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A partition of unity finite element method for three-dimensional transient diffusion problems with sharp gradients

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Abstract

An efficient partition of unity finite element method for three-dimensional transient diffusion problems is presented. A class of multiple exponential functions independent of time variable is proposed to enrich the finite element approximations. As a consequence of this procedure, the associated matrix for the linear system is evaluated once at the first time step and the solution is obtained at subsequent time step by only updating the right-hand side of the linear system. This results in an efficient numerical solver for transient diffusion equations in three space dimensions. Compared to the conventional finite element methods with h-refinement, the proposed approach is simple, more efficient and more accurate. The performance of the proposed method is assessed using several test examples for transient diffusion in three space dimensions. We present numerical results for a transient diffusion equation with known analytical solution to quantify errors for the new method. We also solve time-dependent diffusion problems in complex geometries. We compare the results obtained using the partition of unity finite element method to those obtained using the standard finite element method. It is shown that the proposed method strongly reduces the necessary number of degrees of freedom to achieve a prescribed accuracy.

Keywords. Finite element method; Partition of unity method; Three-dimensional diffusion problems; Enrichment functions; Heat conduction; Sharp gradients

1 Introduction

Despite the relatively simple model represented by the scalar transient diffusion equation, its numerical solution can still be a serious challenge when the solution diffuses with steep boundary layers. This is often the case if steep gradients occur in the solution that arises for example from cooling a solid at a uniform temperature in contact with a fluid at a different temperature. Depending on the temperature differences, the resulting thermal stresses can be severe and may result in plastic deformations or even cracking, see for instance [46, 48]. For example in glass manufacturing, the molten glass is often cooled down quickly to the room temperature. To control the annealing process it is important to resolve the thermal boundary layers accurately so that the resulting thermal stress can be evaluated. On the other hand, using standard numerical methods to evaluate such steep boundary layers, highly refined meshes become necessary [29, 3]. Considering that the problem is time dependent, evaluating the solution progress over refined meshes and for many hundreds or thousands of time steps can become a serious numerical burden. This can be a significant numerical challenge in two-dimensional problems and even more so in three dimensions [17, 40]. In this work we focus on resolving transient steep boundary layers in three-dimensional problems using the finite...
Although we focus on heat diffusion, the problem is also relevant to many applications in industrial context and also in natural sciences as for example the applications stemming from cell biology [9], thermal radiation heat transfer [13], Stefan-type problems [37, 4], and optical tomography [18]. In many cases these time-dependent diffusion problems are not trivial to simulate since the geometry can be complex and internal source/sink terms may produce steep gradient fields that propagate within the computational domain. The finite element method (FEM) offers a remarkable level of accuracy and robustness for solving partial differential equations (PDEs) on complex geometries. However, using the standard FEM to deal with transient boundary layers with steep gradients can cause severe numerical difficulties.

To avoid intensive computations it was proposed in the literature to enrich the finite element approximations with high order basis functions. Such enrichment approach was first achieved by exploiting the partition of unity property of the standard polynomial basis functions [26]. The approach is widely known as the partition of unity method (PUM). First, only functions that comprise the asymptotic solution space of the considered PDEs were used for the enrichment [19]. For example, in the context of the partition of unity finite element method (PUFEM) and the generalized finite element method (GFEM), a set of plane waves or Bessel functions were used to enrich the FEM space when solving the Helmholtz equation [45, 20, 28, 41, 44]. In the context of the extended finite element method (XFEM), a basis expressing the displacement around the crack tip from classical expansions in fracture mechanics is used to enrich the FEM [27]. Recently, functions that do not satisfy the PDEs under study are also used for the enrichment [31, 30, 43]. However, these functions exhibit features similar to the physical behaviour of the solution in the sense that they have steep gradients, for example, so that the FEM can obtain the solution with less computational effort. Another approach to enrich the solution space in the FEM was achieved through discontinuous Galerkin methods. If the inter-element continuity is enforced rather than ensured through conformity, the choice of elementary basis functions becomes a lot more flexible. Oscillatory basis functions were used to solve wave problems in the discontinuous enrichment method where Lagrange multipliers are utilized to enforce inter-element continuity [11]. The ultraweak variational formulation is another approach where plane or cylindrical waves were used to enrich the solution space for wave problems [14, 23, 24]. Several other enriched discontinuous Galerkin approaches are also available in the literature, see [21, 22, 33], among others.

In heat transfer problems, enrichment functions were used to retrieve sharp thermal gradients using global and local enrichment functions in the GFEM [34, 36]. The linear basis functions are augmented by tailored enrichments computed on the fly for steady-state problems [34] as well as for transient problems [36]. In a different work for time-dependent geothermal applications, a set of enrichment functions that approximate the solution at each time step, were also utilized [47]. The evolution of thermal gradients with time in this approach requires updating the enrichment functions. Hence, the shape functions must also be updated as the solution progresses in time. A different enrichment strategy was proposed in [29] where the time-dependent enrichment was replaced with a set of stationary basis functions. The combination of these functions covers the spatial as well as the temporal solution features. This can significantly reduce the computational costs for any time marching scheme as the linear system of equations built at the first time step can be reused for all subsequent time steps after updating the right-hand side. Thus, solving the linear system can be reduced to a backward/forward substitution if an LU decomposition is performed at the first time step. The work was also developed to solve the coupled problem of heat conduction and radiation in grey media with a single radiation frequency [30] and in glass cooling with a wide spectrum of frequencies [31]. Approaches based on the PUM are also utilized to capture discontinuity in the heat or its gradient in two-dimensional problems [7, 42] and in three-dimensional problems [43] as well as for the discontinuity in solidification problems [6]. A major advantage of such methods is the ease of formulation. Moreover, the implementation in existing codes can be carried out without any large scale restructuring of the code. However, it should be noted that compared to standard finite element methods the majority of enrichment approaches suffer from ill-conditioning of the associated linear systems. The conditioning issue is mainly linked to the number of enrichment functions such that increasing the number of functions leads to the deterioration of the conditioning. This has been reported in many works on the PUFEM, see for example [5]. However, it should also be noted that the errors can be significantly reduced by including...
only a few enrichment functions which keeps relatively low condition numbers [29]. Enrichment functions are also used with a discontinuous Galerkin method to solve advection-diffusion problems [12]. A method employing Lagrange multipliers was also implemented for spatially-varying advection fields in [38] as well as for unsteady advection-diffusion problems in [39].

