Pyramid finite elements for discontinuous and continuous discretizations of the neutron diffusion equation with applications to reactor physics

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ABSTRACT

When using unstructured mesh finite element methods for neutron diffusion problems, hexahedral elements are in most cases the most computationally efficient and accurate for a prescribed number of degrees of freedom. However, it is not always practical to create a finite element mesh consisting entirely of hexahedral elements, particularly when modelling complex geometries, making it necessary to use tetrahedral elements to mesh more geometrically complex regions. In order to avoid hanging nodes, wedge or pyramid elements can be used in order to connect hexahedral and tetrahedral elements, but it was not until 2010 that a study by Bergot established a method of developing correct higher-order basis functions for pyramid elements. This paper analyses the performance of first and second-order pyramid elements created using the Bergot method within continuous and discontinuous finite element discretisations of the neutron diffusion equation. These elements are then analysed for their performance using a number of reactor physics benchmarks. The accuracy of solutions using pyramid elements both alone and in a mixed element mesh is shown to be similar to that of meshes using the more standard element types. In addition, convergence rate analysis shows that, while problems discretized with pyramids do not converge as well as those with hexahedra, the pyramids display better convergence properties than tetrahedra.

1. Introduction

For 3D finite element problems the most commonly used element types are tetrahedra and hexahedra (Bathe, 1996; Dhatt et al., 2012). Studies have shown that in general hexahedral elements are superior in terms of computational efficiency and accuracy to tetrahedral elements of the same order (Cifuentes and Kalbag, 1992; Benzley et al., 1995). An example of the difference between the two may be understood by comparing tri-linear hexahedral elements to linear tetrahedral elements. The tri-linear hexahedral elements have coupling between the different parametric co-ordinates whereas the linear tetrahedral elements do not. This difference means that the tetrahedral elements are less accurate overall than hexahedral elements. However, while various robust mesh generation techniques, such as advancing front and Delaunay, exist to mesh complex geometrical domains with tetrahedral elements, no general technique exists for hexahedral elements (Frey and George, 2008), due to the geometrically stiff structure of hexahedra (Schneiders, 2000; Puso and Solberg, 2006). Often the only reliable and robust way of systematically generating a fully hexahedral mesh for a complex geometrical domain is to generate a tetrahedral mesh and then split each tetrahedron into four hexahedra (Garcia, 2002), a process which substantially increases the cost of generating the mesh.

Because of this it is desirable to use algorithms that create a mixed mesh of elements (Hitschfeld-Kahler, 2005). Doing so allows for a mesh which is predominantly composed of hexahedra, with tetrahedra used where necessary to mesh the more complex parts of the geometry. This presents a challenge due to the fact that the tetrahedra have triangular faces while hexahedra faces are quadrilateral, meaning that a mixed mesh of just these two element types would require hanging nodes. In order to overcome this problem mesh generators will include a mix of prismatic (wedge) and pyramid elements. Such elements may be used to create a link without the need for hanging nodes due to the fact that they have both triangular and quadrilateral faces. Whether wedges, pyramids, or a mixture of both are required for this purpose is dependent on problem geometry.

Another application of pyramid elements is for connecting regions of elements with varying mesh refinement. A structure of pyramid and tetrahedral elements may connect two regions of structured hexahedral
elements of different size without the need for hanging nodes. For example octree based mesh generators will use pyramids in order to eliminate hanging nodes in the refinement process (Dawes et al., 2009).

Developing the basis functions and quadrature for prismatic elements is not particularly complex, as they are essentially a triangle extruded into a third dimension (Dhath et al., 2012). However, pyramid elements are more complicated due to their non-polynomial nature. The set of basis functions for a first-order pyramid with five nodes has been known for some time (Coulomb et al., 1997), but an optimal set of basis functions for higher order pyramid elements was not fully understood and approximations based on a template approach were used (Felippa, 2004). More recently, a technique for generating effective basis functions for higher order pyramids has been developed (Bergot et al., 2010), enabling stable and effective solutions.

