

Unisolvency for Polynomial Interpolation in Simplices with Symmetrical Nodal Distributions

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Abstract In one dimension, nodal locations that are distinct are necessary and sufficient to ensure that a unique polynomial interpolant exists for data provided at a set of nodes, i.e. that the set of nodes is unisolvent. In multiple dimensions however, unisolvency for a polynomial interpolant of degree p is not ensured even with nodal locations that are distinct and a set of n nodes, with n equal to the cardinality of a set of polynomial basis functions of at most degree p . In this paper a set of equations is derived for simplices of one to three dimensions with symmetrical nodal distributions to identify a combination of symmetry orbits that can provide a unisolvent set of nodes. The results suggest that there is a unique combination of symmetry orbits that can provide a unisolvent set of nodes for each degree of polynomial interpolant. Consequently, all other combinations of symmetry orbits cannot provide a unisolvent set of nodes for a degree p polynomial interpolant. This is verified numerically up to degree 10 for triangles and degree 7 for tetrahedra. The results suggest that the same is also true for higher-order polynomial interpolants. This significantly reduces the number of combinations of symmetry orbits that needs to be considered. For example, for a tetrahedron with a degree seven interpolant, only one combination of symmetry orbits needs to be considered instead of the 161 different combinations of symmetry orbits that provide a set of nodes with n equal to the cardinality of the set of basis functions of at most degree seven. For a symmetrical nodal distribution in a simplex, the conditions presented are necessary but not sufficient to have a unisolvent set of nodes for polynomial interpolation.

Keywords Unisolvency · Multidimensional interpolation · Simplices · Symmetry orbits

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1 Introduction

1.1 Preliminaries

In this paper only polynomial interpolation is considered. Therefore, when a unisolvent set of nodes is mentioned, it implies a unisolvent set of nodes for polynomial interpolation.

A function might only be known at a finite set of nodes located within a domain. The value of the function on this set of nodes, known as the data, can be used to construct an interpolant to estimate the function elsewhere in the domain. A polynomial interpolant of degree p , denoted as \mathcal{P}_p , must satisfy

$$\mathcal{P}_p(\mathbf{x}_i) = y_i, \quad \forall i \in \{1, \dots, n\}, \quad (1)$$

where \mathbf{x}_i and y_i are the coordinates and value of the data, respectively, of the i -th node in a set of n nodes. A set of nodes is unisolvent if there is a unique polynomial that satisfies Eq. (1). For a set of nodes to satisfy Eq. (1) the number of nodes in the set must be equal to the cardinality of the basis, i.e. $n = N_{p,d}^*$, where

$$N_{p,d}^* \equiv \binom{p+d}{d}, \quad (2)$$

and d is the number of dimensions. The cardinality for one to three dimensions is $N_{p,1}^* = (p+1)$, $N_{p,2}^* = (p+1)(p+2)/2$, and $N_{p,3}^* = (p+1)(p+2)(p+3)/6$.

A set with $n = N_{p,d}^*$ nodes is unisolvent if and only if its Vandermonde matrix has a non-zero determinant. In one dimension, all that is required to have a unique polynomial interpolant are distinct nodal locations [2]. In multiple dimensions, distinct nodal locations are necessary but are insufficient to ensure unisolvency [2,9].

1.2 Non-unisolvency in multiple dimensions

Consider a square non-singular Vandermonde matrix with one row per node and one column per basis function. Swapping two rows in the Vandermonde matrix, which is the equivalent of switching the location of two nodes in a set of nodes, changes the sign of the determinant of the matrix. Since the determinant depends continuously on the nodal locations, the determinant of the Vandermonde matrix varies smoothly as the locations of the nodes are changed. Therefore, if two nodes in a simplex switch locations, the intermediate value theorem indicates that there is at least one set of nodal locations where the determinant of the Vandermonde matrix is zero, and thus the set of nodes is non-unisolvent. In one dimension, two nodes cannot change locations without having their paths cross, which is where the determinant of the Vandermonde

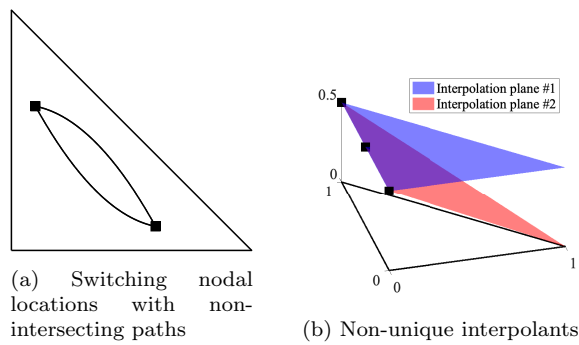


Fig. 1: How non-unisolvency arises in multiple dimensions.

matrix goes to zero since the nodal locations are no longer unique. However, in multiple dimensions there is an infinite number of paths that two nodes can take to switch locations without crossing each other, as shown in Fig. 1a.

When a set of nodes is non-unisolvent, there is not a unique polynomial interpolant that matches the data at each of the nodes. A simple example of this is shown in Fig. 1b. In this case, there is an infinite number of linear interpolants since the data at the three nodes vary linearly. However, if the data at the three nodes did not vary linearly, there would exist no linear interpolant that satisfies Eq. (1). This concept also applies in three or more dimensions as well as to higher order polynomial interpolants.

1.3 The need for unisolvency

Interpolation using multidimensional simplices requires a unisolvent set of nodes and it is common for all of the nodes to be in symmetry orbits [14,4]. With a unisolvent set of nodes, other interpolation aspects can be considered, such as minimizing the interpolation error, which is the difference between the function and an interpolant. The set of nodes that minimizes the Lebesgue constant, which enters into the bounds of the interpolation error in the infinity norm, is known as the Lebesgue nodes [3]. An alternative to Lebesgue nodes are Fekete nodes, which seek to maximize the determinant of the Vandermonde matrix [13]. Maximizing the determinant of the Vandermonde matrix helps minimize the Lebesgue constant but the Lebesgue constant of a set of Fekete nodes cannot be lower than for a set of Lebesgue nodes. Fekete and Lebesgue nodes with all the nodes in symmetry orbits have been generated on simplices of various dimensions for polynomial interpolants of numerous degrees [21,1,18].

Another important area where unisolvency is important is for certain methods that approximate derivatives in order to solve partial differential equations numerically. Various methods exist where unisolvency is necessary, such as node-based finite-element methods [6,11], flux reconstruction methods [23,

22], and multidimensional summation-by-parts methods with operators that have $n = N_{p,d}^*$ [12,17]. Various flux reconstruction operators are constructed in a paper by Witherden and Vincent using all of the combinations of symmetry orbits that give $n = N_{p,2}^*$. [23]. The process was subsequently repeated by Witherden *et al.* in three dimensions [22]. The authors of those papers derived flux reconstruction operators for triangles and found that over a thousand symmetrical nodal distributions were non-unisolvent, or a little more than half of all nodal distributions considered. Similarly, for tetrahedra over a hundred symmetrical nodal distributions were derived that were found to have non-unisolvent sets of nodes, which represent about 18% of all the sets of nodes considered. The authors of this paper suspect that the majority of operators that were derived with non-unisolvent sets of nodes did not use the unique combination of symmetry orbits that can provide a unisolvent set of nodes for triangles, which is derived in this paper.

1.4 Contributions from this paper

The presence of non-unisolvent sets of nodes in multiple dimensions is well known [2,9]. However, there is an incomplete understanding of the necessary conditions for a set of nodes to be unisolvent. It has been demonstrated for example that a set of nodes is unisolvent if the nodes lie in a lattice of a particular arrangement [5,15]. This lattice arrangement is sufficient but not necessary to have a unisolvent set of nodes and is somewhat limiting in terms of the nodal locations. Hesthaven and Teng [10] investigated spectral methods on tetrahedra which require unisolvent node sets. The authors noted that the sufficient conditions for unisolventy presented in [5] are strict and not necessary and consequently did not use them. On the other hand, little is known of the conditions that are necessary for unisolventy in multiple dimensions, other than the requirement that all of the nodal locations be distinct. This paper considers the conditions that are necessary, but not necessarily sufficient, to have a unisolvent set of nodes in triangles and tetrahedra when all the nodes are in symmetry orbits. These conditions are significantly less restrictive than the sufficient conditions from [5,15] and thus allow for several unisolvent sets that do not satisfy the sufficient conditions.