In the present work, we propose a PUFEM approach for transient diffusion problems in three space dimensions. Unlike previous work where extra enrichment functions are added to recover the solution in the extra dimension. The exponential functions proposed in this work can be designed to have steep gradients in one, two or three space dimensions. Hence, it is possible to solve three-dimensional problems with the same number of enrichment functions needed in two-dimensional problems. However, the achieved saving in the total number of degrees of freedom required for solving a problem is far higher in the three-dimensional problem compared to its two-dimensional counterpart. The proposed approach has the same useful features of the work proposed in [29] such that the same enrichment can be reused for all time steps. Hence, it will also be possible to decompose the system matrix at the first time step and then reuse the decomposition for all other steps. However, so far the approach proposed in [29] was used for solving simple geometries in two dimensions. We show that the approach can also be very useful for complicated geometries in three space dimensions such as in industrial applications. The saving in the computational time especially for three-dimensional problems can downscale industrial applications to run on a single processor of a standard desktop computer. Such applications would otherwise require multi-cores or even a cluster to simulate. It is worth noting that the enrichment approach for heat transfer problems offers a further advantage in comparison to that used for wave problems. In the PUFEM for wave modelling, the number of enrichment functions taken in three dimensions is far larger than that of two dimensional cases. For example, if about 30 plane waves are used in a two-dimensional case, in a three-dimensional one about 100 plane waves would be used [25]. However, in the case of heat transfer problems, where Gaussian-type enrichment functions are incorporated in the field approximation, it is sufficient to add a-priori information into the two-dimensional enrichment functions to describe the field behaviour in three dimensions while keeping the number of enrichment functions unchanged, typically 5 [16], which is demonstrated in the current work.

The remainder of this paper is organized as follows. In section 2 the considered boundary value problem is introduced together with its weak formulation. Next, the enrichment approach is presented in section 3. To investigate the efficiency of the approach a number of numerical test examples are considered in section 4. Finally, in section 5, we finish with some concluding remarks.

2 Weak formulation of three-dimensional diffusion problems

In the current study we are interested in the three-dimensional transient diffusion problems governed by the following boundary-value equation

\[
\frac{\partial \phi}{\partial t} - \lambda \nabla^2 \phi = f(t,x), \quad (t, x) \in [0, T] \times \Omega,
\]

where \([0, T]\) is a given time interval, \(\Omega \subset \mathbb{R}^3\) is a three-dimensional open bounded domain with a boundary \(\Gamma\). Here, \(x = (x, y, z)^T\) denotes the spatial coordinates, \(t\) is the time variable, \(\lambda\) is the diffusion coefficient, and \(f\) represents the effects of internal source/sink terms. The material properties are accounted for in (1) by the diffusion coefficient \(\lambda\). The equation is equipped with an initial condition as

\[
\phi(0, x) = \phi_0(x), \quad x \in \Omega,
\]

where \(\phi_0\) is a defined function. On the boundary \(\Gamma\), the solution satisfies

\[
\eta \phi + \lambda \frac{\partial \phi}{\partial n} = g(t, x), \quad (t, x) \in [0, T] \times \Gamma,
\]

where \(n\) is the outward unit normal on the boundary \(\Gamma\), and \(g\) is a prescribed boundary function. In the current work, we only consider a Robin-type boundary conditions, hence, we take \(\eta = 1\). It is also possible
to consider a Dirichlet-type boundary conditions in a similar way but using a large value for $\eta$ as a penalty factor [15]. Indeed, compared to other numerical methods such as those using Lagrange multipliers [2], the penalty method can be easily used to enforce Dirichlet boundary conditions without adding any extra unknowns. It should also be noted that the penalty formulation was effectively implemented in the context of meshfree methods [49] but not in the PUFEM. However, we expect similar behaviour when using with the PUFEM. Furthermore, no spurious oscillations have been detected in our simulations obtained for the unknowns. It should also be noted that the penalty formulation was effectively implemented in the context of meshfree methods [49] but not in the PUFEM. However, we expect similar behaviour when using with the PUFEM. Furthermore, no spurious oscillations have been detected in our simulations obtained for the considered value of $\eta$. The equations (1)-(3) have been widely used in the literature to model diffusion problems including heat transfer. In this case, $\phi$ represents the temperature and $\lambda$ the heat conduction coefficient. On the boundary of the computational domain, the heat energy which diffuses through the boundary $\Gamma$ is proportional to the boundary temperature and its gradient with respect to the outward unit normal direction $\mathbf{n}$ on the boundary $\Gamma$. The ambient temperature is reflected through the boundary function $g$.

To solve the initial boundary-value problem defined by the equations (1)-(3), we use the well-established Rothe approach [8] in which we first integrate the equations in time and then a finite element method is used for the spatial discretization. First, the time domain $[0, T]$ is divided into $N_t$ uniform subintervals $[t_n, t_{n+1}]$ with duration $\Delta t = t_{n+1} - t_n$ for $n = 0, 1, \ldots, N_t$. To denote the value of a generic function $\omega$ at time $t_n$ we use the notation $\omega_n$. For the time integration of (1) over the time domain we consider a $\theta$-time stepping scheme. Hence, the semi-discrete formulation of the diffusion equation (1) can be written as

$$\frac{\phi^{n+1} - \phi^n}{\Delta t} - (1 - \theta)\lambda \nabla^2 \phi^{n+1} - \theta \lambda \nabla^2 \phi^n = (1 - \theta)f^{n+1} + \theta f^n,$$  

(4)

where the parameter $\theta$ is defined based on the chosen time stepping scheme. For $\theta = 0$, the time stepping scheme (4) reduces to the first-order backward Euler method

$$\frac{\phi^{n+1} - \phi^n}{\Delta t} - \lambda \nabla^2 \phi^{n+1} = f^{n+1}(x), \quad x \in \Omega,$$  

(5)

$$\phi^{n+1} + \lambda \frac{\partial \phi^{n+1}}{\partial n} = g^{n+1}(x), \quad x \in \Gamma.$$

The first equation in (5) can be rearranged as

$$\phi^{n+1} - \lambda \Delta t \nabla^2 \phi^{n+1} = \Delta t f^{n+1} + \phi^n.$$  

(6)

Note that the first-order backward Euler scheme (5) is unconditionally stable for linear problems. Therefore, the choice of $\Delta t$ may be solely based on the accuracy to be achieved in the computed solutions. The solution $\phi^{n+1}$ at a given time instant $t_{n+1}$ can be obtained by solving the equation (6) at this time instant. To solve the equation using the finite element method, we multiply (6) by a test function $w$ and then integrate over $\Omega$

$$\int_{\Omega} w \phi^{n+1} d\Omega - \int_{\Omega} \lambda \Delta t w \nabla^2 \phi^{n+1} d\Omega = \int_{\Omega} w \left( \Delta t f^{n+1} + \phi^n \right) d\Omega, \quad \forall w \in H^1(\Omega),$$  