This paper examines the performance of pyramid elements generated using the Bergot method when applied to neutron diffusion problems in reactor physics using both continuous and discontinuous finite element discretizations. The solution of the neutron diffusion problem is important in the fields of reactor physics, nuclear criticality safety assessment and radiation shielding as it enables the use of Diffusion Synthesis Acceleration (DSA) and Nonlinear Diffusion acceleration (NDA) (Schunert et al., 2017) for neutron transport methods (Larsen, 1984).

After providing some background theory and describing Bergot’s method for generating the pyramid element basis functions a variety of verification test cases will be used to demonstrate that pyramid elements may be effectively used within reactor physics problems without causing an excessive negative impact on accuracy or convergence in comparison to a case where more standard hexahedral elements are used. These are not intended to prove the superiority of pyramid elements over any other element type in terms of accuracy or computational efficiency, but instead to show that any computational disadvantages of pyramids, if they exist, are small, so that they may be used safely in problems where their geometric properties are useful.

2. Neutron diffusion discretization

The neutron diffusion equation is an elliptic partial differential equation (PDE) derived through simplification of the neutron transport equation. The equation describes the neutron scalar flux $\phi$ ($\text{cm}^{-2}\text{s}^{-1}$) at position $r$ and neutron energy $E$. The equation is written as:

$$V \cdot D(r, E) \nabla \phi(r, E) - \Sigma_{r}(r, E) \phi(r, E) + S(r, E) = 0$$ (1)

where the diffusion coefficient $D$ (cm) and the neutron removal cross-section $\Sigma_r$ (cm$^{-1}$) are material properties of the medium. The neutron source $S$ (cm$^{-3}$s$^{-1}$) is a combination of neutrons generated through fission, neutrons entering energy level $E$ due to scatter from another energy level, and any fixed (extraneous) neutron sources present.

The discretization of the diffusion equation in a finite element (FEM) framework is described using the bilinear and linear forms. The inner product is given as $()$ on the discretization $\mathcal{L}^2(V)$ for spatial domain $V$ with boundary $\partial V$ and set of element edges $\mathcal{e}$, such that:

$$(a, b)_{\mathcal{L}^2(V)} = \int_{V} ab \, dV$$ (2)

The discontinuous Galerkin (DG-FEM) discretization of the neutron diffusion equation, as described in (Adams and Martin, 1992), is not stable for all problems. Discontinuous formulations of elliptic problems necessitate the addition of a penalty term to ensure stability (Di Pietro and Ern, 2012). This paper uses the modified interior penalty (MIP) scheme in order to stabilise the discontinuous diffusion equation (Wang and Ragusa, 2010). The bilinear form for this case is given as:

$$\alpha(\phi, \phi') = (\mathcal{S}, \phi')_{V} + (\nabla \phi', \nabla \phi)_{V} + \{\{\phi\}, \{\nabla \phi'\}|_{\mathcal{e}}\} + \{(\phi|_{\mathcal{e}}, |\nabla \phi'\mathcal{e}|_{\mathcal{e}})\} + (\{\phi\}, \{\nabla \phi'\})_{V}$$

$$\phi(\phi, \phi')_{V} - \frac{1}{2}(\phi', \nabla \phi)_{V} - \frac{1}{2}(D \phi', \phi'')_{V}$$ (3)

where $\kappa$ represents the penalty term at element edge or domain boundary.

The expressions

$$\{\phi\} = \hat{\mathbf{n}}^{+} \phi^{+} + \hat{\mathbf{n}}^{-} \phi^{-} \quad \text{and} \quad \{(\phi, \phi')\} = (\phi^{+} + \phi^{-})/2$$ (4)

are the boundary flux jump and average respectively, with $+$ and $-$ representing either side of an element face. $\hat{\mathbf{n}}$ represents the outward pointing normal vector at each face.

It should be noted that the penalisation of the boundary conditions in equation (3) does not strictly represent a bare boundary as stated. This is due to the boundary treatment introduced by the MIP scheme (Wang and Ragusa, 2010) in order to improve the stability and robustness of the method. This can be done since the main aim of these equations is to use them as DSA for DG-FEM$S_0$ transport. Section 4.3 will demonstrate the errors generated by this method and also demonstrate how removing the boundary penalisation removes them.

