# A partition of unity finite element method for time-dependent diffusion problems using multiple enrichment functions

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**Abstract**

An enriched partition-of-unity (PU) finite element method is developed to solve time-dependent diffusion problems. In the present PU formulation, an exponential solution describing the spatial diffusion decay is embedded in the finite element shape function. It results in an enriched approximation, which is in the form of local asymptotic expansion. The temporal decay in the solution is embedded naturally in the PU expansion so that, unlike previous works in this area, the same system matrices may be used for every time step. In comparison with the traditional finite element analysis with $p$-version refinements, the present approach is much simpler, more robust and efficient, and yields more accurate solutions for a prescribed number of degrees of freedom. On the other hand, the notorious difficulty encountered in the meshless method in satisfying the essential boundary conditions is circumvented. Numerical results are presented for a transient diffusion equation with known analytical solution. The performance of the method is analysed on two applications: the transient heat equation with a single source and with multiple sources. The aim of such a method compared to the classical finite element method is to solve time-dependent diffusion applications efficiently and with an appropriate level of accuracy.

**Keywords.** Finite-element method; partition-of-unity method; time-dependent equations; diffusion problems

## 1 Introduction

In recent decades, finite element methods have offered a remarkable level of accuracy and robustness required for solving complex potential problems governed by steady-state differential equations (PDEs) of elliptic type. However, engineering applications often involve time-dependent partial differential equations which have to be solved on complex geometries, thus suggesting the use of discretization of both space and time variables. In practice, the focus is on unstructured meshes where a non-trivial reconstruction scheme is required to have a high-order spatial accuracy. Most classical finite element methods for unstructured grids proposed to date employ linear or quadratic elements. However, solving time-dependent diffusion equations using the finite element methods is still a considerable task in the case of unstructured meshes; particularly when these equations have to be solved in conjunction with PDEs of hyperbolic type. It is well known that the solutions of these coupled problems present steep fronts, boundary layers, and even shock discontinuities, which need to be resolved accurately in applications and often cause severe numerical difficulties.

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Time-dependent diffusion equations are used in many physical and engineering applications, for example, to describe cooling down of molten glass or heat transfer in enclosures. In glass manufacturing, a hot melt of glass is cooled down to room temperature. This annealing must be monitored carefully to avoid excessive temperature differences, which may affect the quality of the product or even lead to cracking [1]. To control the annealing process, the transient diffusion equations may be used to predict accurately the temperature evolution in the glass. In addition, time-dependent diffusion equations are also used to model several problems in thermal radiation heat transfer [2] and optical tomography [3] among others. In general, thermal radiation has to be modelled by equations that involve the direction- and frequency-dependent thermal radiation field due to the energy transport by photons. However, using asymptotic expansions, the full radiative transfer equation can be replaced by a class of non-stationary diffusion equations equipped with Robin boundary conditions that depend on space and time but not direction. Such practical time-dependent diffusion problems are not trivial to simulate since the geometry can be complex and internal source/sink term may produce steep gradient (solution peaks) propagating along the computational domain. It is well-known that unstructured grids can be highly advantageous based on their ability to provide local mesh refinement near important diffusion features and structures. As a consequence, the ability to provide local mesh refinement where it is needed leads to improve accuracy for a given computational cost as compared to methods that use structured meshes.

One solution that has emerged in the literature is the idea of injecting enrichment functions into the finite element approximation space. These techniques fall under the general heading of Partition of Unity Methods (PUM) [4], so-called because the partition of unity property of traditional interpolating shape functions allows enrichment functions to be undistorted through their combination with these shape functions. The enrichment functions may be of different characters. Ideally they comprise either the asymptotic solution space or sets of functions known to be complete for the PDE at hand. An example of taking enrichment functions from asymptotic fields is found in the eXtended Finite Element Method (XFEM), where a basis for expressing the displacement found locally around crack tips is found from classical expansions found in fracture mechanics [5]. There is also a large body of literature in the meshless methods [6] and boundary element [7] communities using similarly derived enrichment functions for cracks. An example of taking a set of enrichment functions known to be complete for the PDE is in expressing wave potential as a linear combination of a set of plane waves. Instances of this approach are available in the literature for enriched FEM [8, 9, 10], BEM [11] and ultraweak formulations [12] for the solution of Helmholtz (e.g. acoustic) and elastic wave problems. The PUM idea has also been presented in the context of the Generalised finite element method (GFEM) [13]. Formulations are emerging in which the enrichment functions themselves are determined adaptively [14, 15].

