The Spherical Multipole Expansion of a Triangle

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Abstract

We describe a technique to analytically compute the multipole moments of a charge distribution confined to a planar triangle, which may be useful in solving the Laplace equation using the fast multipole boundary element method (FMBEM). This algorithm proceeds by performing the necessary integration recursively within a specific coordinate system, and then transforming the moments into the global coordinate system through the application of rotation and translation operators. While this method has currently only been implemented in conjunction with a simple piecewise constant collocation scheme, it can be generalized to non-uniform charge densities. This method has shown itself to be accurate and robust when applied to acute triangles, and fast in comparison to the two dimensional quadrature methods which are often employed to evaluate the multipole expansion coefficients of boundary elements.

Keywords: Multipole Expansion, Triangle, Spherical Harmonics, Boundary Element Method, Laplace Equation

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1. Introduction

The behavior of systems under electrostatic forces is governed by the electric field $E$, which can be expressed as the gradient of a scalar potential $\Phi$:

$$E = -\nabla \Phi$$ (1)

In the absence of free charges, the potential $\Phi$ is determined by the Laplace equation,

$$\nabla^2 \Phi = 0$$ (2)

for all points $x$ in the simply connected domain $\Omega$. The Laplace equation admits a unique solution for the field $E$ when the conditions on the boundary of the domain, $\partial \Omega$, are specified. The boundary conditions may be completely specified by associating either a value for the potential $\Phi$ (Dirichlet), or the derivative of $\Phi$ with respect to the surface normal $\frac{\partial \Phi}{\partial n}$ (Neumann), for every point on $\partial \Omega$.

One technique for numerically solving the Laplace equation is the boundary element method (BEM). Compared to other popular methods designed to accomplish the same goal, such as Finite Element and Finite Difference Methods [1], the BEM method focuses on the boundaries of the system rather than its domain, effectively reducing the dimensionality of the problem. BEM also facilitates the calculation of fields in regions that extend out to infinity (rather than restricting computation to a finite region) [2]. These two features make the BEM faster and more versatile than competing methods when it is applicable.

The basic underlying idea of the BEM involves reformulating the partial differential equation as a Fredholm integral equation of the first or second type, defined respectively as,

$$f(x) = \int_{\partial \Omega} K(x, y) \Phi(y) dy$$ (3)

and

$$\Phi(x) = f(x) + \lambda \int_{\partial \Omega} K(x, y) \Phi(y) dy,$$ (4)

where $K(x, y)$ (known as the Fredholm kernel), and $f(x)$ are known, square-integrable functions, $\lambda$ is a constant, and $\Phi(x)$ is the function for which a solution is sought. Discretizing the boundary of the domain into $N$ elements
and imposing the boundary conditions on this integral equation through either a collocation or Galerkin scheme results in the formation of dense matrices which naively cost $O(N^2)$ to compute and store and $O(N^3)$ to solve \cite{3}. This scaling makes solving large problems (much more than $\sim 10^4$ elements) impractical unless some underlying aspect of the equations involved can be exploited. For example, for the Laplace equation there exist iterative methods, such as Robin Hood \cite{4} \cite{5}, which take advantage of non-local charge transfer allowed by the elliptic nature of the equation to reduce the needed storage to $O(N)$ and time of convergence to $O(N^\alpha)$, with $1 < \alpha < 2$.

Another technique that has been used to accelerate the BEM solution to the Laplace equation, and has also found wide applicability in three dimensional electrostatic, elastostatic, acoustic, and other problems, is the fast multipole method (FMM) \cite{3}. The FMM was originally developed by V. Rohklin and L. Greengard for the two dimensional Laplace boundary value problem \cite{6} and N-body simulation \cite{7}. Fast multipole methods are appropriate when the kernel of the equation is separable or approximately separable so that, to within some acceptable error, it may be expressed as \cite{8},

$$K(x, y) \approx \sum_{k=0}^{p} \psi_k(x) \xi_k(y).$$

In the case of the Laplace equation, the kernel is often approximated by an expansion in spherical coordinates, with the functions $\psi_k(x)$ and $\xi_k(y)$ taking the form of the regular and irregular solid harmonics \cite{9}, \cite{10}. This expansion allows the far-field effects of a source to be represented in a compressed form by a set of coefficients known as the multipole moments of the source.

When applying BEM together with FMM in solving the Laplace equation over a complex geometry, it is necessary to determine the multipole moments of various subsets of the surfaces involved. At the smallest spatial scale, this requires a means of computing the individual multipole moments of each of the chosen basis functions (boundary elements). Geometrically, these basis functions usually take the form of planar triangular and rectangular elements, with the charge density on these elements either constant or interpolated between some set of sample points. Since rectangular elements cannot necessarily discretize an arbitrary curved surface without gaps or overlapping elements and can be decomposed into triangles, we consider it sufficient to compute the multipole expansion of basis functions of the triangular type.
2. Mathematical Preliminaries

For an arbitrary collection of charges bounded within a sphere of radius $R$ about the point $x_0$, there is a remote expansion for the potential $\Phi(x)$ given by [11], [7]:

$$\Phi(x) = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} \frac{Q_l^m Y_l^m(\theta, \phi)}{r^{l+1}}.$$  \hspace{1cm} (6)

This approximation converges at all points $|x - x_0| > R$. The coefficients $Q_l^m$ are known as the multipole moments of the charge distribution. The functions $Y_l^m(\theta, \phi)$ (known as the spherical harmonics), are given by:

$$Y_l^m(\theta, \phi) = N_l^m P_l^{|m|}(\cos \theta)e^{im\phi},$$  \hspace{1cm} (7)

where the coordinates $(r, \theta, \phi)$ are measured with respect to the origin $x_0$, and the function $P_l^{|m|}$ is the associated Legendre polynomial of the first kind. Several normalization conventions exist for the spherical harmonics; here we use the Schmidt semi-normalized convention with the normalization coefficients given by:

$$N_l^m = \sqrt{\frac{(l - |m|)!}{(l + |m|)!}}.$$  \hspace{1cm} (8)

When the charge distribution $\sigma(x')$ is confined to a surface $\Sigma$, the moments are given by the following integral:

$$Q_l^m = \int_{\Sigma} \sigma(x) Y_l^m(\theta, \phi) r^l d\Sigma.$$  \hspace{1cm} (9)

Here we have used a bar over the spherical harmonic to denote the complex conjugate. The integral given in equation (9) can be addressed in a straightforward manner through two dimensional Gaussian quadrature [12]. It can also be reduced to a one dimensional Gaussian quadrature if one first computes an auxiliary vector field and applies Stokes’ theorem, as described by Mousa et al [13]. However, for high-order expansions, accurate evaluation of the numerical integration becomes progressively more expensive. It is therefore desirable to obtain an analytic expression of the multipole moments.

For an arbitrary expansion origin and triangular surface element, Equation (9) is very difficult to compute analytically. In order to proceed, we
therefore make two simplifying restrictions on the general problem: we assume that the charge density $\sigma_0$ is constant over the triangle, and that we can always find a special coordinate system $S$ unique to each triangle in which to perform the integral [9].

3. Coordinate system for integration

In order to compute the multipole expansion of the triangle $\Sigma$ defined by points $\{P_0, P_1, P_2\}$, we first must select the appropriate coordinate system to simplify the integration. Without loss of generality, we choose a system so that the vertex $P_0$ lies at the origin, and the $\hat{e}_1$ direction is parallel to the vector $P_2 - P_1$. The plane defined by the triangle is then parameterized by the local coordinates $(u,v)$. Formally, this local coordinate system $S$ can be defined with the following origin and basis vectors:

$$S: \begin{cases} \mathcal{O} = P_0 \\ \hat{e}_0 = \frac{Q - P_0}{|Q - P_0|} \\ \hat{e}_1 = \frac{P_2 - P_1}{|P_2 - P_1|} \\ \hat{e}_2 = \hat{e}_0 \times \hat{e}_1 \end{cases}, \quad (10)$$

where $\{P_0, P_1, P_2\}$ are the points defining the triangle $\Sigma$ in the original coordinate system. The point $Q$ lies at $(h,0)$ in the $(u,v)$-plane and is the closest point to $P_0$, which lies on the line joining the points $P_1$ and $P_2$. It is given by:

$$Q = P_1 + \left( \frac{(P_0 - P_1) \cdot (P_2 - P_1)}{|P_2 - P_1|^2} \right) (P_2 - P_1). \quad (11)$$

Figure (1) shows the arrangement of this coordinate system.