(7)

where the space of the test functions is the conventional Sobolev space $H^1(\Omega)$. Using the divergence theorem and then rearranging the terms, we can write

$$\int_{\Omega} \left( \lambda \Delta t \nabla w \cdot \nabla \phi^{n+1} + w \phi^{n+1} \right) d\Omega - \int_{\Gamma} \lambda \Delta t w \nabla \phi^{n+1} \cdot \mathbf{n} \ d\Gamma = \int_{\Omega} w \left( \Delta t f^{n+1} + \phi^n \right) d\Omega.$$  

(8)

Using the boundary condition in (5) we define the weak formulation: Find $\phi \in H^1(\Omega)$ such that

$$\int_{\Omega} \left( \lambda \Delta t \nabla w \cdot \nabla \phi^{n+1} + w \phi^{n+1} \right) d\Omega + \int_{\Gamma} \Delta t w (\phi^{n+1} - g^{n+1}) d\Gamma = \int_{\Omega} w (\Delta t f^{n+1} + \phi^n) d\Omega.$$  

(9)

A fully discrete system of the diffusion problem (1)-(3) is completed when a spatial discretization is performed for the semi-discrete equation (9). In the current work, this step is achieved using the finite element method.
3 Partition of unity enriched finite element method

A finite element discretization of the computational domain $\Omega_h \subset \Omega$ is given by $\{\Omega^e\}$ where $e = 1, 2, \ldots, N_e$ and $N_e$ being the total number of elements. The partitions $\{\Omega^e\}$ are non-overlapping with $\Omega_h = \Omega^1 \cup \Omega^2 \cup \ldots \cup \Omega^{N_e}$. The subscript $h$ refers to the discrete finite element problem. The conforming finite element space for the solution is defined as

$$\Phi_h = \left\{ \phi_h \in C^0(\Omega) : \phi_h|_{\Omega^e} \in P(\Omega^e), \ \forall \Omega^e \in \Omega_h \right\},$$  

with

$$P(\Omega^e) = \left\{ p(x) : p(x) = \hat{p} \circ Y^{-1}_j(x), \ \hat{p} \in P_m \right\}.$$  

The polynomial $\hat{p}(x)$ is defined on the element $\hat{\Omega}^e$ and $P_m$ is the set of all polynomials of degree $\leq m$ defined on a reference element whereas, $Y_j$ is an invertible one-to-one mapping between the element $\Omega^e$ and the reference element. Hence, the solution approximated using the finite element method and at a given time is defined by

$$\phi_n(x) \equiv \phi_{n,h}(x) = \sum_{j=1}^{N_d} C_{n,j} N_j(x),$$  

where $N_d$ is the total number of nodes in the computational domain $\Omega_h$. The variables $C_{n,j}$ correspond to the nodal values of $\phi_{n,h}(x)$ i.e., $C_{n,j} = \phi_{n,h}(x_j)$ with $j = 1, 2, \ldots, N_d$. The functions $\{N_j\}_{j=1}^{N_d}$ are a set of global nodal basis functions characterized by $N_j(x_j) = \delta_{ij}$ with $\delta_{ij}$ denoting the Kronecker delta.

In each element $\Omega^e$ we define a set of $M$ nodes $\{x_j\}_{j=1}^{M}$ and a set of $M$ basis functions $\{\varphi_j\}_{j=1}^{M}$ in $\Phi_h$.

The basis functions are local restrictions of the global basis functions $\{N_j\}_{j=1}^{N_d}$ on the element $\Omega^e$. The approximation space can then be defined as

$$\tilde{\Phi}_h^0 = \text{span} \left\{ N_h, \ \phi_h = \sum_{j=0}^{M} \varphi_j N_j \right\}.$$  

To improve the finite element approximation (11) which is based on polynomials, we enrich the solution space with exponential basis functions. The enriching functions are chosen to have better approximation properties for solving the diffusion equation with steep boundary layers as the one considered in the present study. Note that we choose the PUFEM because it ensures inter-element continuity in a natural way which simplifies implementing the proposed approach in any existing finite element code with minimal changes.

Here, the following sum of exponential basis functions are used to enrich the solution space

$$G_q(x,y,z) = \frac{\exp \left( - \left( C_1(x-x_0) + C_2(y-y_0) + C_3(z-z_0) \right)^q \right) - \exp \left( - \left( \frac{R_c}{C} \right)^q \right)}{1 - \exp \left( - \left( \frac{R_c}{C} \right)^q \right)},$$  

for $q = 1, 2, \ldots, Q$ with $Q$ being the total number of enrichment functions. In (12), $(x_0, y_0, z_0)$ and $(x, y, z)$ are the control point and any point in the domain $\Omega_h$, respectively. The control point should be placed in the domain part with a zero or a minimum gradient so that the gradient increases in any direction inside the domain and away from the control point. Often the domain part with zero-gradient is within the domain core. Together with the exponent $q$ the parameters $C_1$, $C_2$, $C_3$, $C$ and $R_c$ in (12) control the gradient of the sum of the exponential functions $G_q$ in the three spatial directions. In the parametric studies performed in this work a value range of $[0.1, 2]$ for $C_1$, $C_2$ and $C_3$ with $C \approx \frac{1}{C_1}$ and $R_c \approx \sqrt{\frac{14}{C_1}}$, leads to the best performance of the proposed enrichment. It is possible to optimize these parameters based on a specific problem but such optimization has a limited impact on the enrichment performance as long as these
constants remain within the above mentioned range. Choosing these parameters to be an order of magnitude different may lead to unstable performance for the enriched finite elements. It is also worth noting that if the gradient is only changing in one direction (e.g. x-axis) it is possible to cancel the parameters in other directions i.e. $C_2 = 0$ and $C_3 = 0$. Optimizing the gradient in different directions for each function can reduce the total number of degrees of freedom required to solve the diffusion problem. However, this reduction is often insignificant relatively to the already low number of degrees of freedom needed with the enrichment. In this work, for simplicity, a uniform gradient is considered in all directions. It should be mentioned that an exponential function similar to $G_q$ with $q = 2$ was used in [1] as a weighting function in the context of meshless methods for solving the linear Poisson equation. Single functions similar to $G_q$ with $q = 1$ or 2 were also used as an enrichment for finite elements in previous works [32, 34, 35, 47]. Finally, a sum of functions similar to $G_q$ were first introduced in [29] for solving the two-dimensional diffusion equations. The sum of multiple functions $G_q$ where $q = 1, 2, ..., Q$ is a generalization of the exponential functions considered in the previous work so that the time-dependency of the enrichment is avoided. The enrichment is included in the finite element approximation by expanding the nodal values to be rewritten as

$$C_{n,j} = \sum_{q=1}^{Q} A_{n,j,q} G_q. \quad (13)$$

Thus, the linear system of equations resulting from the enriched finite element formulation is solved for the new unknowns $A_{n,j,q}$ instead of the nodal values $C_{n,j}$ as in the conventional finite element approximation. Hence, using the enriched expansion (13), the finite element approximation (11) becomes

$$\phi_n(x) = \sum_{j=1}^{N_d} \sum_{q=1}^{Q} A_{n,j,q} N_j(x) G_q(x). \quad (14)$$