Roth [19] considered the interpolation properties of sets of nodes in a triangle. Both Fekete and Lebesgue nodes were derived with all of the nodes in symmetry orbits. Table 2.1 in [19] lists all of the combinations of symmetry orbits that give $n = N_{p,2}^*$ for p from 0 to 9 and indicates one combination of symmetry orbits for each degree p that gave the “best configuration”, i.e. the combination of symmetry orbits that was used to derive Fekete and Lebesgue nodes. This combination of symmetry orbits was found by using an equation that was determined empirically, but not proven. When generating Lebesgue points on triangles for polynomial interpolation of up to degree 18, Rapetti *et al.* [18] observed that only one combination of symmetry orbits provides a Vandermonde matrix with a determinant that is non-singular, i.e. a set of

nodes that is unisolvent. This observation suggests that there is a unique combination of symmetry orbits for a triangle that can provide a unisolvent set of nodes. In Section 3.3 a set of equations is derived to identify a combination of symmetry orbits that can provide a unisolvent set of nodes for a triangle. It is verified up to $p = 10$ that the identified combination of symmetry orbits is the unique one that can provide a unisolvent set of nodes. In Section 3.4 a similar approach is taken for tetrahedra and the results are verified up to $p = 7$.

The symmetry orbits for lines, triangles and tetrahedra that are used in the proofs are presented in Section 2. Section 3 demonstrates that some combinations of symmetry orbits cannot provide a set of nodes that is unisolvent. To have Lagrange nodes there needs to be at least one combination of symmetry orbits that provides a unisolvent set of nodes in a simplex for each polynomial degree. This is confirmed in Section 3, where it is demonstrated that there is a unique combination of symmetry orbits that can provide a unisolvent set of nodes for simplices of one to three dimensions. Finally, Section 4 demonstrates that even with the required combination of symmetry orbits to have a unisolvent set of nodes, non-unisolvency can still arise. Hence the conditions provided are necessary, but not sufficient for unisolvency.

2 Symmetry orbits

In this section we discuss barycentric coordinates and present the different symmetry orbits for simplices. We also discuss the use of integration and interpolation weights.

2.1 Construction of the symmetry orbits

Barycentric coordinates are indispensable when considering symmetry orbits for simplices. Barycentric coordinates provide the locations of nodes in an element relative to all of its vertices. For simplices, which have one more vertex than the number of dimensions, there is one more barycentric coordinate than there are dimensions. However, barycentric coordinates for simplices are made unique by enforcing the condition $\sum_{i=1}^{d+1} \lambda_i = 1$ where λ_i is the barycentric coordinate with respect to the i -th vertex. The barycentric coordinate of only one node per symmetry orbit is required since the coordinates of all the other nodes in the same symmetry orbit can be found by permuting the barycentric coordinates of that node. Table 1 lists the different symmetry orbits for simplices of one to three dimensions. The format for the names of the symmetry orbits is $S_{n,d}$, where n indicates the number of nodes in the symmetry orbit and d is the dimension of the simplex.

An alternative perspective to the use of barycentric coordinates is that symmetry orbits arise as the orbits of one point under the action of all the affine transformations of a simplex on itself. For example, if a node is placed at each of the vertices of a simplex, such as a triangle, then this set of nodes forms a symmetry orbit since it is invariant for all affine transformations.

Table 1: Barycentric coordinates of simplex symmetry orbits, where n is the number of nodes in each symmetry orbit ($\lambda_i \neq \lambda_j, \forall i \neq j$).

Simplex	Barycentric group	Barycentric coordinates	n
Line	$S_{1,1}$	$(\frac{1}{2}, \frac{1}{2})$	1
	$S_{2,1}$	$\text{Perm}(\lambda_1, 1 - \lambda_1)$	2
Triangle	$S_{1,2}$	$(\frac{1}{3}, \frac{1}{3}, \frac{1}{3})$	1
	$S_{3,2}$	$\text{Perm}(\lambda_1, \lambda_1, 1 - 2\lambda_1)$	3
	$S_{6,2}$	$\text{Perm}(\lambda_1, \lambda_2, 1 - \lambda_1 - \lambda_2)$	6
Tetrahedron	$S_{1,3}$	$(\frac{1}{4}, \frac{1}{4}, \frac{1}{4}, \frac{1}{4})$	1
	$S_{4,3}$	$\text{Perm}(\lambda_1, \lambda_1, \lambda_1, 1 - 3\lambda_1)$	4
	$S_{6,3}$	$\text{Perm}(\lambda_1, \lambda_1, \frac{1-2\lambda_1}{2}, \frac{1-2\lambda_1}{2})$	6
	$S_{12,3}$	$\text{Perm}(\lambda_1, \lambda_2, \frac{1-\lambda_1-\lambda_2}{2}, \frac{1-\lambda_1-\lambda_2}{2})$	12
	$S_{24,3}$	$\text{Perm}(\lambda_1, \lambda_2, \lambda_3, 1 - \lambda_1 - \lambda_2 - \lambda_3)$	24

With the exception of the centroid symmetry orbit, there are several locations where the nodes can be located within one symmetry orbit. This is demonstrated in Fig. 2 where several distinct groups of nodes are shown that are in the same symmetry orbit.

When we consider a combination of symmetry orbits we are looking for a unisolvent set of nodes with an integer number of symmetry orbits such that $n = N_{p,d}^*$. For example, if we consider the combination of symmetry orbits with two $S_{3,2}$ symmetry orbits then we have $n = N_{2,2}^* = 6$. The nodes in these two symmetry orbits could be anywhere in the symmetry orbit, such as at the black circles, the blue squares, or the red diamonds in Fig. 2a. Alternatively, we can get $n = N_{p,d}^* = 6$ with one $S_{6,2}$ symmetry orbit and the nodes could be, for example, at the black circles or blue squares in Fig. 2b.

Reference simplices are used in this paper to derive the required equations. However, the results are not limited to the reference simplices. Consider the orthogonal basis functions presented in [7] that are constructed using barycentric coordinates. We can thus construct a Vandermonde matrix with these basis functions using only the barycentric coordinates of a given set of nodes. If the determinant of the Vandermonde matrix is non-zero, then the set of nodes is unisolvent. We can then use their barycentric coordinates to form a unisolvent set of nodes on simplices with different vertices.

2.2 Integration and interpolation weights for nodes in symmetry orbits

In this paper we will use both integration and interpolation weights and we define what these entail here. Integration weights are used to integrate the interpolant over the simplex and are used to calculate

$$\int \mathcal{P}_p(\mathbf{x}) d\Omega = \sum_{j=1}^{N_{p,d}^*} y_j w_j, \quad (3)$$

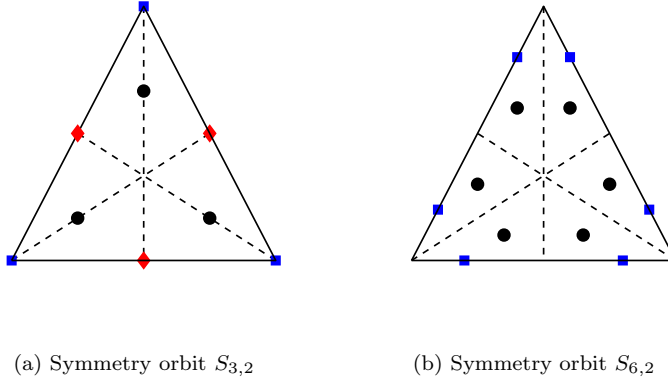


Fig. 2: Symmetry orbits for triangles.

where $d\Omega$ indicates we are integrating over the simplex and w_j is the integration weight for the j -th node. The interpolation weights are used to evaluate the interpolant at a point \mathbf{u}

$$\mathcal{P}_p(\mathbf{u}) = \sum_{j=1}^{N_{p,d}^*} y_j r_j(\mathbf{u}), \quad (4)$$

where r_j is the interpolation weight for the j -th node and its value depends on the point \mathbf{u} . To calculate the integration and interpolation weights we will use Lagrange basis polynomials. These can be used to construct the unique degree p interpolant for a unisolvent set of nodes

$$\mathcal{P}_p(\mathbf{x}_i) = \sum_{j=1}^{N_{p,d}^*} y_j l_j(\mathbf{x}_i), \quad (5)$$

where $l_j(\mathbf{x}_i) = \delta_{ij}$ [20]. We now consider

Theorem 1 *For a regular simplex with all of its nodes in symmetry orbits, the Lagrange bases $l_a(\cdot)$ and $l_b(\cdot)$ are symmetric about a symmetry plane of the simplex if \mathbf{x}_a and \mathbf{x}_b are symmetric about the same plane.*

Proof We denote the plane about which \mathbf{x}_a and \mathbf{x}_b are symmetric as the k -th symmetry plane. We use the transformation $\sigma_k(\mathbf{x}) = \hat{\mathbf{x}}$, where \mathbf{x} and $\hat{\mathbf{x}}$ are symmetric to one another about the k -th symmetry plane. It follows that $\mathbf{x}_a = \sigma_k(\mathbf{x}_b) = \hat{\mathbf{x}}_b$. We want to show that $l_a(\cdot)$ and $l_b(\cdot)$ are symmetric to each other about the k -th symmetry plane. Consider

$$l_a(\sigma_k(\mathbf{x}_i)) = l_a(\hat{\mathbf{x}}_i) = \begin{cases} 1 & \text{if } \hat{\mathbf{x}}_i = \mathbf{x}_a \\ 0 & \text{if } \hat{\mathbf{x}}_i \neq \mathbf{x}_a, \end{cases} \quad (6)$$

where it follows that, $l_a(\sigma_k(\mathbf{x}_i)) = l_b(\mathbf{x}_i) \forall \{1, 2, \dots, N_{p,d}^*\}$. A polynomial of degree p and dimension d is uniquely determined by $N_{p,d}^*$ points. Since $l_a(\sigma_k(\cdot))$

and $\ell_b(\cdot)$ are equal at $N_{p,d}^*$ points, it follows that they are the same polynomial. Therefore, $\ell_a(\cdot)$ and $\ell_b(\cdot)$ are symmetric about the k -th symmetry plane. This analysis can be used for each of the symmetry planes. This completes the proof.