Within $S$ the integration takes place entirely in the $(u,v)$-plane, therefore the integration over the $\theta$ coordinate can be trivially evaluated at $\theta = \pi/2$, and the integral reduces to:

$$Q_l^m = N_l^m P_l^m(0) \int_{\phi_1}^{\phi_2} \int_0^r \sigma_0 e^{-im\phi} r^{l+1} dr d\phi. \quad (12)$$

As can be seen in figure (1) the upper limit on the $r$ integration is given by:

$$r(\phi) = \frac{h}{\cos \phi}. \quad (13)$$
Figure 1: In (1a) the boundary element \( \Sigma \) (shaded region) is shown with arbitrary position and orientation in the global coordinate system. A detailed view of the local coordinate system \( S \), in which the integration is performed, is shown in (1b), where the \( w \) axis points out of the page.

Performing the integration over the \( r \) coordinate leaves us with:

\[
Q_l^m = \left( \frac{N_l^m h^{l+2} P_l^m(0)}{l+2} \right) \left( \prod_{i=1}^{K_{l,m}} \right) \int_{\phi_1}^{\phi_2} e^{-i m \phi} (\cos \phi)^{l+2} d\phi . \tag{14}
\]

The prefactors \( K_{l,m} \) are easy to compute. To address the integral \( \mathcal{I}_{l,m} \), we split our integrand into imaginary and real components, \( \mathcal{I}_{l,m} = \mathcal{A}_{l,m} - i \mathcal{B}_{l,m} \), where:

\[
\mathcal{A}_{l,m} = \int_{\phi_1}^{\phi_2} \frac{\cos(m \phi)}{(\cos \phi)^{l+2}} d\phi . \tag{15}
\]

and

\[
\mathcal{B}_{l,m} = \int_{\phi_1}^{\phi_2} \frac{\sin(m \phi)}{(\cos \phi)^{l+2}} d\phi . \tag{16}
\]
Before evaluating these integrals, we must first introduce the Chebyshev polynomials [14], [15]. The Chebyshev polynomials of the first kind $T_n(x)$ are defined recursively for $n \geq 0$ as:

$$T_0(x) = 1$$
$$T_1(x) = x$$
$$T_{n+1}(x) = 2xT_n(x) - T_{n-1}(x).$$

Similarly, the Chebyshev polynomials of the second kind, $U_n(x)$, are defined as:

$$U_0(x) = 1$$
$$U_1(x) = 2x$$
$$U_{n+1}(x) = 2xU_n(x) - U_{n-1}(x).$$

These polynomials are noteworthy for our purposes because of the two following useful properties:

$$T_n(\cos \phi) = \cos(n\phi)$$
$$U_n(\cos \phi) = \frac{\sin((n + 1)\phi)}{\sin \phi}.$$ 

We can exploit these in order to evaluate $A_{l,m}$ and $B_{l,m}$ recursively. We first address $A_{l,m}$. Using (23) we may rewrite (15) as:

$$A_{l,m} = \frac{\phi_2}{\phi_1} \int_{\phi_1}^{\phi_2} T_m(\cos \phi) \left(\frac{\cos \phi}{\cos \phi}\right)^{l+2} d\phi,$$

which can be expanded in terms of $T_{m-1}(x)$ and $T_{m-2}(x)$ using (19) to give

$$A_{l,m} = 2 \int_{\phi_1}^{\phi_2} T_{m-1}(\cos \phi) \left(\frac{\cos \phi}{\cos \phi}\right)^{l+1} d\phi - \int_{\phi_1}^{\phi_2} T_{m-2}(\cos \phi) \left(\frac{\cos \phi}{\cos \phi}\right)^{l+2} d\phi.$$

This yields the recursion relationship for the $A_{l,m}$:

$$A_{l,m} = 2A_{l-1,m-1} - A_{l,m-2}.$$
Similarly we may use the Chebyshev polynomial of the second kind \( U_2 \) to rewrite (16) as
\[
\mathcal{B}_{l,m} = \frac{\phi_2}{\phi_1} \int_0^{\phi_1} U_{m-1}(\cos \phi) \frac{(\cos \phi)^{l+2}}{\phi^{l+2}} \sin \phi d\phi
\] (28)
and derive the recursion relationship for the \( \mathcal{B}_{l,m} \), which unsurprisingly has the same form:
\[
\mathcal{B}_{l,m} = 2\mathcal{B}_{l-1,m-1} - \mathcal{B}_{l,m-2}.
\] (29)

Given these recursion relationships, we can reduce the integrals \( \mathcal{A}_{l,m} \) and \( \mathcal{B}_{l,m} \) of any degree \( 0 \leq l \) and order \( 0 \leq m \leq l \) into a series of terms, for which only the base cases must be evaluated explicitly. Figure (2) shows a representation of the recursion relationship.

Figure 2: Graphical representation of recursion given in equation (27) up to \( l = 3 \). Circles denote terms which must be computed as a base case, squares denote terms which may be computed by recurrence. The arrows indicate dependence. Higher order terms extend downwards and to the right, as denoted by the dotted lines and arrows.

Specifically, the integrals that are not further reducible by recursion are
the following: \( A_{l,0} \), \( A_{l,1} \), \( B_{l,0} \), and \( B_{l,1} \). Fortunately, all of these base cases have relatively simple solutions that either have a closed form, or a terminating reduction relation. Integrals of the form \( B_{l,0} \) are zero for all \( l \geq 0 \), while the \( B_{l,1} \) are given as follows:

\[
B_{l,1} = I_{l+2}^{1} = \int_{\phi_1}^{\phi_2} \frac{\sin \phi}{(\cos \phi)^{l+2}} d\phi
\]  

(30)

whereas both \( A_{l,0} \) and \( A_{l,1} \) are integrals of a power of secant \( I_p^0 \):

\[
I_p^0 = \int_{\phi_1}^{\phi_2} (\sec \phi)^p d\phi
\]  

(31)

with \( A_{l,0} = I_{l+2}^0 \) and \( A_{l,1} = I_{l+1}^0 \). The notation \( I_p^0 \) and these integrals are addressed in Appendix A.

It should be noted that during the process of computing the value of the \( Q_{l,m} \) moment through recursion, the real and imaginary parts of all moments with degree \( \leq l \) and order \( \leq m \) will be computed. These values can be stored so that there is no need to repeat the recursion for each individual moment needed. This is useful when determining the multipole expansion of a boundary element since all moments up to certain maximal degree can be computed in one pass through the recurrence.

4. Multipole moments under coordinate transformation

We can make use of the results of the preceding section to compute the multipole expansion coefficients of the boundary element \( \Sigma \) with respect to an arbitrary origin and set of coordinate axes. Typically, we are most interested in being able to construct the multipole moments \( M_j^k \) of \( \Sigma \) in the coordinate system that has the canonical Cartesian coordinate axes, with an origin at an arbitrary point \( S_0 \). We denote this system as \( S'' \):

\[
S'' : \begin{cases}
\mathcal{O} & = S_0 \\
\hat{e}''_0 & = (1, 0, 0) \\
\hat{e}''_1 & = (0, 1, 0) \\
\hat{e}''_2 & = (0, 0, 1)
\end{cases}
\]  

(32)

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Table 1: Euler angles in terms of the elements of the matrix $U$

| Angle | $U_{22} \neq \pm 1$ | $U_{22} = 1$ | $U_{22} = -1$ |
|-------|-------------------|--------------|---------------|
| $\alpha$ | $\text{atan2}\left(\frac{-U_{21}}{\sin \beta}, \frac{-U_{20}}{\sin \beta}\right)$ | 0 | $\pi$ |
| $\beta$ | $\cos(U_{22})$ | $\text{atan2}(U_{10}, U_{00})$ | $\text{atan2}(U_{01}, U_{11})$ |
| $\gamma$ | $\text{atan2}\left(\frac{-U_{12}}{\sin \beta}, \frac{-U_{02}}{\sin \beta}\right)$ | 0 | 0 |