For simplicity in the presentation we define a new set of shape functions $L_{(j-1)Q+q}$ as

$$L_{(j-1)Q+q}(x) = N_j(x) G_q(x), \quad (15)$$

and the new approximation space becomes

$$\tilde{\Phi}_h^1 = \text{span} \left\{ L_h, \phi_h = \sum_{j=1}^{N_d} \sum_{q=1}^{Q} A_{n,j,q} N_j G_q \right\}.$$

The same enrichment functions are applied at all nodes in the computational domain so that a global enrichment approach is followed in this work. In this way the inter-element $C^0$ continuity is naturally ensured and the implementation of the approach in existing codes will require minimum changes. It should be stressed that the new shape functions are composed of the enrichment functions $G_q$ which are written in terms of the global coordinates $x$ multiplied by the nodal polynomial shape functions $N_j$. The shape functions have different approximation properties at different elements based on the behaviour of the global enrichment functions in these elements. These global approximations are made local in the vicinity of a feature of interest such as a steep boundary layer using the local basis functions. The solution of the transient diffusion problem (1)-(3), can have a steep gradient that moves with time. The individual enrichment functions have steep gradients at different locations in the computational domain so that they represent the solution at different stages in time. This feature helps to capture the solution steep gradient as it moves in the domain. This variation in time is captured by the sum of enrichment functions although the functions themselves are time-independent. Other enrichment functions including time-dependent functions can also be used in our approach without major conceptual modifications. Moreover, the main advantage of the time independent enrichment functions is the possibility to build the assembled matrix for the linear system only at the first time step to be used in subsequent time steps. Since only the right-hand side of the linear system is updated in the time integration process, one may factorize the matrix using an LU decomposition at the
first time step and the solution is computed using backward/forward substitutions. This can significantly increase the efficiency when a large number of time steps is needed compared to updating the matrix and fully solving the system at every time step.

4 Numerical results

In this section we present the numerical results for three numerical test problems solved using the PUFEM approach. To study the efficiency of the approach the results of the first two tests are also compared to the results of the standard FEM with linear finite elements which is often used in industry for solving similar problems. After studying the convergence of the approach we use the PUFEM for retrieving the heat transfer in an industrial geometry. In all the reported computations, the integrals over elements are evaluated numerically using the standard Gaussian quadrature. We ensured in all the presented results that the chosen number of quadrature points is high enough to eliminate the effect of integration errors. Although usually the number of integration points per element is much higher with the PUFEM than with the standard FEM but the total number of integration points in the entire domain with the PUFEM is smaller to that of the corresponding number of the FEM. This is caused by the much higher number of elements needed for the FEM compared to the PUFEM. All the resulting linear systems of algebraic equations are solved using a direct solver.

4.1 Diffusion problem in a cube enclosure

To evaluate the efficiency of the PUFEM approach relative to other high order methods, the convergence rates of the PUFEM are provided in this example. In addition, since the low order FEM is often used in industrial applications to solve heat transfer problems, comparisons between the linear FEM and the PUFEM are also included in this section. First, we aim to examine the PUFEM convergence rate for $h$- and $q$-refinement procedures. To this end we solve the transient diffusion problem (1)-(3) in the cube $\Omega = [0, 2]^3$ with a known analytical solution. The source term $f$, the boundary function $g$ and the initial condition $\phi_0$ are explicitly calculated such that the analytical solution of (1)-(3) is given by

$$\phi(x, y, z, t) = x^\tau (2 - x)^\tau y^\tau (2 - y)^\tau z^\tau (2 - z)^\tau \left(1 - e^{-\lambda t}\right),$$

(16)

where $\tau$ is a parameter used to control the steepness of the solution gradient such that for sharp gradients we increase the value of $\tau$. In this example a fixed value $\tau = 20$ is chosen in the presented simulations. The
Table 1: Relative $L^2$-errors obtained using the PUFEM and the FEM on the considered meshes for the diffusion problem in a cube enclosure using different time steps $\Delta t$. The number of enrichments used in the PUFEM is $Q = 6$.

<table>
<thead>
<tr>
<th>$\Delta t$</th>
<th>PUFEM</th>
<th>FEM-E</th>
<th>FEM-F</th>
<th>PUFEM</th>
<th>FEM-E</th>
<th>FEM-F</th>
</tr>
</thead>
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<td>0.05</td>
<td>8.7124E-03</td>
<td>9.4645E-02</td>
<td>1.2768E-02</td>
<td>8.8473E-03</td>
<td>1.0238E-01</td>
<td>1.5249E-02</td>
</tr>
<tr>
<td>0.01</td>
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<td>8.9109E-02</td>
<td>1.0065E-02</td>
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<td>9.8572E-02</td>
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<tr>
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<td>1.3054E-02</td>
</tr>
</tbody>
</table>

Figure 2: Time evolution of the $L^2$-error obtained using the FEM on different meshes and the PUFEM with different enrichments for the diffusion problem in a cube enclosure using $\Delta t = 0.001$ (left) and $\Delta t = 0.01$ (right).

exact solution has sharp gradient close to the domain core and vanishes on the boundary surface $\Gamma$. To quantify the error in the computed numerical solutions we use the following relative error norms

$$\varepsilon = \frac{\| \phi - \varphi \|_{L^2(\Omega)}}{\| \varphi \|_{L^2(\Omega)}}, \quad \varepsilon_\infty = \frac{\| \phi - \varphi \|_{L^\infty(\Omega)}}{\| \varphi \|_{L^\infty(\Omega)}},$$

where $\| \cdot \|_{L^2(\Omega)}$ is the $L^2$-norm, $\| \cdot \|_{L^\infty(\Omega)}$ is the $L^\infty$-norm, $\phi$ and $\varphi$ are, respectively, the numerical and exact solutions. The considered values for the enrichment parameters are $C_1 = C_2 = C_3 = 1.195$, $C = \frac{1}{1.195}$ and $R_c = \sqrt{\frac{14}{1.195}}$.