For a continuous FEM discretization the bilinear form $\alpha(\phi, \phi')$ and linear form $l(\phi')$ combine to create the variational form:

$$\alpha(\phi, \phi') = (\mathcal{S}, \phi')_{V} + (\nabla \phi', \nabla \phi)_{V} + (\kappa \phi, \phi')_{V} - \frac{1}{2}(\phi', \nabla \phi)_{V} - \frac{1}{2}(D \phi', \phi'')_{V}$$

and

$$l(\phi') = (S, \phi')_{V}$$ (6)

Here the boundary conditions of the continuous FEM discretization have been obtained from the discontinuous discretization (equation (3)) by closing the inter-element discontinuities, in order to preserve consistency between the discontinuous and continuous equations. As a consequence, it is similar to the weakly imposed Dirichlet condition of Nitsche (1971).

3. Basis functions and quadrature

Recent studies have lead to the development of a methodology which defines a mathematically rigorous basis for nodal pyramid elements of an arbitrary order (Bergot et al., 2010), which have been shown to produce optimal results. This set of basis functions is defined over the reference or parent element shown in Fig. 1.

The number of degrees of freedom $n$ of a pyramid of order $r$ is given by the formula:

$$n = \frac{1}{6}(r + 1)(r + 2)(2r + 3)$$ (7)

which is equal to the dimension of the finite element space $H_{r}$.

![Fig. 1. Reference pyramid element.](image-url)
In order to obtain a set of basis functions it is first necessary to obtain a set of expressions which form an orthogonal base of \( \hat{P} \). This is done through the use of Jacobi polynomials, where \( P_m^\alpha(x) \) is a Jacobi polynomial of order \( m \) which is orthogonal for the weighting \((1-x)\alpha(1+x)\beta\) (Szegö, 1975). The orthogonal basis of the finite element space over a pyramid is then defined as:

\[
\psi^{i,j,k}(x, y, z) = P_i^\alpha\left(\frac{x}{1-z}\right)P_j^\beta\left(\frac{y}{1-z}\right)(1-z)^m P_k^{\max(i,j)}(2z-1)
\]

for values of \( i, j \) and \( k \) where:

\[
0 \leq i \leq r, \quad 0 \leq j \leq r, \quad 0 \leq k \leq r - \max(i,j)
\]

For a first-order pyramid element the orthogonal base is formed of the following 5 expressions:

\[
\begin{align*}
\psi_1(x, y, z) &= 1 \\
\psi_2(x, y, z) &= x \\
\psi_3(x, y, z) &= y \\
\psi_4(x, y, z) &= 4z - 1 \\
\psi_5(x, y, z) &= \frac{y}{1-z}
\end{align*}
\]

(10)

Once the orthogonal basis is defined it is used to create a Vandermonde (VDM) matrix in which the values within each row are one of the orthogonal basis functions evaluated for all \( M_i \) where \( M_i \) is the location of degree of freedom \( i \) on the reference pyramid.

\[
VDM_{ij} = \psi_i(M_j), \quad 1 \leq (i, j) \leq n
\]

(11)

For a first-order element with the orthogonal base as shown above and node positions as shown in Fig. 1 the VDM matrix will be as follows:

\[
\begin{bmatrix}
1 & 1 & 1 & 1 & 1 \\
-1 & -1 & 1 & 1 & 0 \\
1 & -1 & -1 & 1 & 0 \\
1 & -1 & -1 & -1 & 1 \\
-1 & 1 & 1 & -1 & 1 \\
-1 & 1 & 1 & -1 & 0 \\
\end{bmatrix}
\]

(12)

The VDM matrix is then inverted and multiplied with the orthogonal base vector to obtain the set of basis functions \( N \).

\[
N = VDM^{-1}\psi
\]

(13)

producing, for a first-order element, the following set of basis functions:

\[
\begin{align*}
N_{1}^{1st} &= \frac{1}{4}\left(1 - x + y - z + \frac{y}{1-z}\right) \\
N_{1}^{2st} &= \frac{1}{4}\left(1 - x + y - z + \frac{y}{1-z}\right) \\
N_{1}^{3st} &= \frac{1}{4}\left(1 - x + y - z + \frac{y}{1-z}\right) \\
N_{1}^{4st} &= \frac{1}{4}\left(1 - x + y - z + \frac{y}{1-z}\right) \\
N_{1}^{5st} &= z
\end{align*}
\]

(14)

This method may be followed for any positive integer value of \( r \) to obtain a set of basis functions of that order.