Therefore, we must first construct the coordinate transformation $A : S \rightarrow S''$, and then determine how this coordinate transform operates on the coefficients $Q_{lm}^m$ of the multipole expansion given in $S$. The rigid motion $A : S \rightarrow S''$ can be specified by a rotation $U : S \rightarrow S'$ followed by a translation $T : S' \rightarrow S''$. We can describe the translation by the displacement $\Delta = S_0 - P_0$, and the rotation $U$ by the Euler angles $(\alpha, \beta, \gamma)$ following the $Z - Y' - Z''$ axis convention of [16] and [17]. The Euler angles allow us to write the rotation $U$ as the composition of three successive rotations $U = U_{Z''}(\gamma)U_{Y'}(\beta)U_Z(\alpha)$. Explicitly, $U$ is given by

$$U = \begin{bmatrix}
\cos \gamma & -\sin \gamma & 0 \\
\sin \gamma & \cos \gamma & 0 \\
0 & 0 & 1
\end{bmatrix} \begin{bmatrix}
\cos \beta & 0 & -\sin \beta \\
0 & 1 & 0 \\
\sin \beta & 0 & \cos \beta
\end{bmatrix} \begin{bmatrix}
\cos \alpha & -\sin \alpha & 0 \\
\sin \alpha & \cos \alpha & 0 \\
0 & 0 & 1
\end{bmatrix} \tag{33}
$$

and can be related to the basis vectors of the coordinate system $S$ by:

$$U = \begin{bmatrix}
U_{00} & U_{01} & U_{02} \\
U_{10} & U_{11} & U_{12} \\
U_{20} & U_{21} & U_{22}
\end{bmatrix} = \begin{bmatrix}
\hat{e}_0 \\
\hat{e}_1 \\
\hat{e}_2
\end{bmatrix}^T \tag{34}
$$

It is well known that the Euler angles $(\alpha, \beta, \gamma)$ do not uniquely describe an arbitrary rotation matrix $U$, however, a unique description is not necessary for our purposes. A convenient set of choices is given in table (1). With the transformation $A : S \rightarrow S''$ specified by the Euler angles $(\alpha, \beta, \gamma)$ and the displacement $\Delta$, we can determine the multipole moments of $\Sigma$ in $S''$ through the application of theorems (1) and (2).

Theorem (1), from Wigner [18], originates in quantum mechanics [19]. It appears when needing to express the result of the action of the rotation operator $D_l^m(\alpha, \beta, \gamma)$ upon a particular eigenstate $|l, m\rangle$ of total angular momentum $l$, which is associated with the spherical harmonic $Y_l^m(\theta, \phi)$, in terms
of the eigenstates of the rotated frame $|l', m'\rangle$. Note that since total angular momentum is conserved, this rotation operator does not mix states with a distinct value of $l$ (thus $l = l'$). Specifically, Wigner’s theorem tells us the matrix elements of the rotation operator $D^l(\alpha, \beta, \gamma)$, which is a member of the $(2l+1) \times (2l+1)$ matrix representation of $SO(3)$. A more succinct version of this theorem is given in [17], and is restated here in slightly a modified form.

**Theorem 1.** Assume there are two coordinate systems which share the same origin $S : (O, \hat{e}_0, \hat{e}_1, \hat{e}_2)$ and $S' : (O, \hat{e}_0', \hat{e}_1', \hat{e}_2')$, that are related by the rotation $U \in SO(3)$ specified by the Euler angles \{\alpha, \beta, \gamma\} such that $\hat{e}_i' = U \hat{e}_i$, for $i = 0, 1, 2$. Furthermore assume that there is a function $F(\theta, \phi)$ that can be expanded in terms of the spherical harmonics $Y^m_l(\theta, \phi)$ such that:

$$F(\theta, \phi) = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} Q^m_l Y^m_l(\theta, \phi)$$

then there exists a function $f(\theta', \phi')$ such that

$$f(\theta', \phi') = F(\theta(\theta', \phi'), \phi(\theta', \phi')) = \sum_{l=0}^{\infty} \sum_{m'=-l}^{l} q^m_l Y^m_l(\theta', \phi')$$

where the coefficients $q^m_l$ are given by:

$$q^m_l = \sum_{m=-l}^{l} D^l_{m', m}(\alpha, \beta, \gamma) Q^m_l$$

and elements of the Wigner matrix $D^l_{m', m}(\alpha, \beta, \gamma)$ are given by:

$$D^l_{m', m}(\alpha, \beta, \gamma) = e^{im' \gamma} d^{l}_{m', m}(\beta) e^{im \alpha}$$

with

$$d^{l}_{m', m}(\beta) = \left[\frac{(l + m'!)(l - m')!}{(l + m)! (l - m)!}\right]^{1/2} \times \sum_{\sigma} \left\{ (-1)^{l-m'-\sigma} \left(\begin{array}{c} l + m \\ l - m' - \sigma \end{array}\right) \left(\begin{array}{c} l - m \\ \sigma \end{array}\right) \times \left(\cos \frac{\beta}{2}\right)^{2\sigma + m' + m} \left(\sin \frac{\beta}{2}\right)^{2l - 2\sigma - m' - m} \right\}$$
where the summation over $\sigma$ is for all values where the entries of binomial coefficients are non-negative.

The direct evaluation of the coefficients $D_{m',m}^l(\alpha,\beta,\gamma)$ through the use of the expressions given by Wigner is known to be inefficient, as well as numerically unstable for large values of $l$ and certain angles [20]. However, given the wide applicability of spherical harmonics to quantum chemistry, fast multipole methods, and other areas, there has recently been a large effort to develop efficient and stable methods to perform such rotations in both real and complex spherical harmonic bases. The current state of the field of spherical harmonic rotation is well summarized by [21], with the algorithm developed by Pinchon et al. [16] being one of the fastest and most accurate. We will provide a brief description their algorithm here.

To avoid the need of complex matrix-vector multiplication, the method proposed by Pinchon et al. [16] is executed in the basis of real spherical harmonics $S_{0}^{m} (\theta, \phi)$. The real spherical harmonics as defined by Pinchon (note the difference in the normalization convention) are related to our definition of the complex spherical harmonics given in equation (7) by

$$S_{0}^{m} (\theta, \phi) = \sqrt{\frac{2l+1}{4\pi}} Y_{0}^{m} (\theta, \phi)$$

(40)

$$S_{l}^{m} (\theta, \phi) = \begin{cases} \frac{1}{\sqrt{2}} \left( \sqrt{\frac{2l+1}{4\pi}} \right) [Y_{l}^{m} (\theta, \phi) + (-1)^{m} Y_{l}^{-m} (\theta, \phi)] & : m > 0 \\ \frac{i}{\sqrt{2}} \left( \sqrt{\frac{2l+1}{4\pi}} \right) [(-1)^{m} Y_{l}^{m} (\theta, \phi) - Y_{l}^{-m} (\theta, \phi)] & : m < 0 \end{cases}.$$  

(41)

To apply a rotation to the set of multipole moments $\{Q_{l}^{m} \}$ with $l$ fixed and $m$ ranging from $-l$ to $l$ we first must calculate the corresponding real basis $\{R_{l}^{m} \}$ coefficients, such that

$$\sum_{m=-l}^{l} Q_{l}^{m} Y_{l}^{m} (\theta, \phi) = \sum_{m=-l}^{l} \frac{4\pi}{2l+1} R_{l}^{m} S_{l}^{m} (\theta, \phi),$$

(42)

using the relations given in (40) and (41). Then, to prepare this set of moments $\{R_{l}^{m} \}$ for the rotation operator we arrange them to form the column vector $\mathbf{R}_{l}$:

$$\mathbf{R}_{l} = \left[ R_{l}^{-1}, R_{l}^{-l+1}, R_{l}^{-l+2}, \ldots, R_{l}^{-l-1}, R_{l}^{l} \right]^T.$$  

(43)

The application of the Wigner $D_{l}$-matrix to this column vector produces the corresponding vector of rotated moments $\mathbf{r}_{l}$. For efficiency, the $D_{l}$-matrix is
itself decomposed into several matrices, each of which may be applied to the vector $\mathbf{R}_l$ in succession:

$$\mathbf{r}_l = \mathcal{D}^l(\alpha, \beta, \gamma)\mathbf{R}_l = [X_l(\alpha)J_l(\beta)J_l(\gamma)]\mathbf{R}_l$$  \hspace{1cm} (44)$$