First, to test the convergence of the time discretization scheme for the PUFEM we consider four time steps of different sizes. The PUFEM solution is obtained on a uniform mesh composed of 216 hexahedral elements and 343 nodes, where the computational domain is discretized into 6 uniform intervals in the $x$, $y$ and $z$ directions and the resulting elements are all cubes of edge length $h = \frac{2}{6}$. The approximation is then enriched with six enrichment functions ($Q = 6$) which makes the total number of degrees of freedom 2058 in the PUFEM. To solve the problem with the FEM using a similar number of degrees of freedom a uniform coarse mesh composed of 1000 hexahedral elements and 1331 nodes is considered where the domain...
is discretized into uniform cubes of edge length $h = \frac{2}{10}$. The FEM solution on this mesh is referred to as FEM-E. A fine mesh is also considered with the domain discretized into 15625 hexahedral elements and 17576 nodes so that the resulting elements are uniform cubes of edge length $h = \frac{2}{25}$. The FEM solution on this mesh is referred to as FEM-F where the total number of degrees of freedom is 13.5 times higher than the PUFEM. Figure 1 shows the three considered meshes.

The PUFEM solution errors are compared to the FEM errors at two instances namely, $t = 0.05$ and $t = 0.1$ using $\Delta t = 0.05$, 0.01, 0.001 and 0.0005 for the diffusion coefficient $\lambda = 0.1$. The results, listed in Table 1, show that the $L^2$-error is reduced in all the cases if a finer time step is considered. For example the PUFEM $L^2$-error at $t = 0.05$ is reduced from $\varepsilon = 8.7124E-03$ for $\Delta t = 0.05$ to $\varepsilon = 8.3246E-03$ for $\Delta t = 0.0005$. Similarly the FEM-E $L^2$-error is reduced from $\varepsilon = 9.4645E-02$ to $\varepsilon = 8.7630E-02$ and FEM-F from $\varepsilon = 1.2768E-02$ to $\varepsilon = 9.3254E-03$. When comparing the errors for the same $\Delta t$ it can be seen that the PUFEM always leads to one order of magnitude smaller errors than the FEM-E where both methods use a similar number of degrees of freedom. Although the FEM-F involves a total number of degrees of freedom order of magnitude higher but the PUFEM again leads to smaller errors. For example at $t = 0.05$ and for $\Delta t = 0.001$ the errors obtained with the PUFEM, FEM-E and FEM-F are, respectively, 8.3288E-03, 8.7709E-02 and 9.3653E-03. The results in the table also show that at $t = 0.05$ for FEM-F the $L^2$-error improves from around 0.013 for $\Delta t = 0.05$ to 0.009 for $\Delta t = 0.001$. Refining the time step further shows insignificant improvement in the $L^2$-error. At the same time and for the PUFEM the $L^2$-error is around 0.009 for $\Delta t = 0.05$ and improves to 0.008 for $\Delta t = 0.01$. Again further time step refinement shows insignificant improvement in the $L^2$-error. This suggests that the spatial $L^2$-error is around 0.008 for both FEM-F and the PUFEM. Note that using the PUFEM, it is possible to achieve this error with $\Delta t = 0.01$ while for FEM-F it is necessary to reduce the time step to $\Delta t = 0.001$ to achieve this error. This behaviour suggests that the PUFEM is able to tolerate a much larger time step without losing much accuracy compared to a fine FEM mesh. Furthermore, as time progresses it can be seen that the PUFEM $L^2$-error accumulates at a smaller rate compared to FEM-E and FEM-F. For example for $\Delta t = 0.001$ the PUFEM $L^2$-error increases from 8.3288E-03 at $t = 0.05$ to 8.5356E-03 at $t = 0.1$, which is around 2.5% increase. For the same case the FEM-E $L^2$-error increases by 10.2% and FEM-F by 28.4%. This suggests that the PUFEM accumulates spatial errors at a smaller rate in time.

To further compare the accumulation of spatial errors in time of both methods, we illustrate in Figure 2...
Table 2: The PUFEM solution errors and average convergence rates $\alpha_h$ and $\alpha_q$ of the considered meshes and enrichment numbers, respectively, for the diffusion problem in a cube enclosure using $\Delta t = 0.001$ and two values of the diffusion coefficient.

<table>
<thead>
<tr>
<th>$h$</th>
<th>$Q$</th>
<th>$\alpha_q$</th>
<th>$\alpha_h$</th>
<th>$Q$</th>
<th>$\alpha_q$</th>
<th>$\alpha_h$</th>
</tr>
</thead>
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<tr>
<td>4/32</td>
<td>2</td>
<td>0.077</td>
<td>0.46</td>
<td>2</td>
<td>0.077</td>
<td>0.77</td>
</tr>
<tr>
<td>3</td>
<td>0.034</td>
<td>0.073</td>
<td>0.32</td>
<td>3</td>
<td>0.028</td>
<td>0.073</td>
</tr>
<tr>
<td>3/32</td>
<td>0.028</td>
<td>0.066</td>
<td>0.026</td>
<td>3/32</td>
<td>0.0085</td>
<td>1.98</td>
</tr>
<tr>
<td>2</td>
<td>0.0085</td>
<td>0.018</td>
<td>0.0078</td>
<td>2</td>
<td>0.0027</td>
<td>1.98</td>
</tr>
<tr>
<td>32</td>
<td>2.00</td>
<td>1.98</td>
<td>2.77</td>
<td>32</td>
<td>2.77</td>
<td>1.98</td>
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<tr>
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</tr>
</tbody>
</table>

the $L^2$-errors obtained using the PUFEM with $Q = 4$ and $Q = 6$ where the former is denoted by PUFEM-4 while the latter by PUFEM-6. The results obtained for the $L^\infty$-error are displayed in Figure 3. The FEM and the PUFEM discretizations are chosen so that the error at the first time step is smaller with FEM-F than PUFEM-6 and smaller with PUFEM-6 than FEM-C. At the same time step PUFEM-4 has the largest error. This will help to minimize the effect of the initial error on the FEM cases as they start from smaller errors. However, it is always possible to refine the PUFEM discretization so that a smaller error is obtained. The errors are plotted for 1000 time steps when the step size is $\Delta t = 0.001$ and for 100 time steps when $\Delta t = 0.01$. The considered value of heat conduction is kept at $\lambda = 0.1$. On the same plots we also include the errors obtained using the FEM-D and another coarser mesh FEM-C composed of 8000 hexahedral elements and 9261 nodes where the elements are cubes of edge length $h = 2/20$. Even though FEM-F starts with the smallest error in the first time step in all cases, it becomes larger than that of PUFEM-6 at time $t = 0.04$ when $\Delta t = 0.001$ and around 3 time steps when $\Delta t = 0.01$. In fact, for $\Delta t = 0.01$ the FEM-F error becomes higher than that of PUFEM-4 at around 50 time steps. Similarly, FEM-C starts at smaller errors than PUFEM-4 but it accumulates errors faster which leads to higher errors eventually for both $\Delta t = 0.001$ and $\Delta t = 0.01$. Hence, one may conclude that the PUFEM accumulates spatial errors at a smaller rate in time than the FEM. One reason might be the much higher number of elements with the FEM which may lead to faster increase of round-off errors especially for time-domain problems involving many time steps.