As well as the basis functions it is also necessary to define a quadrature scheme across the pyramid element for accurate numerical integration. For the standard hexahedral reference element, a cube of side length 2 centred on the origin, the quadrature is formed by taking 1D Gauss-Legendre quadrature between \(-1\) and \(1\) and applying it in three dimensions (Stroud, 1971). The methodology for quadrature over a pyramid suggested in (Bergot et al., 2010) is similar to this except that while standard Gauss-Legendre quadrature is used across the \(x\) and \(y\) directions, this formulation uses a Gauss-Jacobi quadrature between 0 and 1 along the \(z\) direction.

For a quadrature of order \( n_q \) the 1D Gauss-Legendre \( Q^L \) and Gauss-Jacobi \( Q^J \) quadrature points are vectors for \( 1 \leq n \leq n_D \) where \( n_D = \frac{r}{2} + 1 \) is the number of 1D quadrature points for quadrature of order \( n_q \) (\( n_q \) is always even so \( n_D \) is always an integer). The 3D pyramid quadrature coordinates on the reference pyramid, denoted by \( \Theta \), are then given by the formula:

\[
\begin{align*}
\Theta_i^{Q^L} &= (1 - Q^L(1))(Q^L(i)) \\
\Theta_i^{Q^J} &= (1 - Q^J(1))(Q^J(i)) \\
\Theta_i^{Q^J} &= Q^J(k)
\end{align*}
\]

(15) (16) (17)

The 1D quadrature weightings for Gauss-Legendre and Gauss-Jacobi are given by the vectors \( w_L \) and \( w_J \) respectively, again of length \( n_D \). The quadrature weighting for each point on the pyramid is given by:

\[
\begin{align*}
\omega_{ij}^{Q^J} &= \prod_{k=1}^{n_D} w_{L_{ij}}(j)w_{J_k}(k)
\end{align*}
\]

(18)

\[
1 \leq i, j, k \leq n_D
\]

4. Results

This section contains a series of FEM neutron diffusion verification test problems which make use of the pyramid elements described previously. These results aim to study various aspects of the performance of the pyramid elements and compare and contrast with more common element types. Most of the structured finite element meshes for these problems were generated using a python script, although GMSH (Geuzaine and Remacle, 2009) was used for some of the problems.

4.1. \( L_2 \)-error

An \( L_2 \)-error analysis is performed for homogeneous solutions of the neutron diffusion equation using a structured mesh consisting entirely of structured pyramid elements. Results are taken for the diffusion equation solved with both a continuous FEM formulation and for discontinuous DG-FEM with an MIP penalty scheme (Wang and Ragusa, 2010). The \( L_2 \)-error is analysed on a homogeneous cubic problem of dimension 1.0cm x 1.0cm x 1.0cm. The exact solution of the MMS problem is:

\[
\phi(x, y, z) = (2x^2 - x^4)(2y^2 - y^4)(2z^2 - z^4)
\]

(19)

yielding a solution where all boundaries are reflective.

The results of the \( L_2 \)-error analysis are plotted in Figs. 2 and 3. The characteristic length is an expression roughly corresponding to the size of the element, here it is calculated simply as the cubic root of the number of elements. For a properly set up finite element code it is

![Fig. 2. \( L_2 \)-Error plot for continuous diffusion.](image-url)
expected that, when printed on logarithmic scales, we would expect that the $L_2$-error will scale almost linearly with characteristic length and with a gradient of 2 for first-order elements and 3 for second-order elements. These plots demonstrate that the pyramid elements are properly displaying this behaviour. The characteristic length parameter is obtained by taking the cube root of the number of elements. It should be noted that because hexahedra and pyramids have a different number of nodes per element direct comparison between the two element types should not be made from this data.

4.2. Linking regions of varying refinement

It is possible to use pyramid and tetrahedral elements to create a structure that will link two regions of structured hexahedral elements where one region has elements with a side length of double the other. This is achieved first by creating a pyramid element with its base on the surface of a larger hexahedron and its apex at a point in the centre of four of the surfaces of four smaller hexahedra, as demonstrated in Fig. 4.