We now use the results from Theorem 1 to prove the following two theorems.

Theorem 2 *If all the nodes are in symmetry orbits in a regular simplex, then the integration weights are identical for all of the nodes in the same symmetry orbit.*

Proof The integration of the interpolant over the simplex gives

$$\begin{aligned} \int \mathcal{P}_p(\mathbf{x})d\Omega &= \int \sum_{j=1}^{N_{p,d}^*} y_j \ell_j(\mathbf{x})d\Omega \\ &= \sum_{j=1}^{N_{p,d}^*} y_j \int \ell_j(\mathbf{x})d\Omega \\ &= \sum_{j=1}^{N_{p,d}^*} y_j w_j, \end{aligned} \quad (7)$$

where $w_j = \int \ell_j(\mathbf{x})d\Omega$. As was demonstrated in Theorem 1, a regular simplex with all of its nodes in symmetry orbits has Lagrange basis functions that are symmetric to each other about the symmetry planes. Therefore, the integral of the Lagrange basis functions, and consequently the integration weights, for all of the nodes in the same symmetry orbit are identical. This completes the proof.

Theorem 3 *Consider a regular simplex with all of its nodes in symmetry orbits. The interpolation weights for nodes that are symmetric about a symmetry plane are identical when interpolating the solution to a point on the same plane.*

Proof Let \mathbf{u} be a point on a symmetry plane of the simplex. When we evaluate the interpolant we find

$$\begin{aligned} \mathcal{P}_p(\mathbf{u}) &= \sum_{j=1}^{N_{p,d}^*} y_j \ell_j(\mathbf{u}) \\ &= \sum_{j=1}^{N_{p,d}^*} y_j r_j, \end{aligned} \quad (8)$$

where $r_j = \ell_j(\mathbf{u})$. It was shown in Theorem 1 that for two nodes located symmetrically about a symmetry plane, their Lagrange basis functions are

symmetric to each other about the same plane. Let \mathbf{x}_a and \mathbf{x}_b be two nodes located symmetrically about the symmetry plane that \mathbf{u} is located on. We have $\ell_a(\mathbf{u}) = \ell_b(\mathbf{u})$ and therefore $r_a = r_b$. If node \mathbf{u} is on two or more symmetry planes, then this same process can be used to relate additional interpolation weights. This completes the proof.

3 Interpolation with symmetry orbits

Some helpful relations that are used in the following subsections to derive equations are

$$\sum_{k=0}^b k = \frac{b(b+1)}{2} \quad (9)$$

$$\sum_{k=0}^b k^2 = \frac{b(b+1)(2b+1)}{6} \quad (10)$$

$$\sum_{k=a}^b (-1)^k = \frac{(-1)^b + (-1)^a}{2} \quad (11)$$

$$\left\lfloor \frac{x}{y} \right\rfloor = \frac{x - \text{mod}(x, y)}{y} \quad (12)$$

$$\text{mod}(x, 2) = \frac{1 - (-1)^x}{2}, \quad (13)$$

where $\lfloor x \rfloor$ is the floor operator, which returns the largest integer that is smaller or equal to x , and $\text{mod}(x, y)$ is the modulo operator, which returns the remainder of x divided by y . The ceiling operator $\lceil x \rceil$, which returns the smallest integer that is greater or equal to x , is also used in the following sections.

These equations will be used in the derivation of equations to determine the unique combination of symmetry orbits that can provide a unisolvent set of nodes. The derivation of equations for the line, triangle and tetrahedron follow a similar format. For each simplex an equation will be derived by requiring that $n = N_{p,d}^*$. An equation is also derived to determine if there is a node at the centroid of the simplex or not. For the triangle and tetrahedron an additional equation is derived by considering the integration of the polynomial interpolant over the simplex. Finally, for the tetrahedron, two additional equations are derived by considering the interpolation of data from the nodes in the symmetry orbits to other points that are on various symmetry planes.

In the derivation of the equations that involve the integration of the interpolant, the number of variables (weights) and the number of equations to consider is reduced since all the nodes are in symmetry orbits. The reduction in the number of interpolation and integration weights that need to be considered was demonstrated in Theorems 2 and 3, while the reduction in the number of equations is shown in subsequent theorems.

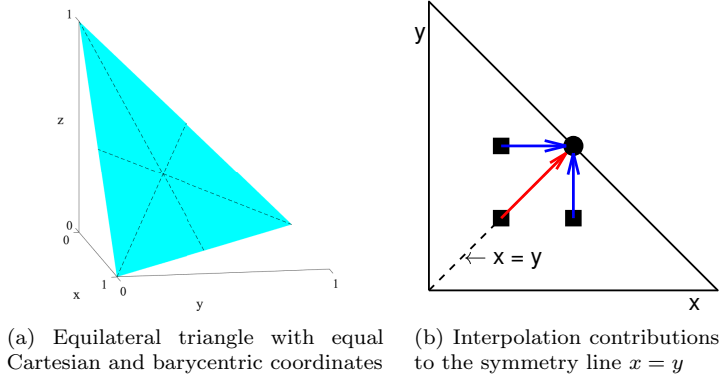


Fig. 3: Symmetry lines and contributions for a triangle.

3.1 Example of a combination of symmetry orbits that cannot provide a unisolvent set of nodes

In this subsection it is demonstrated that certain combinations of symmetry orbits cannot provide a unisolvent set of nodes, regardless of where the nodes are located within the symmetry orbit. A $p = 2$ interpolant on a triangle requires unique nodal locations and $n = \mathbf{N}_{p,2}^* = 6$ to be uniquely defined. The $S_{6,2}$ symmetry orbit provides the required six nodes. The parametrized x and y nodal locations for these six nodes in the $S_{6,2}$ symmetry orbit on a right triangle with vertices at $(0, 0)$, $(1, 0)$, and $(0, 1)$ are

$$\frac{1}{3} \times \begin{bmatrix} 1 - t_1 + 2t_2 & 1 + 2t_1 - t_2 \\ 1 - t_1 - t_2 & 1 - t_1 + 2t_2 \\ 1 + 2t_1 - t_2 & 1 - t_1 - t_2 \\ 1 + 2t_1 - t_2 & 1 - t_1 + 2t_2 \\ 1 - t_1 - t_2 & 1 + 2t_1 - t_2 \\ 1 - t_1 + 2t_2 & 1 - t_1 - t_2 \end{bmatrix},$$

where t_1 and t_2 are free parameters that allow the nodes to be anywhere in the symmetry orbit when $t_1, t_2 > 0$ and $t_1 + t_2 \leq 1$ [16]. To ensure none of the nodes are collocated $t_1 \neq t_2$ and $t_1, t_2 \neq 0$. A Vandermonde matrix is constructed with this set of nodes with the monomial basis

$$\mathbf{V} = \begin{bmatrix} 1 & \frac{1-t_1+2t_2}{3} & \frac{1+2t_1-t_2}{3} & \frac{(1-t_1+2t_2)^2}{9} & \frac{(1-t_1+2t_2)(1+2t_1-t_2)}{9} & \frac{(1+2t_1-t_2)^2}{9} \\ 1 & \frac{1-t_1-t_2}{3} & \frac{1-t_1+2t_2}{3} & \frac{(1-t_1-t_2)^2}{9} & \frac{(1-t_1-t_2)(1-t_1+2t_2)}{9} & \frac{(1-t_1+2t_2)^2}{9} \\ 1 & \frac{1+2t_1-t_2}{3} & \frac{1-t_1-t_2}{3} & \frac{(1+2t_1-t_2)^2}{9} & \frac{(1+2t_1-t_2)(1-t_1-t_2)}{9} & \frac{(1-t_1-t_2)^2}{9} \\ 1 & \frac{1+2t_1-t_2}{3} & \frac{1-t_1+2t_2}{3} & \frac{(1+2t_1-t_2)^2}{9} & \frac{(1+2t_1-t_2)(1-t_1+2t_2)}{9} & \frac{(1-t_1+2t_2)^2}{9} \\ 1 & \frac{1-t_1-t_2}{3} & \frac{1+2t_1-t_2}{3} & \frac{(1-t_1-t_2)^2}{9} & \frac{(1-t_1-t_2)(1+2t_1-t_2)}{9} & \frac{(1+2t_1-t_2)^2}{9} \\ 1 & \frac{1-t_1+2t_2}{3} & \frac{1-t_1-t_2}{3} & \frac{(1-t_1+2t_2)^2}{9} & \frac{(1-t_1+2t_2)(1-t_1-t_2)}{9} & \frac{(1-t_1-t_2)^2}{9} \end{bmatrix}. \quad (14)$$

The rank of this Vandermonde matrix is five, and thus the determinant is zero. This indicates that the set of nodes is non-unisolvent for any value of t_1 and

t_2 . In fact, $\text{rank}(\mathbf{V})$ can be lower but not greater for certain values of t_1 and t_2 . It was previously observed and demonstrated that this symmetry orbit cannot provide a unisolvent set of nodes for a $p = 2$ interpolant [8]. Other examples can be demonstrated for both triangles and tetrahedra with combination of symmetry orbits that give $n = N_{p,d}^*$ but cannot provide a unisolvent set of nodes. Sections 3.2, 3.3 and 3.4 demonstrate a method of determining which combinations of symmetry orbits can provide a unisolvent set of nodes.