Our final aim in this example is to investigate the $h$- and $q$-convergence of the PUFEM. The convergence rates can help to evaluate the relative performance of the method in comparison to other high order methods. In Table 2 we summarize the errors of the PUFEM solution for the time step $\Delta t = 0.001$ and two values of the diffusion coefficient $\lambda = 0.1$ and $\lambda = 0.01$. The table shows how the error is reduced when we refine the mesh from $h = 4/32$ to $h = 3/32$ and then $h = 2/32$. For each mesh we can also observe the reduction of the error for an increase in the number of enrichment functions from $Q = 2$ to $Q = 4$ and then $Q = 6$. The average convergence rates $\alpha_h$ and $\alpha_q$ for $h$- and $q$-convergence are also listed in the respective columns/rows.

Examining the results some interesting patterns can be noticed. First, although the enrichment leads to the same accuracy for fewer degrees of freedom but using a small number of enrichment functions can slow down the convergence rate. For example, the trilinear finite element optimum convergence rate for $h$-refinement in the $L^2$-error norm should be $\alpha_h = 2$. This rate is reduced to a number smaller than one when two enrichment functions are used in the simulations. This can be seen for $\lambda = 0.1$ for which the average convergence rate is $\alpha_h = 0.46$. However, this number seems to increase to $\alpha_h = 0.77$ for $\lambda = 0.01$ where the solution exhibits steeper gradients in this case. Although the average rate $\alpha_h$ is decreased from 2 to 0.46 for $Q = 2$ but it recovers for $Q = 4$ to 1.92 and significantly increases to 3.49 for $Q = 6$. This suggests that...
the average convergence rate is increased as we increase the number of enrichment functions $Q$ which is similar to the behaviour observed in wave problems [10]. The $h$-convergence rate less than one is observed for the smallest considered number of enrichment functions i.e. $Q = 2$, and can be attributed to the fact that the method being in its pre-asymptotic regime. For the case $\lambda = 0.01$ when the solution gradient is steeper the convergence rate shows even higher increases with increasing $Q$ as can be seen in Table 2 where $\alpha_h$ increases to 2.43 for $Q = 4$ and 4.07 for $Q = 6$. Next, we turn our attention to the convergence rate when adding more enrichment functions and keeping the mesh fixed. Again for the considered coarsest mesh with $h = \frac{4}{32}$, the $q$-convergence rate seems to be smaller than one i.e. $\alpha_q = 0.83$. This number remains practically unchanged when the steepness of the solution gradient is increased by taking $\lambda = 0.01$. The same observation made above about the method being in its pre-asymptotic regime can also be made for the coarsest considered mesh where the $q$-convergence rate is also smaller than one. This behaviour is completely different when the mesh is refined to $h = \frac{3}{32}$ and then to $h = \frac{2}{32}$ where the convergence rate is increased to $\alpha_q = 2.00$ and $\alpha_q = 2.77$, respectively. Again, the effect of changing $\lambda = 0.01$ seems insignificant on these rates of convergence.

It should also be stressed that the results presented in Table 2 suggest that the convergence rate in the PUFEM increases with increasing the number of enrichment functions $Q$ and also by refining the mesh. However, it should be noted that this $q$- and $h$-refinements will also increase the condition number of the resulting linear system of algebraic equations. In fact increasing $Q$ to 8 or 10 start to deteriorate the results as the conditioning of the linear system of equations starts to become very poor. Similarly, having highly refined meshes with $Q = 6$ will also lead to conditioning problems for both diffusion coefficients. The results obtained in this study suggest that having between 4 and 6 enrichment functions with relatively coarse meshes, leads to the most efficient solutions.

4.2 Diffusion problem in a sphere enclosure

In the second test example we aim to evaluate the performance of the PUFEM in computing heat transfer solutions with gradients varying at different rates in different directions. Unlike the previous example where the gradient is uniformly varying in the three dimensions, this problem cannot be reduced to a two-dimensional problem. We consider a sphere that is exposed to a heat source maximized at the point (2,2,2)
Figure 5: Temperature distributions obtained for the diffusion problem in a sphere enclosure using the FEM (top) and the PUFEM (bottom) at three different instances $t = 0.02$, 0.05 and 0.1 (from left to right).

and exponentially damped away from this point. The source is amplified on the surface sphere closest to the point and exponentially diffuses away from it. The rate at which the intensity is damped varies in different directions. The problem is again governed by the equations (1)-(3) where the computational domain is a unit sphere centered at $(1, 1, 1)$. The source intensity is given by

$$f(x, y, z) = \gamma \exp\left(-\sqrt{(z - 2)^2 + 1}\right) \exp\left(-(x - 2)^2 - (y - 2)^2\right),$$

(18)

where $\gamma$ is a constant fixed to 15000 in our simulations. Unlike the first example, where the heat gradient is varied at the same rate in all three dimensions, this test serves in evaluating the enrichment efficiency in a more challenging problem in term of variation of solution gradients. The thermal conductivity of the sphere material is $\lambda = 0.01$. The domain is initially at temperature $\phi_0 = 0$ and the boundary condition is set to $g = 0$. Although, the gradient of the solution is different in each spatial direction i.e. $x, y$ and $z$, the same value is considered for the enrichment parameters $C_1, C_2$ and $C_3$ so that $C_1 = C_2 = C_3 = 0.225$ while $S = \frac{1}{0.225}$ and $R_c = \sqrt{\frac{11}{0.225}}$.

In this example the linear FEM is used to create a reference solution using an $h$-refinement convergence study. It should be mentioned that the results obtained in this convergence study confirm the conclusions made in the previous example that the PUFEM leads to a significant reduction in the total number of degrees of freedom compared to the FEM. However, comparing the FEM to the PUFEM in terms of degrees of freedom is not performed in this example as it is not possible to measure the error. There is no analytical solution available for the problem. To measure the error using a numerical reference solution on a highly refined mesh will lead to an improved geometry representation compared to the geometry representation with the coarse mesh used with the PUFEM. The FEM reference solution is obtained on a dense mesh composed of 59611 tetrahedron elements and 11360 nodes and is used for qualitative comparisons with the PUFEM solution. On the other hand the PUFEM solution is obtained on a coarse mesh of 1972 tetrahedron elements and 564 nodes and using four enrichment functions ($Q = 4$). For illustration purpose the two considered meshes are displayed in Figure 4. The time domain is discretized using $\Delta t = 0.001$. 