Four more pyramids are then generated, each with its base as the surface of one of the four smaller hexahedral elements, and its apex at the corresponding corner of the larger hexahedron, demonstrated in Fig. 5.

Once these five pyramids are generated the remaining space may be naturally filled with four tetrahedral elements. This leads to a structure of nine pyramids and tetrahedra which connects the hexahedral regions without any hanging nodes, shown in Fig. 6.

In order to study the impact of using this technique on solution accuracy and convergence a method of manufactured solutions problem is generated for a discontinuous Galerkin diffusion problem in a homogeneous region of size $1.0 \text{cm} \times 1.0 \text{cm} \times 1.0 \text{cm}$. A low and high refinement mesh are generated by dividing the problem into cubic hexahedral elements of size length 0.05 cm and 0.025 cm respectively.

Fig. 7 shows a cropped view of a finite element mesh where a region of elements of low refinement connected to a region of elements of high refinements, joined by the pyramid and tetrahedral structure defined in Figs. 4–6.

The exact solution for the MMS problem is the same as for the first $L_2$-error analysis, given by equation (19). The discontinuous diffusion problem is again set up using the MIP scheme. The solution is obtained using a conjugate gradient (CG) solver with aggregation-based algebraic multigrid (AGMG) used as the preconditioner (Notay, 2010, 2012; Napov and Notay, 2012; Notay, 2014).

Table 1 shows results obtained for the MMS solution on all three meshes, using both first-order and second-order elements. The values indicate that the introduction of the pyramids and tetrahedra as a link between two refinement regions does have some negative impact on the convergence of the problem, leading to an increase in iteration number. However maximum absolute error is less than that for the coarse problem in the first-order case and not significantly higher in the second-order case, indicating that the link does not introduce excessive error to the problem. This conclusion is supported by the $L_2$-error which in both cases lies somewhere in between that for the low and high refinement cases. It is also worth considering that some of the extra error introduced may be down to the sudden change in mesh refinement, and
Table 1
Convergence and error data for MMS solution for structured hexahedra of single and mixed refinement. Solutions obtained with conjugate gradient preconditioned with AGMG. Convergence RMS residual of $1.0 \times 10^{-5}$.

<table>
<thead>
<tr>
<th>First-Order Elements</th>
<th>Low Refinement</th>
<th>High Refinement</th>
<th>Mixed Refinement</th>
</tr>
</thead>
<tbody>
<tr>
<td>Number of Elements</td>
<td>8000</td>
<td>64000</td>
<td>38000</td>
</tr>
<tr>
<td>Iterations to Solve</td>
<td>10</td>
<td>11</td>
<td>29</td>
</tr>
<tr>
<td>Maximum Absolute</td>
<td>$1.67 \times 10^{-3}$</td>
<td>$4.18 \times 10^{-4}$</td>
<td>$7.06 \times 10^{-4}$</td>
</tr>
<tr>
<td>Error</td>
<td>$1.15 \times 10^{-1}$</td>
<td>$2.88 \times 10^{-4}$</td>
<td>$4.96 \times 10^{-4}$</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Second-Order Elements</th>
<th>Low Refinement</th>
<th>High Refinement</th>
<th>Mixed Refinement</th>
</tr>
</thead>
<tbody>
<tr>
<td>Number of Elements</td>
<td>8000</td>
<td>64000</td>
<td>38000</td>
</tr>
<tr>
<td>Iterations to Solve</td>
<td>15</td>
<td>14</td>
<td>40</td>
</tr>
<tr>
<td>Maximum Absolute</td>
<td>$1.32 \times 10^{-3}$</td>
<td>$1.67 \times 10^{-6}$</td>
<td>$1.98 \times 10^{-5}$</td>
</tr>
<tr>
<td>Error</td>
<td>$1.48 \times 10^{-1}$</td>
<td>$1.84 \times 10^{-6}$</td>
<td>$4.60 \times 10^{-6}$</td>
</tr>
</tbody>
</table>

not entirely because of the pyramid elements.