3.2 Lines

Since there is a unique combination of symmetry orbits that provides $n = N_{p,1}^*$ for a given p , it is trivial to select the number of symmetry orbits required to have a unisolvent set of nodes for a given p in one dimension. Nonetheless, the methodology that is used to calculate the unique combination of symmetry orbits that can provide a unisolvent set of nodes for two- and three-dimensional simplices is first presented in one dimension. The equations are simple in one dimension and simplify the generalization to two and three dimensions.

There are two symmetry orbits in one dimension: $\mathbf{n}_{\text{Sym,1D}} = [n_{S_{1,1}}, n_{S_{2,1}}]^T$, where $n_{S_{1,1}}$, indicates the number of $S_{1,1}$ symmetry orbits and analogously for $n_{S_{2,1}}$. Two equations are derived that form a set of linear Diophantine equations, i.e. a system of equations with integers as solutions, that is used to solve for all the entries in $\mathbf{n}_{\text{Sym,1D}}$.

3.2.1 First equation

The first equation requires that the number of nodes is equal to the cardinality, i.e.

$$\begin{aligned} n &= N_{p,1}^* \\ [1, 2]\mathbf{n}_{\text{Sym,1D}} &= p + 1, \end{aligned} \quad (15)$$

where 1 and 2 are the number of nodes in the symmetry orbits $S_{1,1}$ and $S_{2,1}$, respectively.

3.2.2 Second equation

To ensure that no nodes are collocated, there can either be one or no centroid symmetry orbit. To determine the value of $n_{S_{1,1}}$ we consider the following theorem.

Theorem 4 *There is a node at the centroid of a line if and only if $\text{mod}(p, 2) = 0$.*

Proof Eq. (15) indicates that if $n_{S_{1,1}} = 0$, then $p + 1$ must be even for $n_{S_{2,1}}$ to be an integer. Therefore, $n_{S_{1,1}}$ is zero when $p + 1$ is even and one when $p + 1$ is odd. The value for $n_{S_{1,1}}$ can thus be calculated with

$$n_{\text{eq:cent.}} = 1 - \text{mod}(p, 2), \quad (16)$$

which completes the proof.

The equation that must be satisfied is thus

$$[1, 0] \mathbf{n}_{\text{Sym,1D}} = n_{\text{eq:cent.}}. \quad (17)$$

3.2.3 System of equations

Combining Eqs. (15) and (17) gives

$$\begin{bmatrix} 1 & 2 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} n_{S_{1,1}} \\ n_{S_{2,1}} \end{bmatrix} = \begin{bmatrix} N_{p,1}^* \\ n_{\text{eq:cent.}} \end{bmatrix}. \quad (18)$$

If we solve Eq. (18) we find

$$\begin{aligned} \begin{bmatrix} n_{S_{1,1}} \\ n_{S_{2,1}} \end{bmatrix} &= \begin{bmatrix} 1 & 2 \\ 1 & 0 \end{bmatrix}^{-1} \begin{bmatrix} N_{p,1}^* \\ n_{\text{eq:cent.}} \end{bmatrix} \\ &= \begin{bmatrix} 0 & 1 \\ 1/2 & 1/2 \end{bmatrix} \begin{bmatrix} N_{p,1}^* \\ n_{\text{eq:cent.}} \end{bmatrix} \\ &= \begin{bmatrix} n_{\text{eq:cent.}} \\ \frac{N_{p,1}^* + n_{\text{eq:cent.}}}{2} \end{bmatrix}. \end{aligned} \quad (19)$$

This system of equation always provides integer solutions. Consider when p is even, then $N_{p,1}^*$ is odd and $n_{\text{eq:cent.}} = 1$. Alternatively, if p is odd, then $N_{p,1}^*$ is even and $n_{\text{eq:cent.}} = 0$. Therefore, either $N_{p,1}^*$ and $n_{\text{eq:cent.}}$ are both even or both odd. Therefore, their sum is even and divisible by two. We have thus shown that there is a unique combination of symmetry orbits to provide a unisolvent set of nodes in one dimension. This method is extended to two dimensions in the following subsection.

3.3 Triangles

For a triangle there are three unique symmetry orbits:

$$\mathbf{n}_{\text{Sym,2D}} = [n_{S_{1,2}}, n_{S_{3,2}}, n_{S_{6,2}}]^T.$$

3.3.1 First equation

The first equation that is required is

$$\begin{aligned} n &= N_{p,2}^* \\ [1, 3, 6] \mathbf{n}_{\text{Sym,2D}} &= \frac{(p+1)(p+2)}{2}, \end{aligned} \quad (20)$$

where 1, 3 and 6 are the number of nodes in the symmetry orbits $S_{1,2}$, $S_{3,2}$, and $S_{6,2}$, respectively.

3.3.2 Second equation

There can either be one or no node at the centroid, i.e. $n_{S_{1,2}} \in \{0, 1\}$. The value of $n_{S_{1,2}}$ is determined by

Theorem 5 *There is a node at the centroid of a triangle if and only if $\text{mod}(p, 3) = 0$.*

Proof We begin by manipulating Eq. (20) to have $n_{S_{1,2}}$ on the right-hand side

$$[0, 1, 2]\mathbf{n}_{\text{Sym},2\text{D}} = \frac{\frac{(p+1)(p+2)}{2} - n_{S_{1,2}}}{3}. \quad (21)$$

In order to have integer solutions it follows that

$$\text{mod}\left(\frac{(p+1)(p+2)}{2}, 3\right) = \text{mod}(n_{S_{1,2}}, 3). \quad (22)$$

It is clear that $(p+1)(p+2)/2$ is always an integer since it is the product of two consecutive integers, thus one of them is even and divisible by two. If $n_{S_{1,2}} = 0$, then either $p+1$ or $p+2$ is divisible by 3, which implies that $\text{mod}(p, 3) \neq 0$. On the other hand, if $n_{S_{1,2}} = 1$, then neither $p+1$ nor $p+2$ is divisible by 3, which implies that $\text{mod}(p, 3) = 0$. This completes the proof.

An equation that returns one if $\text{mod}(p, 3) = 0$, and zero otherwise is given by

$$n_{\text{eq:cent.}} = 1 - \left\lfloor \frac{\text{mod}(p, 3)}{3} \right\rfloor. \quad (23)$$

The equation that must be satisfied is thus

$$[1, 0, 0]\mathbf{n}_{\text{Sym},2\text{D}} = n_{\text{eq:cent.}}. \quad (24)$$

3.3.3 Third equation

If a set of nodes is unisolvent, then there exists a unique interpolant and its integral over the triangle can thus be calculated. The unique interpolant of degree p can be constructed with $N_{p,d}^*$ basis functions, such as monomials. In order to integrate the unique interpolant exactly, each individual basis function must be integrated exactly, which gives $N_{p,d}^*$ equations. There is an equal number of variables since each node has an integration weight. However, we can reduce the number of equations and variables we need to consider since all the nodes are in symmetry orbits. This is considered in

Theorem 6 *If all of the nodes are in symmetry orbits and the triangle has the same Cartesian and barycentric coordinates, then only the basis functions $x^a y^b z^c$ with $a \geq b \geq c \geq 0$ and $a + b + c = p$ need to be considered for the integration of the basis functions over the triangle.*

Proof A triangle with matching Cartesian and barycentric coordinates, such as the one in Fig. 3a, is equilateral, which means its symmetry lines align with the symmetry planes $x = y$, $x = z$ and $y = z$. Furthermore, as a result of Theorem 2, all the nodes in the same symmetry orbit share the same integration weight. The monomials in two dimensions are $x^a y^b$ with $a + b \leq p$, which is equivalent to $x^a y^b z^c$ with $a + b + c = p$. We use the symmetry plane $x = y$ for our example and we consider both nodes that are on one of the symmetry planes and pairs of nodes that are located symmetrically about a symmetry plane, which would be in the same symmetry orbit. The coordinates of the nodes on the symmetry plane are (x_i, x_i, z_i) , and the coordinate of the other nodes are (x_j, y_j, z_j) , and (y_j, x_j, z_j) . $\mathcal{S}_{x=y}$ and $\mathcal{S}_{x \neq y}$ are the sets for the nodes that are and are not on the symmetry plane $x = y$, respectively. The integration of the basis function $x^a y^b z^c$ over the triangle is given by

$$\sum_{i \in \mathcal{S}_{x=y}} w_i x_i^{a+b} z_i^c + \sum_{j \in \mathcal{S}_{x \neq y}} w_j (x_j^a y_j^b z_j^c + y_j^a x_j^b z_j^c) = \int_0^1 \int_0^{1-y} x^a y^b (1-x-y)^c dx dy, \quad (25)$$

which is identical to the equation for the integration of the basis $x^b y^a z^c$. Therefore, only basis functions with $a \geq b$ need to be considered. The analysis can be repeated with the symmetry planes $x = z$ and $y = z$, which indicates that only basis functions with $a \geq b \geq c \geq 0$ need to be considered, which is the desired result.