In this notation, the $X_l$ matrices effect a rotation about the $z$-axis, while the $J_l$ matrices perform an interchange of the $y$ and $z$ axes. The advantage to this method is that the $X_l$ matrices have a simple sparse form whose action on the vector $\mathbf{R}_l$ can be computed quickly, as they consist only of non-zero diagonal and anti-diagonal terms. For example, for $l = 2$:

$$X_2(\alpha) = \begin{pmatrix} \cos(2\alpha) & 0 & 0 & 0 & \sin(2\alpha) \\ 0 & \cos(\alpha) & 0 & \sin(\alpha) & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & -\sin(\alpha) & 0 & \cos(\alpha) & 0 \\ -\sin(2\alpha) & 0 & 0 & 0 & \cos(2\alpha) \end{pmatrix}.$$  \hspace{1cm} (45)$$

The interchange matrices $J_l$, on the other hand, are completely independent of the rotation angles and therefore only need to be computed once. While the computation of $J_l$ is beyond the scope of this paper, there is an elegant recursive scheme to compute them up to any degree $l$ given by Pinchon et al. \[16\]. After the rotated moments $\mathbf{r}_l$ have been computed in the real basis, we need only convert them back to the complex basis through the inverse of equations (40) and (41) to obtain the set of moments $\{q'^m_l\}$.

Now that we have obtained the multipole moments $\{q'^m_l\}$ in the coordinate system $S'$, we need to determine how they are modified by a displacement of the expansion origin. This can be accomplished by the application of theorem (2). This theorem, presented by Greengard and Rohklin \[6\], \[7\], is a principle part of the fast multipole method, applied during the operation of gathering the multipole expansions of smaller regions into larger collections, and describes how a multipole expansion about one origin can be re-expressed as an expansion about a different origin. Graphically, this is represented in figure \[3\].

**Theorem 2.** Consider a multipole expansion with coefficients $\{O^m_n\}$ due to charges located within the sphere $D$ with radius $a$ centered about the point $\mathbf{P}_0$. This expansion converges for points outside of sphere $D$. Now consider the point $\mathbf{S}_0 \notin D$ such that $\Delta = \mathbf{S}_0 - \mathbf{P}_0 = (\rho, \alpha, \beta)$. We may form a new multipole expansion about the point $\mathbf{S}_0$ due to the charges within $D$ which
converges for points outside of the sphere \( D' \) which has its center at \( S_0 \) and radius \( a' = \rho + a \). The multipole moments of the new expansion \( \{M_j^k\} \) are given by:

\[
M_j^k = \sum_{n=0}^{j} \sum_{m=-n}^{m=n} O_{j-n}^{k-m} \frac{A^n_n A_{j-n}^k \rho^n Y_{n}^{-m}(\alpha, \beta)}{A_j^k}
\]

\[(46)\]

where

\[
A^n_n = \frac{(-1)^n}{\sqrt{(n-m)!(n+m)!}}.
\]

\[(47)\]

Immediately applying this theorem to the set of moments \( \{q_m^{n'j}\} \) results in the final objective of obtaining the multipole moments of the boundary element \( \Sigma \) in the coordinate system \( S'' \). However, the number of arithmetic operations required by the application of theorem (2) scales like \( O(p^4) \). This high cost can be mitigated by the use of a special case of theorem (2), by White et al. [22], and is stated in a form similar to that stated by [23], [24] below:

**Theorem 3.** Consider the situation given in theorem (2), in the case that the point \( S_0 \notin D \) is such that \( \Delta = S_0 - P_0 = (\rho, 0, 0) \). That is, \( S_0 \) lies on the \( z \)-axis above \( P_0 \). We may form a new multipole expansion about the point \( S_0 \), with the multipole moments of the new expansion \( \{M_j^k\} \) given by:

\[
M_j^k = \sum_{n=0}^{j} O_{j-n}^k A^n_n A_{j-n}^k \rho^n Y_0^{-n}(0, 0) \frac{A_j^k}{A_j^k}.
\]

\[(48)\]

Theorem (3) by itself is of course only directly applicable in rare circumstances. However, White et al. [22] noted that it can be applied to perform a multipole-to-multipole translation along any axis needed if a rotation is performed through the use of theorem (1) before and after the translation operation. The first rotation applied aligns the \( z \)-axis with the vector \( S_0 - P_0 \), while the second rotation is the inverse of the first. The use of the rotation operator together with the axial translation has a cost which scales like \( O(p^3) \), which for high-degree expansions can provide useful acceleration when compared to the implementation of theorem (2) alone.
Figure 3: Multipole to multipole translation. The solid shaded area indicates the region where the original multipole expansion \( \{O_n^m\} \) does not converge, the striped area indicates the region where the new multipole expansion \( \{M_{jk}^l\} \) does not converge.

5. Application to higher order basis functions

There are many schemes for function interpolation over triangular domains, such as the natural orthogonal polynomial basis put forth by [25], [26], [27] and [28], and the more commonly used variations on Lagrange and Hermite interpolation [29], [30], [31], [32]. For the sake of simplicity, we avoid these more advanced interpolation schemes in favor of a simpler but less well-conditioned bivariate monomial basis for the charge density. This basis is well suited to the method of integration described in the preceding sections, as it can be represented more naturally in the same coordinate system \( S \). Making a change of basis from some other interpolation method to the bivariate monomials is relatively straightforward; however, we will defer discussion of this change of basis and its application to low-order Lagrange interpolation to Appendix B.

We make the assumption that the interpolated charge density on the triangle can be expressed in terms of the local orthogonal coordinates \((u, v)\)
Figure 4: Planar boundary elements with various orders of charge density interpolation. Height above the element indicates the value of the local charge density.

by:

\[
\sigma(u,v) = \begin{cases} 
\sum_{a=0}^{N} \sum_{b=0}^{N-a} s_{a,b} u^a v^b : (u,v) \in \Sigma \\
0 : (u,v) \notin \Sigma
\end{cases}
\]  

(49)

where \(N\) is the order of the interpolation, the variables \((u,v)\) are as defined in figure (1), and \(s_{a,b}\) are the interpolation coefficients. For an example of various orders \(N\) of interpolation, see figure (4). It is possible to perform a change of basis on the interpolating polynomials [33] to compute the \(s_{a,b}\) coefficients in terms of the coefficients of some other polynomial basis; we leave discussion of this change of basis to Appendix B. As can be seen from figure (1) the local coordinates \((u,v)\) in terms of the polar coordinates \((r,\phi)\) are given by

\[
u(r,\phi) = r \cos \phi
\]

(50)

\[
v(r,\phi) = r \sin \phi.
\]

(51)

Inserting our expression for the charge density (49) and local coordinates (51) into (12) and exchanging the order of integration and summation results in:

\[
Q^m_{l} = \sum_{a=0}^{N} \sum_{b=0}^{N-a} s_{a,b} N^m_{l} P^m_{l}(0) \int_{\phi_1}^{\phi_2} \int_{0}^{r(\phi)} (\cos \phi)^a (\sin \phi)^b e^{-im\phi} e^{a+b+l+1} dr d\phi.
\]

(52)

Performing the integration over the \(r\) coordinate leaves us with:

\[
Q^m_{l} = \sum_{a=0}^{N} \sum_{b=0}^{N-a} \left( \frac{s_{a,b} h^{a+b+l+2}}{a+b+l+2} \right) N^m_{l} P^m_{l}(0) \int_{\phi_1}^{\phi_2} \frac{(\sin \phi)^b e^{-im\phi}}{(\cos \phi)^{b+l+2}} d\phi.
\]

(53)
We compute the integrals of the form $I_{l,m}^b$ by splitting into imaginary and real components, $I_{l,m}^b = A_{l,m}^b - iB_{l,m}^b$:

$$A_{l,m}^b = \int_{\phi_1}^{\phi_2} \frac{(\sin \phi)^b \cos(m \phi)}{\cos \phi)^{b+l+2}} d\phi$$

$$B_{l,m}^b = \int_{\phi_1}^{\phi_2} \frac{(\sin \phi)^b \sin(m \phi)}{\cos \phi)^{b+l+2}} d\phi.$$ (54)

Using (23), we may rewrite (54) as

$$A_{l,m}^b = \int_{\phi_1}^{\phi_2} \frac{(\sin \phi)^b T_m(\cos \phi)}{\cos \phi)^{b+l+2}} d\phi.$$ (56)