Figs. 8 and 9 visualise the absolute error from the specified manufactured solution for each of the three meshes, along a plane at $y = 0.5$. The error is scaled by the same factor for all first-order cases, and similarly but with a larger factor for all second-order cases. These images demonstrate that there is some error introduced by the addition of the linkage, but that it is of roughly the same magnitude as in the coarse problem.

These results demonstrate that for structured hexahedral FEM problems where more refined meshes are required in certain regions of the geometry, this may be used to link the areas of differing refinement without introducing excessive error. The cost of this is weaker convergence.

4.3. Small light water reactor (LWR) (Takeda benchmark model 1)

The Takeda benchmarks (Takeda and Ikeda, 1991) are a set of 3D neutron transport benchmarks. A visualization of the problem as a finite element mesh is shown in Fig. 10. This section will examine Takeda model 1, a small light water reactor (LWR) core with six neutron energy groups. The case for which the control rod is fully inserted will be studied, as the alternative case contains a void region which diffusion codes are ill-suited to.

This problem is selected because of the structured nature of the geometry. This makes it possible to create a mesh of fully structured cubic hexahedra which models the problem correctly. The problem may be converted into a fully structured pyramid mesh by dividing each hexahedral element into six pyramid elements, with the pyramid bases sitting on each face of the cube.

By running this benchmark for varying refinements with both structured hexahedra and structured pyramids, for both first and second-order elements, we may observe the impact on accuracy of using the pyramids.

Most studies which utilise the Takeda benchmark are for neutron transport problems instead of diffusion, however a 2005 study (Ziver et al., 2005), which uses the Takeda problems to test the P$_0$ transport code EVENT (de Oliveira, 1986). EVENT uses a continuous finite element discretization of the second-order even-parity form of the neutron transport equation with a spherical harmonic (P$_N$) angular discretization. Here we use the EVENT results for the P$_1$ case which is equivalent to diffusion for steady-state problems.

Figs. 11 and 12 show the criticality ($K_{\text{eff}}$) solutions for our continuous and discontinuous diffusion codes for the Takeda 1 model discretized using first and second-order hexahedra and pyramids. The benchmark $K_{\text{eff}}$ found by EVENT in (Ziver et al., 2005) is also shown.

The results demonstrate that our continuous diffusion case converges well to a very similar value of $K_{\text{eff}}$ as for the EVENT benchmark. The pyramid elements display convergence towards a value for $K_{\text{eff}}$ which is very close to that of a hexahedron for both 1st and second-order cases. This indicates no significant loss of accuracy when using pyramid elements in this case.

For the discontinuous diffusion case the simulations converge to a slightly lower value of $K_{\text{eff}}$. This discrepancy is due to the fact that the MIP scheme which is being used for the discontinuous diffusion problem penalises at the problem boundaries (Wang and Ragusa, 2010) (Equation (46)). This means that for problems with vacuum (bare) boundaries the neutron loss at these boundaries is increased. It is possible to alter the MIP formulation so that on the boundaries no penalty term is applied, with regular MIP used for the rest of the problem. Such a method is shown in Fig. 13 and it is clear from these results that the modification allows the MIP scheme to properly match the results from the continuous formulation. However, the authors are not aware of a
Fig. 9. Absolute error distribution for homogeneous MMS problem with second-order elements.

(a) Low refinement hexahedra.

(b) High refinement hexahedra.

(c) Low and high refinement hexahedra linked with pyramids and tetrahedra.

Fig. 10. Structured hexahedra mesh of Takeda model 1. Core is surrounded by a reflector with a control rod.

Fig. 11. Criticality results for Takeda model 1 benchmark with control rod inserted. First-order elements.

Fig. 12. Criticality results for Takeda model 1 benchmark with control rod inserted. Second-order elements.

Fig. 13. Criticality results for Takeda model 1 benchmark with control rod inserted. Comparison of continuous and modified MIP formulations for first-order elements.
proof that this modified form of the MIP with unpenalised boundaries, or one similar to it, is unconditionally stable.

Despite these issues with the MIP boundaries, the results in Figs. 11 and 12 still provide evidence that there is no significant loss of accuracy when using pyramid elements for the discontinuous case.