A further classification of enrichment includes the use of functions that *approximate* the solution in some way. While this may be less rigorous mathematically, these methods are attractive for practical use in cases in which no suitable analytical solution space is available to form the enrichment basis. We give evidence in this paper that such approximate enrichment functions allow for improved accuracy for a prescribed number of degrees of freedom. All of these PUM methods are easy to formulate and implementation in existing codes may be carried out without large-scale restructuring of the code. Some care needs to be taken to avoid (or at least ameliorate) problems of ill-conditioning which are reported in many PUM works. However, in spite of the potential for ill-conditioned systems, these approaches have been consistently shown to reduce errors in comparison with conventional piecewise polynomial bases. Enrichment functions have recently been applied to problems involving thermal transients. van der Meer *et al.* [16] developed a set of algorithms to study time-dependent geothermal problems using enrichment functions that approximate the solution at each time step. The evolution of thermal

gradients with time is considered by updating the shape functions so that they remain optimal at each time. O'Hara *et al.* [17] presented a global-local GFEM formulation for transient heat transfer, in which a linear interpolative basis is augmented by an exponential function of space or space and time as well. Time dependent shape functions are used to handle the transient nature of the problem, and these are supplemented by local analysis using various techniques in regions of high thermal gradient.

In the current work, we introduce a PUM approach for the solution of transient diffusion problems which uses a multiplicity of approximate enrichment functions. We use Gaussian functions of varying standard deviations as enrichment, and these are used in combination with a piecewise linear Lagrangian polynomial finite element space so that the global Gaussian surfaces are modulated locally. A notable feature of the approach is that the same (enriched) approximation space is used at each time step. The more rapidly varying enrichment functions are useful for early time steps around localised thermal sources, while other (flatter) enrichment functions become important both in the far-field and more generally as a steady state is approached. This means that there is no requirement for time-dependent shape functions, and the same system matrix may be reused at every time step. Further, the approach may be generalised by locating different Gaussian functions at different centres, allowing the efficient solution of problems with multiple sources.

This paper is organised in the following fashion. In section 2 we introduce the governing PDE for transient diffusion, the initial and boundary conditions and the transformation to the weak form. The Partition of Unity enrichment is presented in section 3, and its effectiveness is demonstrated for a range of numerical test cases in section 4. We close in section 5 with some concluding remarks.

## 2 Boundary value problem and weak form

Given an open bounded domain $\Omega \subset \mathbb{R}^2$ with a boundary $\Gamma$ and a given time interval $[0, T]$, we are interested in this paper to study the following transient diffusion equations: find $u : ]0, T[\times\Omega \longrightarrow \mathbb{R}^2$ such that

$$\frac{\partial u}{\partial t} - \lambda \nabla^2 u = f(t, \mathbf{x}), \qquad (t, \mathbf{x}) \in ]0, T[\times\Omega \tag{1}$$

where $\mathbf{x} = (x, y)^T$ denotes the spatial coordinates, $t$ is the time variable, $\lambda$ is the diffusion coefficient, and $f$ represents the effects of internal sources/sinks. We consider an initial condition

$$u(t = 0, \mathbf{x}) = u_0(\mathbf{x}), \qquad \mathbf{x} \in \ \Omega \tag{2}$$

where $u_0$ is a prescribed initial field. The above equations are to be solved subject to the boundary condition

$$\alpha u + \frac{\partial u}{\partial \mathbf{n}} = g(t, \mathbf{x}), \qquad (t, \mathbf{x}) \in ]0, T[\times\Gamma \tag{3}$$

where $\mathbf{n}$ is the outward unit normal on the boundary $\Gamma$, and $g$ is a given boundary function.

To integrate the equations (1)-(3) we divide the time interval into $N_t$ subintervals $[t_n, t_{n+1}]$ with length $\Delta t = t_{n+1} - t_n$ for $n = 0, 1, \ldots, N_t$. We use the notation $w^n$ to denote the value of a generic function $w$ at time $t_n$. We may consider a $\theta$-time stepping integration scheme, in which the semi-discrete formulation of the diffusion problem (1) is given by

$$\frac{u^{n+1} - u^n}{\Delta t} - (1 - \theta)\lambda \nabla^2 u^{n+1} - \theta \lambda \nabla^2 u^n \quad = \quad (1 - \theta) f^{n+1} + \theta f^n \tag{4}$$