Expanding this using (19) gives

$$A_{l,m}^b = 2 \int_{\phi_1}^{\phi_2} \frac{(\sin \phi)^b T_{m-1}(\cos \phi)}{\cos \phi)^{b+l+1}} d\phi - \int_{\phi_1}^{\phi_2} \frac{(\sin \phi)^b T_{m-2}(\cos \phi)}{\cos \phi)^{b+l+2}} d\phi,$$ (57)

which yields the recursion relationship for the $A_{l,m}^b$:

$$A_{l,m}^b = 2A_{l-1,m-1}^b - A_{l,m-2}^b.$$ (58)

Similarly for the $B_{l,m}^b$, we have:

$$B_{l,m}^b = 2B_{l-1,m-1}^b - B_{l,m-2}^b.$$ (59)

Reducing the integrals $A_{l,m}^b$ and $B_{l,m}^b$ with this recursion relationship leaves us with the task of evaluating the base case integrals that are not further reducible: $A_{l,0}^b$, $A_{l,1}^b$, $B_{l,0}^b$, and $B_{l,1}^b$. Integrals of the form $B_{l,0}^b$ are zero for all $l \geq 0$ and $b \geq 0$, while the remaining base cases can all be expressed as:

$$A_{l,0}^b = I_{l+1}^b,$$ (60)

$$A_{l,1}^b = I_{l+2}^b,$$ (61)

$$B_{l,1}^b = I_{l+2}^b.$$ (62)

where

$$I_p^q = \int_{\phi_1}^{\phi_2} \frac{(\sin \phi)^q}{(\cos \phi)^p} d\phi.$$ (63)

The solution of $I_p^q$ is addressed in Appendix A.

The application of the coordinate transform to the moments $Q_{l,m}^n$ then follows as detailed in section (4). A summary of the full method by which to compute the multipole moments of a triangle is detailed in algorithm (1).
Algorithm 1 Computing the multipole moments of a triangular boundary element.

**Input:** Triangle Σ : \{P_0, P_1, P_2\} and associated charge density interpolation coefficients \{s_{ab}\}.

1: Compute height \( h \) and coordinate system \( S \) for triangle Σ according to equation (10).
2: for \( l = 0 \) to \( p \) do
3:     for \( m = 0 \) to \( l \) do
4:         for all \( s_{a,b} \neq 0 \) do
5:             Compute the prefactor \( K_{a,b}^{l,m} \) according to equation (53).
6:             Recursively compute the integral \( T_{l,m}^{b} \) according to equations (58) and (59).
7:         end for
8:     Compute the multipole moment \( Q_{l}^{m} = \sum_{a} \sum_{b} K_{a,b}^{l,m} T_{l,m}^{b} \) and \( Q_{-l}^{-m} = Q_{l}^{m} \).
9: end for
10: Compute the Euler angles (\( \alpha, \beta, \gamma \)) of the rotation \( U : S \rightarrow S' \) according to table (1).
11: Using theorem (1) compute the effect of the rotation \( U \) on the set of moments; \( \{Q_{l}^{m}\} \rightarrow \{q_{l}^{m'}\} \).
12: Using theorem (2) alone, or according to (22) through the use of theorem (1) and theorem (3) together, compute the effect of the translation \( \Delta : S' \rightarrow S'' \) on the moments; \( \{q_{l}^{m'}\} \rightarrow \{q_{l}^{m''}\} \).

**Output:** The multipole moments \( \{q_{l}^{m''}\} \) of the triangle Σ in coordinate system \( S'' \).
6. Numerical Results

In order to gain some understanding of the accuracy and efficiency of the algorithm presented in this work, some numerical tests were performed with regard to the problem of evaluating the electrostatic potential of a uniformly charged triangle. This simple scenario was chosen because there exists an analytic solution to the potential of a uniformly charged triangle [5], which makes absolute accuracy comparisons feasible. All of the following tests were performed in double precision.

Since the integrals required to compute the multipole expansion of boundary elements are typically evaluated using numerical quadrature, a straightforward two dimensional Gauss-Legendre quadrature method was used as a benchmark against which to compare the speed and accuracy of the analytic algorithm. The benchmark numerical integration is performed by first converting the integral over the triangular domain given by the points \{P_0, P_1, P_2\} to an integral over a rectangular domain through the use of a slightly modified version of the transform described by Duffy [34]. We can then write the surface integral given in equation (9) as:

\[
Q^m_l = \int_0^{L_2} \int_0^{L_1} \sigma_0 Y^m_l(\theta, \phi) |\mathbf{r}| \frac{\partial \mathbf{r}}{\partial u} \times \frac{\partial \mathbf{r}}{\partial v} \, dv \, du = \int_0^{L_2} \int_0^{L_1} f(u, v) \, dv \, du ,
\]

where \(\mathbf{r}(u, v) = \mathbf{t}(u, v) - \mathbf{x}_0\), and \(\mathbf{t}(u, v)\) is given by

\[
\mathbf{t} = \begin{bmatrix}
(P_0 + u \mathbf{n}_1 + v (1 - u/L_1) \mathbf{n}_2) \cdot \hat{x} \\
(P_0 + u \mathbf{n}_1 + v (1 - u/L_1) \mathbf{n}_2) \cdot \hat{y} \\
(P_0 + u \mathbf{n}_1 + v (1 - u/L_1) \mathbf{n}_2) \cdot \hat{z}
\end{bmatrix} ,
\]

with \(L_i = |P_i - P_0|\) and \(\mathbf{n}_i = (P_i - P_0)/L_i\), where \(i = 1, 2\), and the point \(\mathbf{x}_0\) is the origin of the expansion. The two dimensional integral over the \((u, v)\)-plane is then performed using \(m\)-th order two dimensional Gauss-Legendre quadrature [14], given by:

\[
Q^m_l = \frac{L_1 L_2}{4} \sum_{i=1}^{m} \sum_{j=1}^{m} w_i w_j f(u_i, v_j)
\]

where

\[
u_i = \frac{L_2}{2} (x_i + 1) \]
\[
v_j = \frac{L_2}{2} (x_j + 1)
\]
while $w_i$ and $x_i$ are the one-dimensional Gauss-Legendre weights and abscissa, respectively. These can be calculated as described by Golub et al. [35]. The orders of the quadrature rules that were considered were $m = \{4, 6, 8, 10\}$. It should be noted that this numerical integration routine is not the most efficient possible, and is only meant to provide a point of reference to a more commonly used means of computing the multipole coefficients. There are several techniques to accelerate the numerical integration over the benchmark we provide, such as adaptive quadrature [36] or quadrature rules specifically formulated for triangular domains. For example, Cowper [37] gives a 6-point rule with a degree of precision of 4, and a 12-point rule with a degree of precision of 6, which require roughly 3 times fewer function evaluations than the corresponding $4 \times 4$ and $6 \times 6$ two-dimensional rules used in this study. However, the computation of the weights and abscissa for an arbitrary order quadrature rule on a triangular domain is more complicated than the simple two-dimensional scheme, which are trivially generated from the one dimensional Gauss-Legendre weights and abscissa. For the sake of simplicity, these adaptive techniques and triangle-specific quadrature rules were not considered for this study.

The first study consisted of 100 randomly generated acute triangles, whose vertices were chosen to lie on the unit sphere. For each triangle the charge density was selected such that, at a single collocation point (the centroid), the potential as evaluated by the direct method was unity. This was done in order to normalize the scale of the absolute error such that the smallest measurable error is on the order of $10^{-15}$. Then, the multipole expansion of each triangle (up to degree $n = 32$) about the origin $x_0 = (0, 0, 0)$ was formed and $10^4$ points $x$ were selected within the volume $1 < |x - x_0| < 100$. These points had angular coordinates that followed a uniform distribution over the unit sphere, but the radial coordinate was chosen with a higher weight towards smaller radii in order to provide sufficient statistics in this region. At each point the absolute error between the direct potential and the potential given by the multipole expansion was computed for expansions of degree $n = \{1, 2, 4, 8, 16, 32\}$. Using the algorithm described in this work to compute the multipole coefficients, the absolute error on the potential is plotted as a function distance from the expansion origin divided by the radius of the region enclosing the charge in figure (5). For comparison, the accuracy of the multipole expansion when using two-dimensional Gauss-Legendre quadrature to compute the multipole coefficients is shown in figure (7).