The result of Theorem 6 is to limit the values that a , b and c can take to

$$p - b - c = a_{\min} = a = a_{\max} = p - b - c \quad (26)$$

$$c = b_{\min} \leq b \leq b_{\max} = \left\lfloor \frac{p-c}{2} \right\rfloor \quad (27)$$

$$0 = c_{\min} \leq c \leq c_{\max} = \left\lfloor \frac{p}{3} \right\rfloor. \quad (28)$$

The total number of equations that remain is

$$\begin{aligned} n_{\text{eq:elem}} &= \sum_{c=c_{\min}}^{c_{\max}} \sum_{b=b_{\min}}^{b_{\max}} 1 \\ &= \sum_{c=0}^{c_{\max}} (b_{\max} + 1 - b_{\min}) \\ &= \sum_{c=0}^{c_{\max}} \frac{-6c + (2p+3) + (-1)^{p+c}}{4} \\ &= \frac{(2p+3)(c_{\max}+1) - 3c_{\max}(c_{\max}+1) + (-1)^p \frac{1+(-1)^{c_{\max}}}{2}}{4} \\ &= \frac{2(p^2 + 6p + 9) - 2 \bmod(p, 3)^2 + 3(-1)^p \left(1 + (-1)^{\lfloor \frac{p}{3} \rfloor}\right)}{24}. \end{aligned} \quad (29)$$

Since all the nodes in a symmetry orbit share the same weight for the integration over the simplex, the equation that must be satisfied is

$$[1, 1, 1] \mathbf{n}_{\text{Sym},2\text{D}} \leq n_{\text{eq:elem}}. \quad (30)$$

We have proven that only the subset of basis functions with $a \geq b \geq c \geq 0$ needs to be considered. However, Theorem 6 does not rule out that there are additional basis functions that do not need to be considered, which is why there is an inequality. Nonetheless, the results to be presented in Section 3.3.4 suggest that Eq. (30) is an identity for a unisolvent set of nodes, i.e.

$$[1, 1, 1] \mathbf{n}_{\text{Sym},2\text{D}} = n_{\text{eq:elem}}. \quad (31)$$

3.3.4 System of equations

Combining Eqs. (20), (24) and (31) and assuming that Eq. (31) holds for a unisolvent set of nodes gives

$$\begin{bmatrix} 1 & 3 & 6 \\ 1 & 0 & 0 \\ 1 & 1 & 1 \end{bmatrix} \begin{bmatrix} n_{S_{1,2}} \\ n_{S_{3,2}} \\ n_{S_{6,2}} \end{bmatrix} = \begin{bmatrix} N_{p,2}^* \\ n_{\text{eq:cent.}} \\ n_{\text{eq:elem}} \end{bmatrix}. \quad (32)$$

We can solve this linear system to get

$$\begin{aligned} \begin{bmatrix} n_{S_{1,2}} \\ n_{S_{3,2}} \\ n_{S_{6,2}} \end{bmatrix} &= \begin{bmatrix} 1 & 3 & 6 \\ 1 & 0 & 0 \\ 1 & 1 & 1 \end{bmatrix}^{-1} \begin{bmatrix} N_{p,2}^* \\ n_{\text{eq:cent.}} \\ n_{\text{eq:elem}} \end{bmatrix} \\ &= \begin{bmatrix} 0 & 1 & 0 \\ -\frac{1}{3} & -\frac{5}{3} & 2 \\ \frac{1}{3} & \frac{2}{3} & -1 \end{bmatrix} \begin{bmatrix} N_{p,2}^* \\ n_{\text{eq:cent.}} \\ n_{\text{eq:elem}} \end{bmatrix} \\ &= \begin{bmatrix} n_{\text{eq:cent.}} \\ -\frac{N_{p,2}^* - n_{\text{eq:cent.}}}{3} - 2n_{\text{eq:cent.}} + 2n_{\text{eq:elem}} \\ \frac{N_{p,2}^* - n_{\text{eq:cent.}}}{3} + n_{\text{eq:cent.}} - n_{\text{eq:elem}} \end{bmatrix}, \quad (33) \end{aligned}$$

which always provides integer solutions since $(N_{p,2}^* - n_{\text{eq:cent.}})/3$ was demonstrated to always be an integer in Theorem 5. Consequently, Eq. (33) provides the unique combination of symmetry orbits needed to have a unisolvent set of nodes for a triangle.

Vandermonde matrices are constructed for all of the different combinations of symmetry orbits that give $n = N_{p,2}^*$ for $1 \leq p \leq 10$. The free parameters for the nodal locations are kept as variables and are thus included in the Vandermonde matrices, as was done in Eq. (14). The rank of the Vandermonde matrix constructed with the free parameters is calculated using the rank function in MATLAB. The rank of the Vandermonde matrix can be lower, but not greater, for certain nodal locations within the symmetry orbits, as is demonstrated in Section 4. Table 2 thus provides the highest possible rank of each of

Table 2: Combinations of symmetry orbits that provide $n = N_{p,2}^*$ and the highest possible rank of the Vandermonde matrices constructed using these symmetry orbits.

p	$n = N_{p,2}^*$	$\mathbf{n}_{\text{Sym},2\text{D}}$	$\text{rank}(\mathbf{V})$	$\text{rank}(\mathbf{V}) = N_{p,2}^*$	Solution to Eq. (32)
0	1	[1,0,0]	1	✓	✓
1	3	[0,1,0]	3	✓	✓
2	6	[0,2,0]	6	✓	✓
		[0,0,1]	5		
3	10	[1,3,1]	9	✓	✓
		[1,1,1]	10		
4	15	[0,5,0]	12	✓	✓
		[0,3,1]	15		
		[0,1,2]	14		
5	21	[0,7,0]	15	✓	✓
		[0,5,1]	20		
		[0,3,2]	21		
		[0,1,3]	20		
6	28	[1,9,0]	18	✓	✓
		[1,7,1]	24		
		[1,5,2]	27		
		[1,3,3]	28		
		[1,1,4]	27		
7	36	[0,12,0]	21	✓	✓
		[0,10,1]	27		
		[0,8,2]	32		
		[0,6,3]	35		
		[0,4,4]	36		
		[0,2,5]	35		
		[0,0,6]	32		

the Vandermonde matrices and indicates that the only combination of symmetry orbits that provides $\text{rank}(\mathbf{V}) = n = N_{p,2}^*$ is the one that satisfies Eq. (33). The results summarized in Table 2 agree with the example of non-unisolvency presented in 3.1. Furthermore, Table 2 demonstrates that the combinations of symmetry orbits that satisfy Eq. (30) but not Eq. (31) cannot provide a unisolvent set of nodes. This strongly suggests that Eq. (31) must be satisfied to have a unisolvent set of nodes. The same result was also observed for $p \in \{8, 9, 10\}$.

3.4 Tetrahedra

The five symmetry orbits for a tetrahedron are:

$\mathbf{n}_{\text{Sym},3\text{D}} = [n_{S_{1,3}}, n_{S_{4,3}}, n_{S_{6,3}}, n_{S_{12,3}}, n_{S_{24,3}}]^T$. Five equations are derived following the same procedure used for the one- and two-dimensional simplices.

3.4.1 First equation

The first equation is

$$n = N_{p,3}^* \\ [1, 4, 6, 12, 24]\mathbf{n}_{\text{Sym},3\text{D}} = \frac{(p+1)(p+2)(p+3)}{6}, \quad (34)$$

where 1, 4, 6, 12, and 24 are the number of nodes in the symmetry orbits $n_{S_{1,3}}$, $n_{S_{4,3}}$, $n_{S_{6,3}}$, $n_{S_{12,3}}$, and $n_{S_{24,3}}$, respectively.