where the parameter $\theta$ has to be chosen depending on the time stepping scheme; by taking $\theta = 0$ the equation (4) is the first-order Backward Euler scheme, whereas use of $\theta = \frac{1}{2}$ in equation (4) yields the second-order Crank-Nicolson scheme. Note that second-order Crank-Nicolson scheme is unconditionally stable for linear problems, so that the choice of $\Delta t$ may be based on accuracy considerations. To find the solution $u^{n+1}$ from (4) one has to solve, at each time level, a linear system of algebraic equations. When $\theta = 0$ the equation (4) becomes

$$\frac{u^{n+1} - u^n}{\Delta t} - \lambda \nabla^2 u^{n+1} = f^{n+1} \tag{5}$$

This can be rearranged as

$$u^{n+1} - \lambda \Delta t \nabla^2 u^{n+1} = F \tag{6}$$

where $F$ is defined as

$$F = \Delta t f^{n+1} + u^n \tag{7}$$

We may proceed as in conventional finite element formulations by multiplying equation (6) by a weighting function, $W$, and then integrating over $\Omega$, yielding

$$\int_\Omega W u^{n+1} d\Omega - \int_\Omega \lambda \Delta t W \nabla^2 u^{n+1} d\Omega = \int_\Omega W F d\Omega \tag{8}$$

Using the divergence theorem one may write

$$\int_\Omega W \nabla^2 u^{n+1} d\Omega = \int_\Gamma W \nabla u^{n+1} \cdot \mathbf{n} d\Gamma - \int_\Omega \nabla W \cdot \nabla u^{n+1} d\Omega \tag{9}$$

Substituting (9) into (8) results in

$$\int_\Omega W u^{n+1} d\Omega - \int_\Gamma \lambda \Delta t W \nabla u^{n+1} \cdot \mathbf{n} d\Gamma + \int_\Omega \lambda \Delta t \nabla W \cdot \nabla u^{n+1} d\Omega = \int_\Omega W F d\Omega \tag{10}$$

or

$$\int_\Omega (\lambda \Delta t \nabla W \cdot \nabla u^{n+1} + W u^{n+1}) d\Omega - \int_\Gamma \lambda \Delta t W \nabla u^{n+1} \cdot \mathbf{n} d\Gamma = \int_\Omega W F d\Omega \tag{11}$$

Substituting the boundary condition in equation (3) gives us the statement of the problem to be solved in weak form, i.e. find $u \in H^1(\Omega)$ such that:

$$\int_\Omega (\lambda \Delta t \nabla W \cdot \nabla u^{n+1} + W u^{n+1}) d\Omega + \oint_\Gamma \lambda \Delta t W (\alpha u^{n+1} - g^{n+1}) d\Gamma = \int_\Omega W F d\Omega \,, \qquad \forall\, W \in H^1(\Omega) \tag{12}$$

where $H^1(\Omega)$ is the Sobolev space. It well-known that the considered time stepping method is unconditionally stable such that the selection of the time steps $\Delta t$ is based only on the accuracy to achieved in the computed solutions.

## 3 Partition of unity enriched finite element method

To solve the weak form (12) with the finite element method, first the domain $\Omega$ is discretized. To perform this step, we generate a quasi-uniform partition $\Omega_h \subset \Omega$ of $N_e$ elements $\mathcal{T}_j$ that satisfy the following conditions:

(i) $\Omega_h = \bigcup_{j=1}^{N_e} \mathcal{T}_j$.

(ii) If $\mathcal{T}_i$ and $\mathcal{T}_j$ are two different elements of $\Omega_h$, then

$$\mathcal{T}_i \cap \mathcal{T}_j = \begin{cases} P_{ij}, & \text{a mesh point, or} \\ \Gamma_{ij}, & \text{a common side, or} \\ \emptyset, & \text{empty set.} \end{cases}$$

(iii) There exists a positive constant $k$ such that for all $j \in \{1, \cdots, N_e\}$, $\frac{r_j}{h_j} > k$ $(h_j \leq h)$, where $r_j$ is the radius of the circle inscribed in $\mathcal{T}_j$ and $h_j$ is the largest side of $\mathcal{T}_j$.

The conforming finite element space for the solution that we use is defined as

$$V_h = \left\{ u_h \in C^0(\Omega) : \quad u_h\big|_{\mathcal{T}_j} \in P(\mathcal{T}_j), \quad \forall\ \mathcal{T}_j \in \Omega_h \right\} \tag{13}$$

with

$$P(\mathcal{T}_j) = \left\{ p(\mathbf{x}) : \quad p(\mathbf{x}) = \hat{p} \circ Y_j^{-1}(\mathbf{x}), \quad \hat{p} \in P_m(\hat{\mathcal{T}}) \right\},$$

where $\hat{p}(\mathbf{x})$ is a polynomial of degree $\leq m$ defined on the element $\hat{\mathcal{T}}_j$ and $P_m(\hat{\mathcal{T}})$ is the set of polynomials of degree $\leq m$ defined on the element of reference $\hat{\mathcal{T}}$. Here $Y_j : \hat{\mathcal{T}} \longrightarrow \mathcal{T}_j$ is an invertible one-to-one mapping.