It should be noted that the minimum possible error obtainable by the
Figure 5: Comparison of the accuracy of the multipole expansion against the direct method of evaluating the potential. Coefficients of the multipole expansion are calculated using the analytic method described in this paper. Absolute error is shown as a function of the ratio $|\mathbf{x} - \mathbf{x}_0|/R$, where $|\mathbf{x} - \mathbf{x}_0|$ is the distance of the evaluation point from the expansion origin, and $R$ is the radius of the smallest sphere enclosing the charge distribution.
multipole expansion is a slightly increasing function of distance. This trend is observed regardless of the technique used to compute the multipole moments of the source so it is likely attributable to round off error in either the direct potential calculation or in the calculation of the potential from the multipole expansion. However for our purposes this is not an important feature, since we are interested in demonstrating how quickly the expansion converges to this limiting error. As a general rule, as the degree of the expansion is increased the multipole approximation will converge to the minimum possible error at a smaller distance from the source. However, this is only true so long as the method used to compute the multipole moments of the expansion respects the oscillatory behavior of the spherical harmonics. For low degree expansions numerical quadrature rules with a small number of function evaluations can compute the the multipole moments exactly to within machine precision. However, as the degree of the expansion is increased the higher order spherical harmonics oscillate more rapidly and progressively more expensive quadrature rules are needed to evaluate the coefficients to equivalent accuracy. This effect can be seen in figure (7). For example, up to an expansion degree of $n = 8$, the $4 \times 4$ Gauss-Legendre quadrature rule is sufficient to compute the multipole coefficients to the same accuracy as our algorithm. However continuing to use the $4 \times 4$ Gauss-Legendre quadrature rule while increasing the degree of the expansion up to $n = 32$ does not result in a more accurate evaluation of the potential. To obtain the full benefit of a high degree expansion one must correspondingly increase the number of function evaluations used by numerical integration.

The second study demonstrates the efficiency of this algorithm as an alternative to simple two dimensional numerical integration. To do this, a comparison was made between the time needed to compute all of the multipole expansion coefficients of a single triangle (up to a certain degree) using the analytic algorithm and the time needed when using numerical integration. This test was carried out on a computer with an Intel i7 processor running at 1.9GHz, results are shown in figure (6). For all but the lowest degree $p \leq 4$ expansions, the performance of the algorithm presented in this work is approximately an order of magnitude faster than the lowest accuracy Gauss-Legendre quadrature rule considered, while for high order expansions $p \geq 16$, it is nearly two orders of magnitude faster than the quadrature rule which obtains equivalent accuracy.
7. Conclusion

We have presented a novel technique to evaluate the multipole expansion coefficients of a triangle. This method evaluates the necessary integrals through recursion within the context of a coordinate system with special orientation and placement. The results of the integration can then be generalized to the case of an arbitrary system through the well known transformation properties of the spherical harmonics under rotation and translation. Furthermore we have demonstrated that the application of this method to the multipole expansion of triangles with uniformly constant charge density compares favorably in terms of accuracy and speed to numerical integration. This method can also be extended to the case of non-uniform charge density, provided the interpolant can be represented as a sum over the bivariate monomials. We expect this method may find use in solving the three dimensional Laplace equation with the fast multipole boundary element method (FMBEM). We speculate that other boundary integral equation (BIE) problems, such as the Helmholtz equation in the low frequency limit \( k \to 0 \), could benefit from this approach if the integrand in the multipole coefficient integrals can be expanded in terms of the solid harmonics. Such will be the study of a following paper.
Figure 7: Comparison of the accuracy of the multipole expansion against the direct method of evaluating the potential. Coefficients of the multipole expansion are computed using two-dimensional Gauss-Legendre quadrature rules of varying precision.
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Appendix A. Integrals

The solutions to the integrals found in equations (30), (31), and (63) can be found in any standard table of integrals [38], [39]; however, for the sake of completeness we include the solutions and reduction formula here. Starting with equation (30) we have an integral of the form

\[
I^1_p = \int_{\phi_1}^{\phi_2} \frac{\sin \phi}{(\cos \phi)^p} d\phi , \tag{A.1}
\]

which may be solved by simple \(u\)-substitution, with \(u = \cos(\phi)\), which yields,

\[
I^1_p = -\int_{\cos \phi_1}^{\cos \phi_2} \frac{du}{u^p} = \left. \frac{u^{1-p}}{p-1} \right|_{\cos \phi_1}^{\cos \phi_2} . \tag{A.2}
\]

The integral in equation (31) is of the type:

\[
I^0_p = \int_{\phi_1}^{\phi_2} (\sec \phi)^p d\phi . \tag{A.3}
\]

This can be addressed with integration by parts, which yields the reduction relation,

\[
I^0_p = \frac{\sin \phi (\sec \phi)^{p-1}}{(p-1)} \bigg|_{\phi_1}^{\phi_2} + \left( \frac{p-2}{p-1} \right) I^0_{p-2} \tag{A.4}
\]

with the non-trivial base case:

\[
I^0_1 = \int_{\phi_1}^{\phi_2} \sec \phi d\phi = \ln |\tan \left( \frac{\phi}{2} + \frac{\pi}{4} \right) |_{\phi_1}^{\phi_2} . \tag{A.5}
\]
Both of the above integrals turn out to be special cases of equation (63), which has the form,

\[ I_p^q = \int_{\phi_1}^{\phi_2} \frac{(\sin \phi)^q}{(\cos \phi)^p} d\phi \]  

(A.6)

where \( p \) and \( q \) are positive integers. When \( p \neq q \), this integral can be simplified by the reduction relation:

\[ I_p^q = -\frac{(\sin \phi)^{q-1}}{(q-p)(\cos \phi)^{p-1}}\bigg|_{\phi_1}^{\phi_2} + \left( \frac{q-1}{q-p} \right) I_p^{q-2} \]  

(A.7)

until the base cases \( I_p^0 \) and \( I_p^1 \) are reached. If \( p = q \), we simply have an integral of a power of tangent,

\[ I_p^p = \int_{\phi_1}^{\phi_2} (\tan \phi)^p d\phi \]  

(A.8)

which in turn can be reduced with

\[ I_p^p = \frac{(\tan \phi)^{p-1}}{p-1} - I_{p-2}^{p-2} \]  

(A.9)

until reaching the non-trivial base case,

\[ I_1^1 = -\ln |\cos \phi|^{\phi_2}_{\phi_1}. \]  

(A.10)

Although most of these integrals do not have a simple closed form, the implementation of the base cases and reduction formula in computer code is a fairly simple task.

**Appendix B. Change of interpolating basis**

Since the calculation of section (5) proceeds assuming that the interpolant on the boundary element can be expressed in the basis of the bivariate monomials, in order to make these results relevant to the various interpolation methods often used (see for example, [29], [30], [31], [32]) we need to be able to change the basis of the interpolant. Explicitly, we would like to express the interpolant as a sum over the bivariate monomials. To do this, we must determine the coefficients of the bivariate monomials in terms of the original interpolation parameters. To motivate this section, we will consider the example task of changing from the bivariate Lagrange to bivariate monomial
basis. The objective we seek is to replace the tedious symbolic manipulation often encountered when performing a polynomial change of basis with a well defined numerical procedure. We expect that the results may apply to a wider class of interpolants other than Lagrange, though this extension is beyond the scope of this paper. To start, we will first introduce some basic definitions, with the assumption that the reader is familiar with the concept of a group and ring such as presented by [40] or [41].