3.4.2 Second equation

Just like the other simplices, there can either be one or no node at the centroid. The value for $n_{S_{1,3}}$ is determined by

Theorem 7 *There is a node at the centroid of a tetrahedron if and only if $\text{mod}(p, 4) = 0$.*

Proof We follow the same approach that was used to prove Theorem 5. Eq. (34) can be manipulated to move $n_{S_{1,3}}$ to the right-hand side

$$[0, 2, 3, 6, 12]\mathbf{n}_{\text{Sym},3\text{D}} = \frac{(p+1)(p+2)(p+3)}{3 \times 4} - \frac{n_{S_{1,3}}}{2}. \quad (35)$$

To have integer solutions it follows that

$$\text{mod} \left(\frac{(p+1)(p+2)(p+3)}{3}, 4 \right) = 2 \cdot \text{mod}(n_{S_{1,3}}, 2). \quad (36)$$

The fraction $(p+1)(p+2)(p+3)/3$ is always an integer since it is the product of three consecutive integers. If $n_{S_{1,3}} = 0$, then one of $p+1$, $p+2$ or $p+3$ is divisible by 4, which indicates that $\text{mod}(p, 4) \neq 0$. On the other hand, if $n_{S_{1,3}} = 1$, then none of $p+1$, $p+2$, and $p+3$ are divisible by 4, which requires that $\text{mod}(p, 4) = 0$. This completes the proof.

The equation that results from Theorem 7 is thus

$$n_{\text{eq:cent.}} = 1 - \left\lceil \frac{\text{mod}(p, 4)}{4} \right\rceil, \quad (37)$$

which returns one if $\text{mod}(p, 4) = 0$ and zero otherwise. The equation that needs to be satisfied is

$$[1, 0, 0, 0, 0]\mathbf{n}_{\text{Sym},3\text{D}} = n_{\text{eq:cent.}}. \quad (38)$$

3.4.3 Third equation

As has been previously demonstrated two dimensions, a unisolvent set of nodes for a tetrahedron will have a unique interpolant and its integral over the tetrahedron can thus be computed. We start with $N_{p,3}^*$ equations and unknowns but we are able to reduce the number of equations and unknowns since we are considering the case with all of the nodes in symmetry orbits. This is considered by

Theorem 8 *If all the nodes are in symmetry orbits and the tetrahedron has the same Cartesian and barycentric coordinates, then only the basis functions $x^a y^b z^c t^d$ with $a \geq b \geq c \geq d \geq 0$ and $a + b + c + d = p$ need to be considered.*

Proof The proof is analogous to the proof for Theorem 6, where a node on a symmetry plane and two nodes symmetrically located about the same symmetry plane are considered. For the symmetry plane $x = y$, it can then be shown that different basis functions of the form $x^a y^b z^c t^d$ and $x^b y^a z^c t^d$ lead to the same equation. This process is repeated for each of the symmetry planes until the desired result is obtained.

As a result of Theorem 8 the range of values for a , b , c , and d that need to be considered are

$$p - b - c - d = a_{\min} = a = a_{\max} = p - b - c - d \quad (39)$$

$$c = b_{\min} \leq b \leq b_{\max} = \left\lfloor \frac{p - c - d}{2} \right\rfloor \quad (40)$$

$$d = c_{\min} \leq c \leq c_{\max} = \left\lfloor \frac{p - d}{3} \right\rfloor \quad (41)$$

$$0 = d_{\min} \leq d \leq d_{\max} = \left\lfloor \frac{p}{4} \right\rfloor. \quad (42)$$

The total number of remaining equations that need to be considered is

$$\begin{aligned} n_{\text{eq:elem}} &= \sum_{d=d_{\min}}^{d_{\max}} \sum_{c=c_{\min}}^{c_{\max}} \sum_{b=b_{\min}}^{b_{\max}} 1 \\ &= \sum_{d=d_{\min}}^{d_{\max}} \sum_{c=c_{\min}}^{c_{\max}} (b_{\max} + 1 - b_{\min}) \\ &= \sum_{d=d_{\min}}^{d_{\max}} \sum_{c=d}^{c_{\max}} \frac{(2p - 2d + 3) - 6c + (-1)^{p-c-d}}{4} \\ &= \frac{1}{12} \sum_{d=d_{\min}}^{d_{\max}} \left(\frac{16d^2 - 8(p+3)d + (p^2 + 6p + 9) - \text{mod}(p-d, 3)^2}{12} \right. \\ &\quad \left. + \frac{3(-1)^p + (-1)^{c_{\max}+d+p}}{24} \right) \end{aligned} \quad (43)$$

where the final equation still contains a summation since it was not possible to find a concise equation with no summation term. Each node in a symmetry orbit has the same integration weight and as such, each symmetry orbit provides one integration weight. The equation that must be satisfied is

$$[1, 1, 1, 1, 1] \mathbf{n}_{\text{Sym},3\text{D}} \leq n_{\text{eq:elem}}. \quad (44)$$

While it has not been proven, the results in Section 3.4.6 again suggest that Eq. (44) is an identity, i.e.

$$[1, 1, 1, 1, 1] \mathbf{n}_{\text{Sym},3\text{D}} = n_{\text{eq:elem}}. \quad (45)$$

3.4.4 Fourth equation

The interpolation of a node on the symmetry line $x = y = z$ is considered. Similar to the integration of basis functions over the simplex, for interpolation we use the $N_{p,3}^*$ basis functions required to have a unique interpolant of degree p and each node has an interpolation weight. Since we are considering the case where all the nodes are in symmetry orbits, we can reduce the number of equations and unknowns we need to consider. This is demonstrated in

Theorem 9 *If all of the nodes are in symmetry orbits, the tetrahedron is symmetric about the planes $x = y$, $x = z$, and $y = z$, and the interpolation is to a node on the symmetry line $x = y = z$, then only the basis functions $x^a y^b z^c$ with $a \geq b \geq c \geq 0$ and $a + b + c \leq p$ need to be considered.*

Proof We consider a node that is on the symmetry line $x = y = z$, a set of three nodes that are on the symmetry planes $x = y$, $x = z$, and $y = z$, and a set of six nodes that are on none of the symmetry planes $x = y$, $x = z$ or $y = z$. Theorem 3 proved that all of the nodes in each of these sets share the same interpolation weight. The node on the symmetry line $x = y = z$ is at (x_i, x_i, x_i) with the interpolation weight r_i , the three nodes on the symmetry planes share the interpolation weight r_j and are at (x_j, y_j, x_j) , (x_j, x_j, y_j) , and (y_j, x_j, x_j) , and the six nodes that are not on any of the symmetry planes share the interpolation weight r_k and are at (x_k, y_k, z_k) , (x_k, z_k, y_k) , (y_k, x_k, z_k) , (y_k, z_k, x_k) , (z_k, x_k, y_k) , and (z_k, y_k, x_k) . The set for the nodes on the symmetry line $x = y = z$ is \mathcal{S}_1 , the set for the nodes on the symmetry planes $x = y$, $x = z$ and $y = z$ is \mathcal{S}_2 , and the set for the nodes that are on none of the symmetry planes is \mathcal{S}_3 . The solution is interpolated to a node on the symmetry line $x = y = z$ and its coordinates are (x_m, x_m, x_m) . The equation for the interpolation of the basis $x^a y^b z^c$ is

$$\begin{aligned} x_m^{a+b+c} &= \sum_{i \in \mathcal{S}_1} r_i x_i^{a+b+c} \\ &+ \sum_{j \in \mathcal{S}_2} r_j (x_j^{a+c} y_j^b + x_j^{a+b} y_j^c + x_j^{b+c} y_j^a) \\ &+ \sum_{k \in \mathcal{S}_3} r_k (x_k^a y_k^b z_k^c + x_k^a z_k^b y_k^c + y_k^a x_k^b z_k^c + y_k^a z_k^b x_k^c + z_k^a x_k^b y_k^c + z_k^a y_k^b x_k^c), \end{aligned} \quad (46)$$

which is identical to the equations for the bases $x^a y^c z^b$, $x^b y^a z^c$, $x^b y^c z^a$, $x^c y^a z^b$, and $x^c y^b z^a$. Therefore, only bases with $a + b + c \leq p$ and $a \geq b \geq c \geq 0$ provide independent equations. This completes the proof.

