 10$^{-11}$</td>
<td>246 256</td>
</tr>
<tr>
<td>1000</td>
<td>102 597 312</td>
<td>1.37 x 10$^{-12}$</td>
<td>492 492</td>
</tr>
</tbody>
</table>

$\varepsilon$, defined as

$$
\varepsilon = \max \left( \frac{\Re(I_1) - \Re(\tilde{I}_1)}{\Re(I_1)}, \frac{\Im(I_1) - \Im(\tilde{I}_1)}{\Im(I_1)}, \frac{\Re(I_2) - \Re(\tilde{I}_2)}{\Re(I_2)}, \frac{\Im(I_2) - \Im(\tilde{I}_2)}{\Im(I_2)} \right)
$$

where $I_1$ and $I_2$ are the integrals, $I_e$, of the single and double layer potential operators respectively and the tilde denotes a reference solution taken using a very high order Gauss-Legendre scheme of 256 points per wavelength in two dimensions. The number of Gauss points and relative error are shown, for comparison, for a high order scheme using 30 Gauss points per wavelength in each direction, as used in earlier work in which good accuracy of solution was found using plane wave basis integral equations [11].

We note the errors in the integrals using the new scheme are of the same order as the high order scheme, but that the required number of Gauss point evaluations has been markedly reduced. The enhancement of the new scheme by the use of numerical steepest descent brings about a further reduction in the number of Gauss point evaluations.

However, although the method of numerical steepest descent greatly reduces the required number of Gauss point evaluations, the method introduces significant extra computation. This arises both in the iterative determination of the integration path and in the introduction of complex arithmetic into calculations involving $\xi, \eta, r$. Table 2 shows the comparison between the three integration schemes in terms of CPU time instead of Gauss point evaluations. CPU times are normalised with respect to the time required for the new scheme at $k = 125$; true timings in CPU seconds on a 3.4GHz Pentium PC may be found by multiplying the normalised timings by 0.147. The timings exclude the (negligible) computation involved in subdividing the element.

It is clear that the new scheme is of complexity $O(k)$, whereas the expected $O(k^2)$ behaviour of the high order scheme is confirmed in the table. The complexity is shown to reduce to better than $O(1)$ when numerical steepest descent is used. The reduced CPU time at large $k$ results from shortening of the paths $\Gamma_{a-c}$ and $\Gamma_{b-d}$ in the complex plane. It is clear that an efficiently written code will adaptively adopt numerical steepest descent only if the wave number exceeds some threshold, a threshold that lies at $k \simeq 1750$ in this example, i.e.
Curved element. We consider the three-noded, curved triangular element having the same corner nodes as the flat triangular element considered in the first example. In the current example the element is curved such that it forms part of the surface of a cylindrical scatterer of unit radius, and whose axis is coincident with the z-axis. The element subtends an angle of $\pi/2$ in the circumferential direction. The quadratic subdivisions for this case are shown in Fig. 6. The location of the collocation point, the plane wave direction and shape function are as for the flat element example.

Tables 3 and 4 show the relative error $\varepsilon$ found using the various schemes when the element spans approximately 550$\lambda$.

It is noticeable that errors found using the numerical steepest descent algorithm are seen to increase somewhat at low wavenumber. This arises from the fact that the integrand becomes less dominated by the oscillatory component, and the coordinate $p$ increases more slowly with the imaginary abscissa, causing elongation of the path solving (23) over which the integral is taken in the complex plane.

<table>
<thead>
<tr>
<th>$k$</th>
<th>High order CPU</th>
<th>$\varepsilon$</th>
<th>New scheme CPU</th>
<th>$\varepsilon$</th>
<th>New scheme (nsd) CPU</th>
<th>$\varepsilon$</th>
</tr>
</thead>
<tbody>
<tr>
<td>125</td>
<td>24.80</td>
<td>$1.38 \times 10^{-12}$</td>
<td>1.00</td>
<td>$1.52 \times 10^{-12}$</td>
<td>16.93</td>
<td>$2.99 \times 10^{-10}$</td>
</tr>
<tr>
<td>250</td>
<td>99.16</td>
<td>$2.92 \times 10^{-12}$</td>
<td>2.16</td>
<td>$4.47 \times 10^{-12}$</td>
<td>18.59</td>
<td>$6.46 \times 10^{-13}$</td>
</tr>
<tr>
<td>500</td>
<td>396.63</td>
<td>$1.23 \times 10^{-11}$</td>
<td>4.37</td>
<td>$1.64 \times 10^{-11}$</td>
<td>15.93</td>
<td>$7.61 \times 10^{-12}$</td>
</tr>
<tr>
<td>1000</td>
<td>1585.71</td>
<td>$1.37 \times 10^{-12}$</td>
<td>8.61</td>
<td>$1.66 \times 10^{-11}$</td>
<td>15.47</td>
<td>$7.62 \times 10^{-12}$</td>
</tr>
</tbody>
</table>

Table 2: Normalised CPU time and relative error $\varepsilon$ for flat triangular element
alongside the number of integration points required and the associated normalised CPU times. The normalisation of CPU times is taken with respect to that required for the flat element integration for the case \( k = 125 \) to allow for clearer interpretation of the effect of element curvature.

The results for the curved element exhibit all the same features as were found for the flat element. The error in the numerical steepest descent computation at the lowest wave number, \( k = 125 \) has increased markedly with the introduction of curvature. It is also evident that, while the curvature has given rise to an increase in CPU time of 20% in the high order scheme and 30-40% in the new scheme, the time for the steepest descent method has increased by 130%. The area of the curved element is 11% larger than the flat element.

In the numerical tests run to date, it is common to find the timings for curved elements to exceed those for flat elements. Generally CPU times are 10-50% higher when curvature is introduced; the case presented in this paper is the example with the highest increase in CPU time we have found so far when corresponding flat and curved elements are compared. The source of the increase in CPU time is not clear, but the cases in which element curvature causes the greatest detriment to the computational efficiency all involve a much greater number of integrals requiring the transformation (26) and integration using (27). Methods for improving the efficiency of the numerical steepest descent procedure for these cases in which \(|\partial g/\partial h|\) is low at the path ends remain a subject for further research.

6. Conclusions. This paper has presented a numerical integration scheme
for the efficient evaluation of the highly oscillatory boundary integrals arising in Partition of Unity enriched approximations in three-dimensional short wave scattering. The two-dimensional integrals are transformed to an equivalent set of 1D integrals that may be evaluated cheaply yet with the high accuracy that is required for the solution of sets of equations that famously suffer from ill-conditioning.

The integration scheme may be enhanced by the use of numerical steepest descent, such that it exhibits better than $O(1)$ complexity. However, the extra computation involved means that this becomes a cost-effective enhancement only for integrals over boundary elements spanning more than about $50\lambda$.

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References


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