Let $R[u,v]$ be the polynomial ring over the real numbers in the variables $u$ and $v$. Then for all $F(u,v) \in R[u,v]$, we may write $F(u,v)$ as the series,

$$F(u,v) = \sum_{a=0}^{n_f} \sum_{b=0}^{m_f} f_{a,b} u^a v^b$$  \hfill (B.1)

where the coefficients $f_{a,b} \in \mathbb{R}$, and $n_f, m_f \in \mathbb{N}_0$. The sum and product operations on this ring are defined in the usual sense as follows; for $F(u,v), G(u,v) \in R[u,v]$, the sum is given by:

$$F(u,v) + G(u,v) = H(u,v) = \sum_{a=0}^{n_h} \sum_{b=0}^{m_h} h_{a,b} u^a v^b \in R[u,v]$$  \hfill (B.2)

where $h_{a,b} = f_{a,b} + g_{a,b}$, and $n_h = \max(n_f, n_g)$ with $m_h$ defined similarly. The product is given by:

$$F(u,v) \cdot G(u,v) = K(u,v) = \sum_{a=0}^{n_k} \sum_{b=0}^{m_k} k_{a,b} u^a v^b \in R[u,v]$$  \hfill (B.3)

where

$$k_{a,b} = \sum_{i=0}^{a} \sum_{j=0}^{b} f_{i,j} \cdot g_{a-i,b-j}$$  \hfill (B.4)

and $n_k = n_f + n_h$ with $m_k$ similarly.

For a given polynomial $F(u,v)$, the greatest integer $a + b$ for which the coefficient $f_{a,b}$ is nonzero is called the maximal combined order of $F(u,v)$. We will denote the set of all bivariate polynomials $F(u,v) \in R[u,v]$ whose maximal combined order is $N$ as $P_N$. In general we may write any polynomial $S^{(N)}(u,v) \in P_N$ as follows

$$S^{(N)}(u,v) = \sum_{a=0}^{N} \sum_{b=0}^{N-a} s_{a,b} u^a v^b.$$  \hfill (B.5)
Consider for example the first order bivariate polynomial,

\[ s^{(1)}(u, v) = s_{0,0} + s_{0,1}u + s_{10}v. \]  (B.6)

This function can be also represented as the matrix vector product:

\[ s^{(1)}(u, v) = (1, u) \begin{bmatrix} s_{0,0} & s_{0,1} \\ s_{1,0} & 0 \end{bmatrix} \begin{pmatrix} 1 \\ v \end{pmatrix}. \]  (B.7)

The ability to write the above example in this manner motivates us to find a map between \( P_N \) and the set of \((N+1) \times (N+1)\) upper left triangular matrices, \( T_N \). In general, we expect that the bivariate polynomial \( S^{(N)}(u, v) \in P_N \), may be written in terms of a matrix vector product involving an upper left triangular matrix \( R^{(N)} \in T_N \) whose entries correspond to the coefficients \( s_{a,b} \) as follows:

\[ S^{(N)}(u, v) = (1, u, \ldots, u^N) \begin{bmatrix} s_{0,0} & s_{0,1} & s_{0,2} & \cdots & s_{0,N} \\ s_{1,0} & s_{1,1} & \cdots & \cdots & s_{1,(N-1)} & 0 \\ s_{2,0} & \cdots & s_{2,(N-2)} & 0 & \cdots & 0 \\ \vdots & \ddots & \ddots & \ddots & \ddots & \vdots \\ s_{N,0} & 0 & \cdots & 0 & 0 & \end{bmatrix} \begin{pmatrix} 1 \\ v \\ \vdots \\ v^N \end{pmatrix}. \]  (B.8)

Clearly, the set \( T_N \) forms a group under matrix addition, and this corresponds to the fact that \( P_N \) is also closed under addition. Unfortunately, \( P_N \) is not closed under the operation of polynomial multiplication \((\cdot)\), because repeated multiplication can produce a polynomial of arbitrarily large order. In order to construct a proper ring from the set \( P_N \) we must restore the property of closure by replacing the traditional product operator \((\cdot)\), with a new operator \((\odot)\) which we will define as multiplication combined with the truncation of terms with combined order larger than \( N \). Formally, for any two polynomials \( F(u, v), G(u, v) \in P_N \), this operator is given by:

\[ F(u, v) \odot G(u, v) = H(u, v) = \sum_{a=0}^{N} \sum_{b=0}^{N-a} h_{a,b} u^a v^b \in P_N \]  (B.9)
where,
\[ h_{a,b} = \sum_{i=0}^{a} \sum_{j=0}^{b} f_{i,j} \cdot g_{a-i,b-j}. \] (B.10)

We note the the (⊙) product defined in equation (B.9) only differs from the definition of normal polynomial multiplication in equation (B.3) by the limits on the summation. This definition leads us to the following lemma.

**Lemma 1.** The set \( P_N \) together with the binary operations + and ⋄ forms a ring.

In light of lemma (1) we would also like to find a binary operator on two matrices \( A, B \in T_N \) which mirrors the action of multiplication on the set \( P_N \) of bivariate polynomials. It is clear from inspection of equations (B.3) and (B.4) that multiplication (·) over the polynomials in \( R[u,v] \) corresponds with the two dimensional convolution (⋆) of the two matrices formed from the monomial coefficients. However, the set \( T_N \) is also not closed under the convolution operator (⋆). To restore this closure we will instead consider a different operator ⊙, specified in definition (1).

**Definition 1.** Let the two matrices \( A \) and \( B \) be elements of \( T_N \), then the action of the binary operator ⊙ on \( A \) and \( B \) produces another matrix \( C \in T_N \), whose elements are given by:

\[
C_{a,b} = \begin{cases} 
\sum_{i=0}^{a} \sum_{j=0}^{b} A_{i,j} B_{a-i,b-j} & a + b \leq N \\
0 & a + b > N 
\end{cases} \] (B.11)

Choosing the ⊙ operator to be defined as the product operation over \( T_N \) produces the following lemma.

**Lemma 2.** The set \( T_N \) together with the binary operations of matrix addition + and the operator ⊙ forms a ring.

To make use of the two rings \((P_N, +, ⊙)\) and \((T_N, +, ⊙)\) in the problem of determining the monomial coefficients of an interpolant, we now need a bijective map between the two which preserves the structure of the operations on each ring. Specifically, we need an isomorphism, \( \Lambda : (P_N, +, ⊙) \to T_N(P_N, +, ⊙) \). Equation (B.8) has already demonstrated the nature of \( \Lambda^{-1} : (T_N, +, ⊙) \to (P_N, +, ⊙) \) as a matrix vector product, and leads us to definitions (2) and (3), and theorem (4).
Definition 2. Since we may write all $F(u,v) \in P_N$ according to equation (B.5), we define the map $\Lambda : P_N \rightarrow T_N$ as $\Lambda(F(u,v)) = R$, where the entries of the matrix $R \in T_N$ are given in terms of the monomial coefficients of $F(u,v)$ by $R_{i,j} = f_{i,j}$ and are zero when $N < i + j$.

Definition 3. For all $R \in T_N$, we define the map $\Lambda^{-1} : T_N \rightarrow P_N$ as follows,

$$\Lambda^{-1}(R) = F(u,v)$$

(B.12)

where the bivariate polynomial $F(u,v) \in P_N$ is given by the following matrix vector product,

$$F(u,v) = u^T R v$$

(B.13)

where the column vectors $u$ and $v$ of length $N + 1$, have their $i$-th entry given (as powers of the variables $u$ and $v$) by $u^i$ and $v^i$ respectively.

Theorem 4. The inverse of the map $\Lambda : P_N \rightarrow T_N$, is given by $\Lambda^{-1} : T_N \rightarrow P_N$, moreover the map $\Lambda$ is a isomorphism from the ring $(P_N, +, \circ)$ to the ring $(T_N, +, \ast)$.

Now that we are in a position to make use of the isomorphism $\Lambda$, we will also make some assumptions on the class interpolants upon which we wish to make the change of basis. The first assumption is that interpolant $\Pi_N(u,v)$ of maximal combined order $N$ may be written in terms of a finite set of basis polynomials $\Phi_N \subset P_N$ as,

$$\Pi_N(u,v) = \sum_j U_j p_j^{(N)}(u,v)$$

(B.14)

where $p_j^{(N)}(u,v) \in \Phi_N$ and the $U_j$ are known as the interpolation coefficients. The second assumption is that any higher order basis function of the interpolant can be expressed as linear combination of products of the first order basis functions. We will term such a class of interpolants as simple according to definition (4).