4.4. Liquid metal fast breeder reactor (LMFBR) reactor physics benchmark

The LMFBR problem is a model of a liquid metal fast breeder reactor defined in (Wood and Oliveira, 1984). A recent study (Hosseini, 2016) provided a set of diffusion results for this problem which will be used here as a comparison. Two discretizations of the LMFBR problem were created. The first is formed entirely from unstructured tetrahedra. The second is predominantly unstructured tetrahedra but with a mix of other elements, including pyramids. This is designed to test the impact of including unstructured pyramids in a mixed mesh. Fig. 14 details the geometry of the LMFBR problem and Fig. 15 shows an example of a full LMFBR mesh. Fig. 16 shows a cut through of the mixed LMFBR mesh to demonstrate how surface pyramids link to interior tetrahedra.

Figs. 17 and 18 show the criticality results for the LMFBR problem for first-order and second-order elements respectively. The results demonstrate that for all cases the continuous diffusion problem matches well with the Hosseini results. As with the Takeda problem the MIP discretization results in a slightly lower $K_{eff}$ due to penalisation at the vacuum (bare) boundaries, but the difference is smaller in this case due to lower leakage. These results demonstrate no significant loss of solution accuracy when using pyramid elements within an unstructured mixed mesh problem.

4.5. Iterative convergence rates of different element types

The type of elements used when forming a FEM problem may have a significant impact on the rate at which iterative solvers may calculate a solution to the problem being examined. This section examines the convergence rate of a heterogeneous problem discretized with pyramid elements and compares it to the convergence rate when alternative elements are used.

A heterogeneous, mono-energetic and fixed source problem with cubic geometry is examined. The problem consists of two materials, a high scatter (thick) material and a low scatter (thin) material, arranged in a checkerboard structure as seen in Fig. 19. The cube has side length of 25 cm and reflective boundaries on all sides. The material properties of the thick and thin region are given in Table 2. This problem is selected because the highly heterogeneous nature makes it a very challenging problem for neutron diffusion codes to solve.

A finite element mesh of the problem for varying refinements is created using structured hexahedra, tetrahedra and pyramids, both first-order and second-order, and a discontinuous solution is calculated using the MIP formulation. In order to generate the solution a preconditioned conjugate gradient is used, alongside a set of three preconditioners. The first is AGMG, an algebraic multigrid preconditioner (Notay, 2010, 2012; Napov and Notay, 2012; Notay, 2014). The other preconditioners used are multilevel preconditioners tailored specifically for discontinuous neutron diffusion problems by projecting a linear
discontinuous problem to either a constant discontinuous or a linear continuous level. These preconditioners are referred to as the “constant” and “continuous” preconditioner for short and are defined in (O’Malley et al., 2017a). For the second-order element problems P-multigrid is used to expand the preconditioners, see (O’Malley et al., 2017b). For both the constant and continuous case AGMG is used for a low-level correction. The convergence criterion is an RMS residual of $10^{-9}$.

Tables 3 and 4 display the results for the first-order and second-order case respectively. It is clear from these results that hexahedral elements lead to the best convergence properties, which is as expected.

### Table 2

<table>
<thead>
<tr>
<th>Thin Region</th>
<th>Thick Region</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\Sigma_t$</td>
<td>0.1</td>
</tr>
<tr>
<td>$\Sigma_a$</td>
<td>1.0</td>
</tr>
<tr>
<td>Fixed Source</td>
<td>0.0</td>
</tr>
</tbody>
</table>

### Table 3

CG iterations to find solution of checkerboard problem with first-order elements.

<table>
<thead>
<tr>
<th>Degrees of Freedom</th>
<th>Hexahedra</th>
<th>Pyramid</th>
<th>Tetrahedra</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>AGMG</td>
<td>Constant</td>
<td>Continuous</td>
</tr>
<tr>
<td>1000</td>
<td>26.0</td>
<td>19.0</td>
<td>11.0</td>
</tr>
<tr>
<td>8000</td>
<td>30.0</td>
<td>198.0</td>
<td>15.0</td>
</tr>
<tr>
<td>64000</td>
<td>178.0</td>
<td>349.0</td>
<td>16.0</td>
</tr>
<tr>
<td>512000</td>
<td>112.0</td>
<td>337.0</td>
<td>18.0</td>
</tr>
<tr>
<td>4096000</td>
<td>29.0</td>
<td>280.0</td>
<td>18.0</td>
</tr>
</tbody>
</table>

### Table 4

CG iterations to find solution of checkerboard problem with second-order elements.