Next, we formulate the finite element solution to $u^n(\mathbf{x})$ as

$$u^n(\mathbf{x}) \simeq u_h^n(\mathbf{x}) = \sum_{j=1}^{N_d} C_j^n N_j(\mathbf{x}) \tag{14}$$

where $N_d$ is the number of solution mesh points in the partition $\Omega_h$. The functions $C_j^n$ are the corresponding nodal values of $u_h^n(\mathbf{x})$. They are defined as $C_j^n = u_h^n(\mathbf{x}_j)$ where $\{\mathbf{x}_j\}_{j=1}^{N_d}$ are the set of solution mesh points in the partition $\Omega_h$. In (14), $\{N_j\}_{j=1}^{N_d}$ are the set of global nodal basis functions of $V_h$ characterized by the property $N_i(\mathbf{x}_j) = \delta_{ij}$ with $\delta_{ij}$ denoting the Kronecker symbol. We introduce $\{\mathbf{x}_1, \cdots, \mathbf{x}_M\}$ as the set of $M$ nodal points in the element $\mathcal{T}_j$. We also define $\{\varphi_j\}_{j=1}^{M}$ as the set of element basis coefficients for $\mathcal{T}_j$ in $V_h$ characterized by the property $\varphi_i(\mathbf{x}_j) = \delta_{ij}$. Hereafter, unless otherwise stated, the subscripts $h$ and $j$ are used to refer to coefficients associated with the whole mesh $\Omega_h$ and a mesh element $\mathcal{T}_j$, respectively. Note that the set $\{\varphi_j\}_{j=1}^{M}$ is a local restriction on the element $\mathcal{T}_j$ of the set of the global basis functions $\{N_j\}_{j=1}^{M}$. The solution space is then defined as

$$\widetilde{V}_h^0 = \text{span} \left\{ N_h,\ u_h = \sum_{j=0}^{M} u_j N_j \right\}$$

Using the partition of unity method [4] it is possible to enrich the solution space with basis functions that have better approximation properties than the conventional polynomial basis functions. To solve an elliptic partial differential equation similar to the one considered here, X. Li proposed a set of exponential functions [18]. Here we propose using the following sum of exponential basis functions to enrich the solution space

$$F_{enr} = \sum_{q=1}^{Q} G_q \tag{15}$$

where

$$G_q = \frac{\exp\left(-\left(\frac{R_0^2}{C^2}\right)^q\right) - \exp\left(-\left(\frac{R_c^2}{C^2}\right)^q\right)}{1 - \exp\left(-\left(\frac{R_c^2}{C^2}\right)^q\right)} \tag{16}$$

with $R_0 := \mid \mathbf{x} - \mathbf{x}_c \mid$ being the distance from the function control point $\mathbf{x}_c$ to the point $\mathbf{x}$. The constants $R_c$ and $C$ control the shape of the exponential function $G_q$. The number of enrichment functions used is $Q$. It should be mentioned that a similar function to $G_q$ were used in [19] as a weight function in the context of meshless methods when solving the linear Poisson equation. From the above, the nodal values might be rewritten as

$$C_j^n = \sum_{q=1}^{Q} A_j^q G_q \tag{17}$$

The finite element method is now used to find the values of the new set of unknowns $A_j^q$ instead of the nodal values $C_j^n$ as before. Using (17) to rewrite (14) we obtain

$$u^n = \sum_{j=1}^{M} \sum_{q=1}^{Q} A_j^q N_j G_q \tag{18}$$

For simplicity the multiplication of $F_{enr}$ with the polynomial shape function is considered to be the new shape function $L_{(j-1)Q+q}$ defined by

$$L_{(j-1)Q+q} = N_j G_q \tag{19}$$

The new solution space then becomes

$$\widetilde{V}_h^1 = \text{span}\left\{ L_h, \qquad u_h = \sum_{j=1}^{M} \sum_{q=1}^{Q} A_j^q N_j G_q \right\}$$