As a result of Theorem 9, the range of values that need to be considered for a , b , and c are

$$b = a_{\min} \leq a \leq a_{\max} = p - b - c \quad (47)$$

$$c = b_{\min} \leq b \leq b_{\max} = \left\lfloor \frac{p - c}{2} \right\rfloor \quad (48)$$

$$0 = c_{\min} \leq c \leq c_{\max} = \left\lfloor \frac{p}{3} \right\rfloor. \quad (49)$$

The number of remaining basis functions that need to be considered for a tetrahedron with all of its nodes in symmetry orbits and an interpolated node on the symmetry line $x = y = z$ is thus

$$\begin{aligned} n_{\text{eq:int},1} &= \sum_{c=c_{\min}}^{c_{\max}} \sum_{b=b_{\min}}^{b_{\max}} \sum_{a=a_{\min}}^{a_{\max}} 1 \\ &= \sum_{c=0}^{c_{\max}} \sum_{b=c}^{b_{\max}} (p + 1 - c - 2b) \\ &= \sum_{c=0}^{c_{\max}} (p + 1 - c)(b_{\max} + 1 - c) - 2 \frac{b_{\max}(b_{\max} + 1) - (c - 1)c}{2} \\ &= \sum_{c=0}^{c_{\max}} \frac{18c^2 - 12(p + 2)c + (2p^2 + 8p + 7) + (-1)^{p+c}}{8} \\ &= \frac{6c_{\max}^3 - 3(1 + 2p)c_{\max}^2 + 2(p^2 + p - 1)c_{\max} + (2p^2 + 8p + 7)}{8} \quad (50) \\ &\quad + \frac{(-1)^p(1 + (-1)^{c_{\max}})}{16}. \end{aligned}$$

Each symmetry orbit has one independent weigh for each node on the symmetry line $x = y = z$, one weight for each group of three nodes on the symmetry planes $x = y$, $x = z$, and $y = z$ but not on the symmetry line $x = y = z$, and one weight for each group of six nodes that are on not on any these symmetry planes. The symmetry orbits $S_{1,3}$, $S_{4,3}$, $S_{6,3}$, $S_{12,3}$ and $S_{24,3}$ each have 1, 2, 2, 3, and 4 independent weights, respectively. Consequently, the equation to satisfy is

$$[1, 2, 2, 3, 4] \mathbf{n}_{\text{Sym},3\text{D}} \leq n_{\text{eq:int},1}. \quad (51)$$

As before, the results in Section 3.4.6 suggest that the following is required for unisolvency

$$[1, 2, 2, 3, 4] \mathbf{n}_{\text{Sym},3\text{D}} = n_{\text{eq:int},1}. \quad (52)$$

3.4.5 Fifth equation

For the fifth and final equation that is considered for a tetrahedron we consider the interpolation of a node that is on the symmetry plane $x = y$, but not on the symmetry line $x = y = z$. This is considered in

Theorem 10 *When all the nodes are in symmetry orbits, the tetrahedron is symmetric about the plane $x = y$, and the interpolation is to a node that is on the symmetry plane $x = y$, but not on the symmetry line $x = y = z$, only the basis functions of the form $x^a y^b z^c$ with $a \geq b \geq 0$, $c \geq 0$ and $a + b + c \leq p$ need to be considered.*

Proof The proof is analogous to the one for Theorem 9 but it only involves the symmetry plane $x = y$. Therefore, the only condition that is derived is that $a \geq b$, which is the desired result.

As a result of Theorem 10, the variables a , b and c are limited to

$$b = a_{\min} \leq a \leq a_{\max} = p - b - c \quad (53)$$

$$0 = b_{\min} \leq b \leq b_{\max} = \left\lfloor \frac{p - c}{2} \right\rfloor \quad (54)$$

$$0 = c_{\min} \leq c \leq c_{\max} = p. \quad (55)$$

The remaining number of basis functions that need to be considered is

$$\begin{aligned} n_{\text{eq:int},2} &= \sum_{c=c_{\min}}^{c_{\max}} \sum_{b=b_{\min}}^{b_{\max}} \sum_{a=a_{\min}}^{a_{\max}} 1 \\ &= \sum_{c=0}^{c_{\max}} \sum_{b=0}^{b_{\max}} (p + 1 - c - 2b) \\ &= \sum_{c=0}^{c_{\max}} (p + 1 - c)(b_{\max} + 1) - b_{\max}(b_{\max} + 1) \\ &= \sum_{c=0}^p \frac{2c^2 - 4(p + 2)c + (2p^2 + 8p + 7) + (-1)^{p+c}}{8} \\ &= \frac{(2p + 3)(p + 2)(p + 4) - 3 \bmod(p, 2)}{24}. \end{aligned} \quad (56)$$

Each symmetry orbit has one free parameter for each node on the symmetry plane $x = y$ and one for each pair of nodes symmetrically located about this symmetry plane. The symmetry orbits $S_{1,3}$, $S_{4,3}$, $S_{6,3}$, $S_{12,3}$ and $S_{24,3}$ therefore each have 1, 3, 4, 7, and 12 free parameters, respectively. Consequently, the equation that must be satisfied is

$$[1, 3, 4, 7, 12] \mathbf{n}_{\text{Sym},3\text{D}} \leq n_{\text{eq:int},2}, \quad (57)$$

where there is once again an inequality but the results in Section 3.4.6 suggest it is in fact an identity, i.e.

$$[1, 3, 4, 7, 12] \mathbf{n}_{\text{Sym},3\text{D}} = n_{\text{eq:int},2}. \quad (58)$$

3.4.6 System of equations

Combining Eqs. (34), (38), (45), (52) and (58), and assuming that these last three hold for a unisolvent set of nodes, gives

$$\begin{bmatrix} 1 & 4 & 6 & 12 & 24 \\ 1 & 0 & 0 & 0 & 0 \\ 1 & 1 & 1 & 1 & 1 \\ 1 & 2 & 2 & 3 & 4 \\ 1 & 3 & 4 & 7 & 12 \end{bmatrix} \begin{bmatrix} n_{S_{1,3}} \\ n_{S_{4,3}} \\ n_{S_{6,3}} \\ n_{S_{12,3}} \\ n_{S_{24,3}} \end{bmatrix} = \begin{bmatrix} N_{p,3}^* \\ n_{\text{eq:cent.}} \\ n_{\text{eq:elem}} \\ n_{\text{eq:int,1}} \\ n_{\text{eq:int,2}} \end{bmatrix}. \quad (59)$$

This system of equation can be solved to give

$$\begin{aligned} \begin{bmatrix} n_{S_{1,3}} \\ n_{S_{4,3}} \\ n_{S_{6,3}} \\ n_{S_{12,3}} \\ n_{S_{24,3}} \end{bmatrix} &= \begin{bmatrix} 1 & 4 & 6 & 12 & 24 \\ 1 & 0 & 0 & 0 & 0 \\ 1 & 1 & 1 & 1 & 1 \\ 1 & 2 & 2 & 3 & 4 \\ 1 & 3 & 4 & 7 & 12 \end{bmatrix}^{-1} \begin{bmatrix} N_{p,3}^* \\ n_{\text{eq:cent.}} \\ n_{\text{eq:elem}} \\ n_{\text{eq:int,1}} \\ n_{\text{eq:int,2}} \end{bmatrix} \\ &= \begin{bmatrix} 0 & 1 & 0 & 0 & 0 \\ 1 & -1 & 0 & 3 & -3 \\ -1/2 & -3/2 & 4 & -4 & 2 \\ -1 & 2 & -4 & 1 & 2 \\ 1/2 & -1/2 & 1 & 0 & -1 \end{bmatrix} \begin{bmatrix} N_{p,3}^* \\ n_{\text{eq:cent.}} \\ n_{\text{eq:elem}} \\ n_{\text{eq:int,1}} \\ n_{\text{eq:int,2}} \end{bmatrix}. \\ &= \begin{bmatrix} n_{\text{eq:cent.}} \\ N_{p,3}^* - n_{\text{eq:cent.}} + 3(n_{\text{eq:int,1}} - n_{\text{eq:int,2}}) \\ -\frac{N_{p,3}^* + n_{\text{eq:cent.}}}{2} - n_{\text{eq:cent.}} + 4(n_{\text{eq:elem}} - n_{\text{eq:int,1}}) + 2n_{\text{eq:int,2}} \\ -N_{p,3}^* + 2n_{\text{eq:cent.}} - 4n_{\text{eq:elem}} + n_{\text{eq:int,1}} + 2n_{\text{eq:int,2}} \\ \frac{N_{p,3}^* - n_{\text{eq:cent.}}}{2} + n_{\text{eq:elem}} - n_{\text{eq:int,2}} \end{bmatrix}. \quad (60) \end{aligned}$$

The terms $N_{p,3}^*$, $n_{\text{eq:cent.}}$, $n_{\text{eq:elem}}$, $n_{\text{eq:int,1}}$, and $n_{\text{eq:int,2}}$ are all integers for $p \geq 0$. The fifth row in Eq. (60) contains the term $(N_{p,3}^* - n_{\text{eq:cent.}})/2$, which is identical to the right-hand side of Eq. (35), and thus is always an integer. It is analogous to show that $(N_{p,3}^* + n_{\text{eq:cent.}})/2$ in the third row of Eq. (60) is also always an integer. Therefore, Eq. (60) returns a solution of integers, which is the unique combination of symmetry orbits to have a unisolvent set of nodes for $p \geq 0$.