<table>
<thead>
<tr>
<th>Degrees of Freedom</th>
<th>Hexahedra</th>
<th>Pyramid</th>
<th>Tetrahedra</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>AGMG</td>
<td>Constant</td>
<td>Continuous</td>
</tr>
<tr>
<td>3375</td>
<td>23.0</td>
<td>25.0</td>
<td>20.0</td>
</tr>
<tr>
<td>27000</td>
<td>43.0</td>
<td>212.0</td>
<td>121.0</td>
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<tr>
<td>216000</td>
<td>67.0</td>
<td>354.0</td>
<td>142.0</td>
</tr>
<tr>
<td>1728000</td>
<td>47.0</td>
<td>351.0</td>
<td>126.0</td>
</tr>
</tbody>
</table>

Fig. 17. Criticality results for LMFBR model. First-order elements.

Fig. 18. Criticality results for LMFBR model. Second-order elements.

Fig. 19. Heterogeneous two material problem with checkerboard structure.
Pyramids and tetrahedra both consistently require more iterations in order to reach convergence. Of particular note is the fact that in almost all cases shown the pyramid elements provide superior convergence to tetrahedra. This provides strong evidence that these pyramid elements have acceptable convergence properties, even for challenging problems.

5. Conclusions

This paper used an established method for forming the basis functions of pyramid elements, developed by Bergot, with the aim of demonstrating their effectiveness in the solution of neutron diffusion problems in reactor physics. It is generally accepted that hexahedral elements are, where practical to mesh, superior to other element types. Pyramid elements are used in circumstances where generating a finite element mesh with purely hexahedral is not practical and a mix of pyramids and tetrahedra are therefore needed. This paper aims to demonstrate that the use of pyramids instead of hexahedral results in a smaller degradation in computational accuracy compared to using tetrahedral elements. Furthermore, this paper also aims to demonstrate the utility of using pyramid elements to act as interface elements between hexahedral elements and tetrahedral elements.

The first results examined the solution accuracy of problems obtained when using pyramids. An L2-error test was used for both a continuous and discontinuous MIP case for structured hexahedral and pyramid entity problems. The pyramids of both first and second-order were shown to demonstrate the ideal L2-error properties that are expected from all finite element types. In addition to this two criticality benchmark problems were studied, a structured problem (Takeda) and an unstructured problem (LMFBR). The results of both of these problems demonstrated that the pyramids converged to the expected answers as the number of degrees of freedom increased at the same rate as for the cases with purely hexahedral or tetrahedral elements. These results collectively provide strong evidence that these pyramid elements do not have any significant impact upon the accuracy of the solutions obtained.

Next an analysis was performed of the localised error generated when using pyramids and tetrahedra to facilitate a change in refine- ment in a structured hexahedral problem. These results demonstrated that such a linkage did create some error but it was of a similar level to the error naturally present in the low refinement region.

Finally, the convergence properties of pyramid elements were studied in comparison to hexahedral and tetrahedral elements. For this convergence study, a test case was constructed which was highly heterogeneous in material composition in order to provide a challenging test case for the different elements. The convergence results from this test case demonstrated that while the convergence of pyramid elements was not as good as hexahedral elements it was in fact superior to that of tetrahedral elements.

Overall the computational test cases presented in this paper demonstrate that pyramid elements may be used within both continuous and discontinuous finite element discretisations of the neutron diffusion equation. Furthermore, the convergence studies indicate that the pyramid elements have a computational accuracy which is greater than both wedge and tetrahedral elements but less than hexahedral as one would expect. Also the computational test cases demonstrate the ability of the pyramid elements to act as interface elements between hexahedral and tetrahedral elements.

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Data Statement

In accordance with EPSRC funding requirements all supporting data used to create figures and tables in this paper may be accessed at the following DOI: https://doi.org/10.5281/zenodo.1136213.

References