The derivatives of the new shape function are then given by

$$\frac{\partial L_{(j-1)Q+q}}{\partial x} = G_q \frac{\partial N_j}{\partial x} - \frac{\exp\left(-\left(\frac{R_0^2}{C^2}\right)^q\right)}{1 - \exp\left(-\left(\frac{R_c^2}{C^2}\right)^q\right)} R_0^{2(j-1)} N_j (x - x_0) \tag{20}$$

$$\frac{\partial L_{(j-1)Q+q}}{\partial y} = G_q \frac{\partial N_j}{\partial y} - \frac{\exp\left(-\left(\frac{R_0^2}{C^2}\right)^q\right)}{1 - \exp\left(-\left(\frac{R_c^2}{C^2}\right)^q\right)} R_0^{2(j-1)} N_j (y - y_0) \tag{21}$$

It is worth remarking that the enrichment functions $F_{enr}$ are written in terms of the global coordinates $\mathbf{x}$, but that they are multiplied by the nodal shape functions $N_j$. In this sense the additional enrichment takes on a local character. The change in the form of the approximation from (14) to (18) is only made locally in the vicinity of a feature of interest, such as source or sink zones.

# 4 Numerical Results

In this section we examine the accuracy and performance of the proposed PU method using three test examples. The first example solves a transient diffusion equation with analytical solution that can be used to quantify errors in the PU method. The second and third examples consider a problem of heat transfer with single and multiple sources, respectively. These last examples are used to qualify the considered PU method for more complicated time-dependent diffusion problems.

In what follows, we shall use the terminology FEM, PUFEM, PUFEM4DoFs, PUFEM6DoFs and PUFEM8DoFs to refer to the standard finite element method, the partition-of-unity finite element method, PUFEM with the number of enrichment functions $Q = 4$, 6 and 8, respectively. All the computations are made on an Intel®Xeon®PC with one processor of 24 GB of RAM and 2.93 GHz. The codes only take the default optimization of the machine, *i.e.* they are not parallel codes.

## 4.1 Accuracy test problem

As a first test example we consider a diffusion problem with a manufactured exact solution in a squared domain $\Omega = [0, 2] \times [0, 2]$. We solve the transient equation (1)-(3) with the reaction term $f$, the boundary function $g$ and the initial condition $u_0$ are explicitly calculated such that the exact solution of the problem (1)-(3) is given by

$$U(x, y, t) = x^k y^k \left(2 - x\right)^k \left(2 - y\right)^k \Big(1 - \exp\left(-\lambda t\right)\Big) \tag{22}$$

where $k$ is parameter set to 20 in our simulations. Note that in order to avoid having the exact solution (22) as a subset of the enrichment space, the solution does not include exponential parts in the space domain. The initial condition is calculated from the analytical solution (22) while homogeneous Dirichlet boundary conditions are imposed on $\Gamma$. To quantify the errors in this test example we consider the $L^2$-norm error defined as

$$\varepsilon_2 = \frac{\|u - U\|_{L^2(\Omega)}}{\|U\|_{L^2(\Omega)}} \tag{23}$$

where $\|\cdot\|_{L^2(\Omega)}$ is the $L^2$ norm, $u$ and $U$ are respectively, the computed and exact solutions. In all computations presented the parameter $\alpha = 1$, the time step $\Delta t = 0.1$ and the diffusion coefficient $\lambda$ is selected to take the values 0.1 and 0.01. The aim of this test example is to compare the results obtained using the proposed partition-of-unity finite element method (PUFEM) to those obtained using the standard finite element method (FEM). To this end we consider three numbers of enrichment functions $Q = 4$, 6 and 8 in the PUFEM referred to as PUFEM4DoFs, PUFEM6DoFs and PUFEM8DoFs, respectively. To study the convergence, each of these enrichment numbers is considered with further $h$-refinements. The same problem is solved with the FEM using $h$-refinement. Figure 1 and Figure 2 show, respectively the convergence and the conditioning of the proposed method for an increasing number of degrees of freedom when $\lambda = 0.1$. The top three plots of Figure 1 compare the convergence of the PUFEM for an increased number of enrichment functions $Q$ while the bottom figures compare the convergence of the PUFEM for $Q = 6$ to the FEM. The numerical results correspond to the simulation times $T = 0.1$,1 and 10 sec. A similar set of results for $\lambda = 0.01$ are shown in Figure 3 and Figure 4.

In the above set of results and for both values of $\lambda$, it is clear that the PU converges much faster compared to the FEM. More than 10000 degrees of freedom are needed with the FEM to achieve an error of about $\varepsilon_2 = 0.001$ whereas with the PUFEM and using 6 enrichment functions