The same approach as Section 3.3.4 is followed here. Vandermonde matrices are constructed for the nodal locations of each of the symmetry orbits that gives $n = N_{p,3}^*$ for $1 \leq p \leq 7$. The rank of the Vandermonde matrices shown in Table 3 for $1 \leq p \leq 4$ indicates the highest possible rank for the particular combination of symmetry orbits. The rank of the Vandermonde matrix can be lower, but not greater, for certain nodal locations within the symmetry orbits being used, as is demonstrated in Section 4. The only combination of symmetry orbits for each degree of interpolant p that has $\text{rank}(\mathbf{V}) = n = N_{p,3}^*$ is the one that satisfies Eq. (60), as expected. The same results were also observed

Table 3: Combinations of symmetry orbits that provide $n = N_{p,3}^*$ and the highest possible rank of the Vandermonde matrices constructed using these symmetry orbits.

p	$n = N_{p,3}^*$	$\mathbf{n}_{\text{Sym},3\text{D}}$	rank(V)	rank(V) = $N_{p,3}^*$	Solution to Eq. (60)
0	1	[1,0,0,0,0]	1	✓	✓
1	4	[0,1,0,0,0]	4	✓	✓
2	10	[0,1,1,0,0]	10	✓	✓
3	20	[0,5,0,0,0]	12		
		[0,2,2,0,0]	17		
		[0,2,0,1,0]	20	✓	✓
4	35	[1,7,1,0,0]	22		
		[1,4,3,0,0]	24		
		[1,4,1,1,0]	30		
		[1,1,5,0,0]	17		
		[1,1,3,1,0]	29		
		[1,1,1,2,0]	35	✓	✓
		[1,1,1,0,1]	31		

for $p \in \{5, 6, 7\}$. This strongly suggests that satisfying Eqs. (45), (52) and (58) is a required conditions for unisolvency for all p .

3.5 Results for simplices of one to three dimensions

Equations were derived to determine the unique combination of symmetry orbits that can provide a unisolvent set of nodes for simplices of one to three dimensions. Table 4 shows the number of combinations of symmetry orbits that provides $n = N_{p,d}^*$ and the unique combination of symmetry orbits that can provide a unisolvent set of nodes.

4 Non-unisolvency

In one dimension, unique nodal locations and the combination of symmetry orbits that provides $n = N_{p,1}^*$ is sufficient to ensure unisolvency. However, in multiple dimensions unique nodal locations and the unique combination of symmetry orbits that can provide a unisolvent set of nodes is still insufficient to ensure unisolvency. The conditions presented are necessary but not sufficient.

Table 4 indicates that $\mathbf{n}_{\text{Sym},2\text{D}} = [0, 2, 0]$ is required to have a unisolvent set of nodes for a $p = 2$ interpolant on a triangle. The Cartesian coordinates for the nodes in these two symmetry orbits on a right triangle with vertices at

Table 4: The combination of symmetry orbits that can provide a unisolvent set of nodes for simplices of one to three dimensions, where n_c is the number of combinations of symmetry orbits that gives $n = N_{p,d}^*$.

p	Line		Triangle		Tetrahedron	
	n_c	$\mathbf{n}_{\text{Sym,1D}}^T$	n_c	$\mathbf{n}_{\text{Sym,2D}}^T$	n_c	$\mathbf{n}_{\text{Sym,3D}}^T$
0	1	[1, 0]	1	[1,0,0]	1	[1,0,0,0,0]
1	1	[0, 1]	1	[0,1,0]	1	[0,1,0,0,0]
2	1	[1, 1]	2	[0,2,0]	1	[0,1,1,0,0]
3	1	[0, 2]	2	[1,1,1]	3	[0,2,0,1,0]
4	1	[1, 2]	3	[0,3,1]	7	[1,1,1,2,0]
5	1	[0, 3]	4	[0,3,2]	22	[0,2,0,4,0]
6	1	[1, 3]	5	[1,3,3]	70	[0,3,2,3,1]
7	1	[0, 4]	7	[0,4,4]	161	[0,3,0,7,1]
8	1	[1, 4]	8	[0,5,5]	308	[1,2,2,8,2]
9	1	[0, 5]	10	[1,4,7]	715	[0,4,0,11,3]
10	1	[1, 5]	12	[0,6,8]	1378	[0,4,3,11,5]

(0, 0), (1, 0) and (0, 1) are

$$\frac{1}{3} \times \begin{bmatrix} 1 - t_1 & 1 - t_1 \\ 1 + 2t_1 & 1 - t_1 \\ 1 - t_1 & 1 + 2t_1 \\ 1 - t_2 & 1 - t_2 \\ 1 + 2t_2 & 1 - t_2 \\ 1 - t_2 & 1 + 2t_2 \end{bmatrix},$$

where t_1 and t_2 are the free parameters for the nodal locations of the two symmetry orbits. The determinant of a Vandermonde matrix constructed with monomials is

$$\det(\mathbf{V}) = \frac{(t_1^2 t_2^2 (t_1 + t_2)(t_1 - t_2)^3)}{27}, \quad (61)$$

which is zero if $t_1, t_2 = 0$ since the nodes of that respective symmetry orbit would be collocated at the centroid, or if $t_1 = t_2$ since the nodes of the two symmetry orbits would be collocated. Additionally, if $t_1 = -t_2$, which does not involve any collocation of the nodes, then the determinant of the Vandermonde matrix is also zero.

Consider the symmetry orbits $\mathbf{n}_{\text{Sym,3D}} = [0, 1, 1, 0, 0]$, which Table 4 indicates is the required combination of symmetry orbits to have a unisolvent set of nodes for a $p = 2$ interpolant in a tetrahedron. The Cartesian coordinates for the nodes in a tetrahedron with vertices at (0, 0, 0), (1, 0, 0), (0, 1, 0), and

$(0, 0, 1)$ are

$$\frac{1}{4} \times \begin{bmatrix} 1 - t_1 & 1 - t_1 & 1 - t_1 \\ 1 + 3t_1 & 1 - t_1 & 1 - t_1 \\ 1 - t_1 & 1 + 3t_1 & 1 - t_1 \\ 1 - t_1 & 1 - t_1 & 1 - 3t_1 \\ 1 - t_2 & 1 + t_2 & 1 + t_2 \\ 1 + t_2 & 1 - t_2 & 1 + t_2 \\ 1 + t_2 & 1 + t_2 & 1 - t_2 \\ 1 - t_2 & 1 - t_2 & 1 + t_2 \\ 1 - t_2 & 1 + t_2 & 1 - t_2 \\ 1 + t_2 & 1 - t_2 & 1 - t_2 \end{bmatrix},$$

where t_1 and t_2 are the free parameters for the nodal locations for the $n_{S_{4,3}}$ and $n_{S_{6,3}}$ symmetry orbits, respectively. The determinant of the Vandermonde matrix constructed with monomials is

$$\det(\mathbf{V}) = -\frac{t_1^6 t_2^7 (3t_1^2 - 4t_2^2)}{64}, \quad (62)$$

which is zero when $t_1 = 0$ or $t_2 = 0$ since the nodes are collocated at the centroid. However, if $3t_1^2 = 4t_2^2$, then the determinant of the Vandermonde matrix is also zero, even though none of the nodes are collocated.

The relation between the nodal locations of two or more symmetry orbits that gives $\det(\mathbf{V}) = 0$ and that is thus non-unisolvent depends on each combination of symmetry orbits. For example, having $t_i = -t_j$ for two different $n_{S_{3,2}}$ symmetry orbits on a triangle may not necessarily lead to a non-unisolvent set of nodes for $p > 2$. Further work is needed to determine if a necessary and sufficient set of conditions to ensure unisolvency can be derived when all the nodes are in symmetry orbits.

5 Conclusions

It was demonstrated that, for polynomial interpolants, there is a unique combination of symmetry orbits that can provide a unisolvent set of nodes for simplices of one to three dimensions. A system of equations was derived to calculate this unique combination of symmetry orbits. The results were verified for $p \leq 10$ for triangles and $p \leq 7$ for tetrahedra by considering all combination of symmetry orbits with $n = N_{p,d}^*$ and calculating the rank of their Vandermonde matrix. Only the combinations of symmetry orbits identified in this paper provide a unisolvent set of nodes. The results from this paper strongly suggest that satisfying Eqs. (31), (45), (52) and (58) is required to have unisolvency for all p .

Consider an interpolant with $p = 7$, there are 7 and 161 combinations of symmetry orbits that give $n = N_{p,d}^*$ for triangles and tetrahedra, respectively. With the equations derived in this paper, only the unique combination of symmetry orbits that can provide a unisolvent set of nodes needs to be considered. This result may prove helpful in the derivation of Fekete and Lebesgue nodes

as well as operators for finite-element, multidimensional summation-by-parts, and flux reconstruction operators.

For symmetrical nodal distribution in a simplex, the conditions derived in this paper are necessary, at least for $p \leq 10$ for triangles and $p \leq 7$ for tetrahedra, but not sufficient to ensure a unisolvent set of nodes for polynomial interpolation. Even with the unique combination of symmetry orbits to have a unisolvent set of nodes and distinct nodal locations, unisolventy is still not guaranteed. The relation between the nodal locations that provides a non-unisolvent set of nodes is different for each degree of interpolants. Further research is required to determine if additional constraints can be added that would guarantee unisolventy for two- and three-dimensional simplices.

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Conflict of interest

The authors declare that they have no conflict of interest.

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