Definition 4. Assume that a given class of two dimensional interpolating polynomials has the set of first order basis functions given by

$$\Phi_1 = \{ p_0^{(1)} , p_1^{(1)} , \ldots , p_m^{(1)} \} \subset P_1 .$$

(B.15)
Now consider all multi-sets $C_i$ of size $1 \leq k \leq N$, formed by making all possible combinations (with repetition allowed) from elements of $\Phi_1$. The number of multi-sets $C_i$ is given by:

$$M = \sum_{k=1}^{N} \binom{m+k}{k}$$

(B.16)

If the class of interpolants is such that any $N$-th order basis polynomial $p_j^{(N)}$ can be written as,

$$p_j^{(N)} = \sum_{i=0}^{M-1} \gamma_{i,j} \prod_{x \in C_i} x$$

(B.17)

where $\gamma_{i,j} \in \mathbb{R}$ and $C_i$ is the $i$-th multi-set of size $k \leq N$, and which for all $x \in C_i$, we have $x \in \Phi_1$, then we will call such a class simple. We will call the set of coefficients $\gamma_{i,j}$ together with the corresponding set of multi-sets $C_i$, the rule of this simple class.

With this definition in mind, we can now approach the problem of converting from a bivariate Lagrange basis to a bivariate monomial basis. Specifically, we wish to find the bivariate monomial coefficients of the polynomial $N$-th order Lagrange interpolant $\Pi_N(u,v)$. Computationally, this amounts to finding the entries of the matrix $\Lambda(\Pi_N(u,v)) = R^{(N)}$ given the set of interpolation coefficients $\{U_j\}$.

We will follow the notation of [29] and [30], who define the first order Lagrange interpolant for a triangle composed of vertices $P_j = (u_j, v_j)$ as:

$$\Pi_1(u,v) = \sum_{j=0}^{2} U_j p_j^{(1)}(u,v)$$

(B.18)

where,

$$p_j^{(1)}(u,v) = \frac{1}{2A}(\tau_{kl} + \eta_{kl}u - \xi_{kl}v)$$

(B.19)

and

$$\tau_{kl} = u_kv_l - v_ku_l$$

(B.20)

$$\xi_{kl} = u_k - u_l$$

(B.21)

$$\eta_{kl} = v_k - v_l$$

(B.22)
while \((j, k, l)\) is any cyclic permutation of \((0, 1, 2)\). The area of the triangle is denoted by \(A\). Within the context of the coordinate system \(S\), we have \(\mathbf{P}_0 = (0,0)\), and \(u_1 = u_2 = h\), so we may directly write down the basis functions \(p_j^{(1)}\) as:

\[
p_0^{(1)}(u, v) = \frac{1}{2A} [(v_1 - v_2)(u - h)]
\]

\[
p_1^{(1)}(u, v) = \frac{1}{2A} [v_2u - hv]
\]

\[
p_2^{(1)}(u, v) = \frac{1}{2A} [-v_1u + hv]
\]

which have the corresponding coefficient matrices of:

\[
R_0^{(1)} = \frac{1}{2A} \begin{bmatrix} h(v_2 - v_1) & (v_1 - v_2) \\ 0 & 0 \end{bmatrix}
\]

\[
R_1^{(1)} = \frac{1}{2A} \begin{bmatrix} 0 & v_2 \\ -h & 0 \end{bmatrix}
\]

\[
R_2^{(1)} = \frac{1}{2A} \begin{bmatrix} 0 & -v_1 \\ h & 0 \end{bmatrix}
\]

To obtain the bivariate monomial coefficients \(\pi_{a,b}\) of the polynomial \(\Pi_1(x, y)\) it is then only a simple matter of summing each matrix weighted with the appropriate Lagrange interpolation coefficient.

\[
\pi_{a,b} = \left[ \sum_{j=0}^{2} U_j R_j^{(1)} \right]_{a,b}
\]

In order to extend this to \(N\)-th interpolation we could again compute the coefficients \(\pi_{a,b}\) explicitly through direct inspection of the \(N\)-th order basis polynomials. However, for higher orders this quickly becomes tedious even with the use of a computer algebra system. Alternatively we can make use of the isomorphism \(\Lambda\) between the rings \((P_N, +, \circ)\) and \((T_N, +, \star)\). We note that since the bivariate Lagrange basis is a simple class of interpolating polynomials, we can express any \(N\)-th order basis functions according to equation \((\text{B.17})\) as:

\[
\Pi_N(u, v) = \sum_{j=0}^{(N+1)(N+2)/2-1} U_j p_j^{(N)}(u, v).
\]

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Furthermore, under the isomorphism $\Lambda$ the rule of the $N$-th order Lagrange basis can be re-expressed in the space of $T_N$ by:

$$R_j^{(N)} = \sum_{i=0}^{M-1} \gamma_{ij} \prod_{x \in C_i} \otimes \Lambda(x)$$  \hspace{1cm} (B.31)

where we use $\prod \otimes$ to denote a repeated product of the $\otimes$ operator over the matrices given by $\Lambda(x)$. This allows us to compute coefficient matrices $R_j^{(N)}$ directly from the first order coefficient matrices $R_j^{(1)}$ solely through matrix summation and the use of the $\otimes$ operator. Then, to compute the bivariate monomial coefficients $\pi_{a,b}$ we only need to perform the sum:

$$\pi_{a,b} = \left[ \sum_{j=0}^{(N+1)(N+2)/2-1} U_j R_j^{(N)} \right]_{a,b}. \hspace{1cm} (B.32)$$

As an example, consider the second order Lagrange interpolant, given by,

$$\Pi_2(u, v) = \sum_{j=0}^{5} U_j p_j^{(2)}(u, v)$$ \hspace{1cm} (B.33)

with the rule of the second order basis functions defined by:

$$p_j^{(2)}(u, v) = p_j^{(1)} \left( 2p_j^{(1)} - 1 \right) = 2 \left( p_j^{(1)} \right)^2 - p_j^{(1)} : 0 \leq j < 3$$ \hspace{1cm} (B.34)

$$p_j^{(2)}(u, v) = 4p_\epsilon^{(1)} p_\delta^{(1)} : 3 \leq j < 6$$ \hspace{1cm} (B.35)

where $\epsilon = j \text{ mod } 3$, and $\delta = (j + 1) \text{ mod } 3$. Using equation (B.31) to re-express equations (B.34) and (B.35) in terms of coefficient matrices, $R_j^{(2)}$, yields:

$$R_j^{(2)} = 2 \left( R_j^{(1)} \otimes R_j^{(1)} \right) - R_j^{(1)} : 0 \leq j < 3 \hspace{1cm} (B.36)$$

$$R_j^{(2)} = 4 R_\epsilon^{(1)} \otimes R_\delta^{(1)} : 3 \leq j < 6 \hspace{1cm} (B.37)$$

Thus the bivariate monomial coefficients of the polynomial $\Pi_2(u, v)$ can be computed in terms of the interpolation coefficients $U_j$ and coefficient matrices $R_j^{(2)}$ of the second order basis functions by:

$$\pi_{a,b} = \left[ \sum_{j=0}^{5} U_j R_j^{(2)} \right]_{a,b}. \hspace{1cm} (B.38)$$
In a similar fashion, this method can be applied to any class of simple interpolants, summarized in algorithm 2.

Algorithm 2 Compute bivariate monomial coefficients of a simple interpolant.

**Input:** Triangle $\Sigma : \{P_0, P_1, P_2\}$ and set of coefficients $\{U_j\}$ of the $N$-th order simple interpolant $S^{(N)}(u, v)$ with rule $(\{\gamma_{i,j}\}, \{C_i\})$.

1: Compute coordinate system $S$ for triangle $\Sigma$ according to equation (10).
2: Compute $(u, v)$ coordinates of $\{P_0, P_1, P_2\}$ in $S$.
3: Form the matrices $R_j^{(1)}$ of the coefficients of the 1st order polynomials in the bivariate monomial basis according to equations (B.26), (B.27), and (B.28).
4: Compute the coefficient matrices $R_j^{(N)}$ of the $N$-th order basis polynomials according to equation (B.31) and the rule $(\{\gamma_{i,j}\}, \{C_i\})$.
5: Sum the coefficient matrices $R_j^{(1)}$ weighted by their interpolation coefficient $U_j$ according to equation (B.32) to obtain the matrix $M$.
6: Map each element of $M$ to the bivariate monomials coefficient $s_{a,b}$ of $S^{(N)}(u, v)$ according to the isomorphism $\Lambda^{-1} : T_N \rightarrow P_N$.

**Output:** The set of bivariate monomials coefficients $\{s_{a,b}\}$ of $S^{(N)}(u, v)$.

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