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Figure 6: Cross-section of the temperature along the line formed by the two points \( (1,1,0) \) and \( (1,1,2) \) for the diffusion problem in a sphere enclosure at three instances \( t = 0.02, 0.05 \) and 0.1 (from left to right).

Figure 5 depicts the results obtained using both methods, the FEM and the PUFEM, at three different instances namely, \( t = 0.02, 0.05 \) and 0.1. The figure shows the sphere face exposed to maximum heat. As it can be seen in the figure the domain is mainly heated at an area of its surface. The heat is then diffused at different rates on the surface around this area and through the depth of the sphere. The plots show similar heat patterns are obtained with both methods and at all times. To further compare the differences in the results we plot the temperature on a radial cross-section passing through the diameter in the \( z \)-direction. Figure 6 shows the temperature obtained with the FEM and the PUFEM on the radial line defined by the two points \( (1,1,0) \) and \( (1,1,2) \). In general both methods predict similar temperatures along the cross section. The temperature varies in the range 4 to 15 at \( t = 0.02 \). The variation is increased to the range 20 to 80 at \( t = 0.1 \). This increased variation in the temperature and its gradient seems to be satisfactorily recovered with both approaches but with a number of degrees of freedom in the PUFEM far lower than in the FEM. Moreover, at the first time step the CPU time needed for building the linear system of equations is 2828.90 s and for solving it 0.38 s when using the PUFEM. This time increases to 85112.56 s and 177.34 s, respectively, when using the FEM. This shows that potentially the PUFEM can achieve similar results at a much lower computational cost. Starting from the second time step both methods become a lot faster as it is only necessary to update the right hand side and then reuse the decomposition stored at the first time step to solve the system by substitution. The PUFEM CPU time needed to update the right hand side is on average 3.92 s and to solve the system is \( 6.66 \times 10^{-3} \) s. The respective times with the FEM are 1.33 s and 0.33 s. The CPU at the initial time step is mainly dominated by finding the decomposition for the linear system of equations. The time needed for building the system is rather insignificant. This behaviour changes at subsequent time steps where the CPU time is mostly used for updating the system. Therefore, the PUFEM requires more time as it involves expensive integrals to evaluate. However, it should be noted that the considered number of degrees of freedom is relatively small for a three dimensional problem i.e. 11360 for the FEM and 2256 for the PUFEM. At much larger systems involving several hundreds thousands of degrees of freedom the CPU time needed for the substitution will again become the bottle neck. Here, it should be noted that all the computations in this paper were run on an Intel(R) Core(TM) i5-4200U @ 1.60GHz x4 with 8 GB of RAM. Therefore it becomes impractical to run large systems of hundreds thousands of degrees of freedom.

To further compare the solutions obtained using the PUFEM and the FEM we also perform cross-sections at the domain surface. We consider the temperature on the domain outer circumference for which a cross-section is performed within the plane defined by \( z = 1 \). We also consider similar cross-sections but within the planes defined by \( x = 1 \) and \( y = 1 \), respectively. Figure 7 exhibits the temperature plots for these three cross-sections at the times \( t = 0.02, 0.05 \) and 0.1. The figure shows the temperature and its gradient variations at different directions. In all cross sections the temperature increases significantly between the first and the last times. Again the heat patterns obtained with the PUFEM and the FEM are very similar.
Figure 7: Radial cross-section of the temperature obtained for the diffusion problem in a sphere enclosure using the FEM and the PUFEM on the plane $z = 1$ with respect to $x$ (first row) and the plane $x = 1$ with respect to $y$ (second row) and the plane $y = 1$ with respect to $z$ (third row). The results are shown at times $t = 0.02, 0.05$ and $0.1$ from left to right.
at all the cross-sections and for all times. It is evident that for the considered conditions, both the FEM and the PUFEM capture the solution dynamics and accurately resolve the moving solution fronts. However, the FEM results are obtained on a fine mesh with 11360 degrees of freedom while the PUFEM results are computed using a coarse mesh with 2184 degrees of freedom which is a significant reduction, 80%, and obviously leads to significant reduction in the computational cost too. One may conclude that the enrichment is also efficient in recovering the heat patterns despite the spatial and temporal variations in the heat gradients for the considered diffusion problem.

4.3 Diffusion problem in a pump part

The last example in this paper is proposed to test the method on a rather complex three-dimensional geometry. The enrichment methods are often studied on simple geometries. Although such studies show that the enrichment approaches perform well but using the method with industrial geometries can involve different complexities. Here, we use the PUFEM to resolve heat transfer patterns in an industrial geometry for the pump part shown in Figure 8. The geometry in this example is based on the file `pump.carter_sup.stp` kindly provided by INRIA on the shape repository AIM@SHAPE\(^1\). In order to define the thermal material properties in the model we also include here the thermal conductivity \(\kappa\) and the density \(\rho\) in the diffusion equation (1). We apply Neumann type boundary conditions in order to describe an ideal heat isolator on some parts of the domain boundary surfaces. Hence, the boundary value problem in this example is given as

\[
\begin{align*}
\frac{\partial \phi}{\partial t} - \kappa \nabla^2 \phi &= \rho f, & \text{in } \Omega, \\
\kappa \frac{\partial \phi}{\partial n} &= 0, & \text{on } \Gamma_a, \\
\kappa \frac{\partial \phi}{\partial n} &= T_r, & \text{on } \Gamma_r, \\
\phi(0, x) &= T_0, & \text{in } \Omega.
\end{align*}
\]  

(19)

The equations (19) are solved in the domain shown in Figure 8 where \(\Gamma_r\) is the surface highlighted with red and \(\Gamma_a = \Gamma \setminus \Gamma_r\). The material properties considered in this example are \(\kappa = 273\text{W/m-K}\) and \(\rho = 2700\text{kg/m}^3\). The domain initial temperature is \(T_0 = 200\text{K}\). An internal heat source is imposed over the entire domain at the rate \(f = 0.01\text{W/kg}\). The ambient temperature is fixed to \(T_a = 0\) on all the domain.

\(^{1}\)http://visionair.ge.imati.cnr.it/ontologies/shapes/
boundary surfaces except for the upper part of the inner surfaces of the holes. The ambient temperature gradient on $\Gamma_r$ is assumed to be $T_r = 293\text{K/m}$. Applying zero Neumann boundary condition is equivalent to fully isolate a boundary surface so that no heat transfer is allowed. On the other hand imposing a relatively high heat gradients around the inner surfaces of the holes would lead to a high rate of heat escape through these surfaces. This effect yields boundary layers formation around the holes in the pump part. Again in this example the same value is considered for the enrichment parameters $C_1, C_2$ and $C_3$ so that $C_1 = C_2 = C_3 = 0.225$ despite the gradient of the solution is different in each spatial direction i.e. $x, y$ and $z$. For the other parameters the considered values are $C = \frac{1}{0.225}$ and $R_c = \sqrt{\frac{11}{0.225}}$. Here, we aim to test the PUFEM in recovering such solution features for a complex geometry as the one considered in this test example.

The computational domain is discretized into 4-noded tetrahedron elements composed of 6783 elements and 1913 nodes as shown in Figure 8. Notice that the relatively large number of element is needed so that the geometry is represented accurately. However, it should also be noted that the FEM requires even a finer mesh to accurately recover the steep heat gradients resulting in this problem. In our simulations, three
exponential functions are used for each enrichment function. The enrichment functions are given as

\[ G_{q,l}(x,y,z) = \frac{\exp\left(-\left(C_1(x-x_l) + C_2(y-y_l) + C_3(z-z_l)\right)^q\right) - \exp\left(-\left(R_C/C\right)^q\right)}{1 - \exp\left(-\left(R_C/C\right)^q\right)}, \]

where for each \( q \) we have \( l = 0, 1, 2 \). The control points \((x_l, y_l, z_l)\) coincide with the center of each hole i.e. \((x_0, y_0, z_0) = (-118.16, 0.0, 18.0), (x_1, y_1, z_1) = (0.0, 0.0, 18.0)\) and \((x_2, y_2, z_2) = (55.44, 63.11, 18.0)\). Thus, expression (14) becomes

\[ \phi_n(x) = \sum_{j=1}^{N_d} \sum_{q=1}^{Q} A_{n,j,q} N_j(x) (G_{q,1}(x) + G_{q,2}(x) + G_{q,3}(x)). \]

The exponential functions are applied in this manner as we expect boundary layers to be forming around the inner surface of each hole in the pump part. The simulation is carried out up to the final time \( t = 10s \) using the time step \( \Delta t = 0.025s \). In the first two examples we establish the convergence of the method and then we ensure its convergence in three-dimensional problems by matching the converged PUFEM solution to a reference FEM solution. After establishing the \( q \)-convergence of the method in the previous examples now we rely on the \( q \)-convergence to ensure that the method has converged into the problem solution. Thus, the solution convergence is ensured by increasing the number of enrichment functions to \( Q = 5 \) and then 6 where similar results are obtained in all the cases. The results displayed in Figure 9 are obtained with \( Q = 4 \). The figure shows the temperature distributions obtained at four different time instances \( t = 2.5, 5, 7.5 \) and 10s. The view angle is chosen to have a suitable view of heat variation at the shown time instances.

At the beginning of the simulation the domain temperature variation is close to zero between different parts of the domain because a constant initial temperature is considered. For the time up to \( t = 2.5s \) the temperature variation is relatively small and so is the heat gradient. However, the energy introduced by the heat source \( f \) causes a steady increase in the domain temperature. Because the domain boundary surfaces \( \Gamma_b \) are fully isolated while the surfaces \( \Gamma_r \) allow heat energy to escape, the increase of the maximum temperature is observed in the parts further away from \( \Gamma_r \). As the time passes the temperature variation grows higher between the parts away from \( \Gamma_r \) and the parts in the vicinity of \( \Gamma_r \). This can be seen, for example, in Figure 9 when comparing the temperature distribution at the time instance \( t = 2.5 \) to \( t = 5.0 \) or \( t = 7.5s \). As the temperature variation increases the heat gradient also increases and steep boundary layers start to form around the holes. The growing heat gradient from zero, at the initial state, to the high values of the gradient at the end of the considered time span \( t = 10s \) can be seen in the figure. The PUFEM has successfully recovered the entire range of gradient variations without the need to update the mesh or the enrichment.

5 Conclusions

A partition of unity finite element method is proposed to solve time dependent diffusion problems with steep gradients in three space dimensions. An approximate solution describing the diffusion decay is embedded in the finite element shape functions. The enrichment considered in the current study to construct the approximation field is exponential and mimics the spatial and temporal behaviour of the solution. These approximation properties can lead to significant savings in the computational costs compared to only spatial approximation enrichments that change at each time step. Especially that the time needed to build the linear system is increased significantly due to the relatively high number of integration points needed to integrate the enrichment functions. Hence, assembling the system matrix only once can significantly improve the efficiency compared to evaluating the system matrix at each time step. The system matrix can be decomposed at the first time step and then reused after updating the right-hand side to solve the
linear system at the following time steps. The advantage of this method compared to the conventional finite element methods is its ability to locally refine the solution by adapting the enrichment functions instead of creating a new mesh. The favorable performance of the developed partition of unity finite element method has been demonstrated using a series of numerical examples, including the non-stationary heat equation with multiple sources. Numerical comparisons have been carried out for all the considered methods in terms of accuracy and efficiency. It is also shown that for a fixed accuracy the total number of degrees of freedom is drastically reduced when the partition of unity finite element method is used. In addition, for a fixed number of degrees of freedom, the proposed partition of unity finite element method shows higher accuracy than the conventional finite element method. The numerical results obtained for the considered test examples show that the partition of unity finite element method has the advantage of requiring less computational resources for the three-dimensional transient diffusion problems than a conventional finite element method widely used in the literature. These features, as well as its slower rate of accumulation of spatial error in time, make it an attractive alternative for diffusion solvers based on finite element techniques. The numerical examples studied in this paper include stationary heat sources. For moving heat sources the stationary enrichment may not be suitable and time-dependent enrichment may become necessary. If the enrichment is time-dependent it will also become necessary to build and solve the FEM resulting linear system of equations at each time step. Hence, one of the advantages of the proposed enrichment approach will be lost. However, developing a stationary enrichment that can deal with a moving heat source can keep this advantage and hence would be a significant extension to the current work. It is also important to note that the PUFEM enables using large elements to retrieve steep heat profiles without the need for small elements. However, requiring an accurate geometry representation may again lead to the need to use small elements. It will be very useful in future developments to consider an Isogeometric PUFEM approach where non-uniform rational basis spline can be used to represent the geometry exactly on a coarse mesh while capturing the steep heat gradients with the enrichment. In such case, highly refined meshes can be avoided.

References


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