H-P FINITE ELEMENT METHOD FOR THE SIMPLIFIED P$_N$ EQUATIONS

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Abstract *The simplified spherical harmonics approximation to the neutron transport equation defines the neutron distribution inside a nuclear reactor core more accurately than the widely used neutron diffusion equation. To solve this equation, a goal oriented h-adaptable finite element method is employed. The proposed adaptive mesh refinement (AMR) method splits mesh cells whose errors are large and whose importance towards the computational goal is high. In this work, the computational goal is set as the maximum averaged power in an assembly of the reactor as this usually is a design constraint. The goal oriented error estimator is compared with the usual Kelly error indicator and also with a uniform global refinement. The goal oriented error estimator demonstrates to be the most accurate strategy in order to minimise the error in the defined quantity of interest and it is as much efficient as standard error estimators to compute the fundamental eigenvalue.*

1 INTRODUCTION

The neutron transport equation describes the distribution of neutrons and rate of fissions inside a nuclear reactor core. The steady-state neutron distribution satisfies an eigenvalue problem and its solution is used as initial condition for time dependent problems. The steady-state problem is also important because it gives a measure of the criticality of the reactor. To solve the neutron transport equation many angular discretizations have been used to approximate this equation as the diffusion approximation, spherical harmonics or discrete ordinates [1]. Because of the size of the problem, for full core calculations the standard method is to use the diffusion approximation. This theory states that the neutron current is proportional to the gradient in the neutron flux, in a similar way to diffusion of species or the heat equation. But the accuracy of the diffusion theory solution for describing the neutron population in a nuclear reactor is limited for a variety of situations: (a) near boundaries or where material properties change suddenly,

(b) near localised sources and (c) in strong absorbing media. In fact strong angular dependence can be associated with strong spatial variation in the neutron flux.

To improve the results of diffusion theory for these situations, a computational method that incorporates higher-order approximations for the angular dependence of the neutron flux must be employed. The simplified spherical harmonics method (SP_N) has been investigated for this purpose. Theoretical basis for the SP_N equations were provided by Brantley and Larsen [2], showing that these equations are high-order asymptotic solutions of the transport equation when diffusion theory is the leading-order approximation.

Unlike the standard spherical harmonics approximation (P_N), the SP_N solution does not converge to the exact transport solution as $N \to \infty$. However it is accurate for usual reactor configurations within acceptable computing times. The main advantage of the simplified spherical harmonics approximation is the reduced number of equation to be solved when compared with P_N approximation. The number of equations increases quadratically as $(N+1)^2$ for spherical harmonics, while it shows increases linearly as $(N+1)$ for SP_N. Also the resulting system of elliptic equations is readily solvable with existing diffusion solvers. In addition the SP_N approximation does not suffer from the ray effects [3] that can adversely affect the discrete ordinates method, S_N.

In this work, to solve the simplified spherical harmonics method an *h*-adaptable finite element method (FEM) is used as it was done for the multigroup diffusion equation in [4]. Adaptive mesh refinement (AMR) techniques aim to locally refine a grid in order to obtain accurate solutions with the minimum computational cost. Standard AMR techniques are based on error estimators in order to indicate which cells have the majority of the error and refine them. While such methods have been demonstrated to be efficient and accurate compared to globally uniform refined meshes, this traditional approach is not optimal for computing the solution in a particular region or determining a quantity of interest. In nuclear engineering, we are interested in accurately solving the neutronic power in the hottest assembly as this temperature is a design restriction.

To address this kind of problem, goal oriented adaptivity has been developed during the last decades [5]. This method derives error estimates for the goal of the computation, rather than for the global error in the solution. Goal oriented error indicators are composed of both the local error, i.e. how well the exact solution is approximated, as well as a quantity that describes how important the accuracy of this solution on a given cell is toward the goal of the computation [6]. In this work, we solve the multigroup SP_N equations with a goal oriented adaptable mesh to accurately solve for the neutron power in the hottest cell of a nuclear reactor core.

The rest of the paper is organised as follows. The simplified P_N equations are reviewed in Section 2. Next, we introduce the *h*-adaptable finite element discretization in Section 3. Section 4 describes how to compute the goal oriented error estimator and the gradient recovery based error estimator. Numerical results for a two-dimensional nuclear reactor benchmark are studied in Section 5. Finally, the main conclusions of the work are summarised in Section 6.

2 SIMPLIFIED P_N EQUATIONS

We consider the eigenvalue problem associated with the multi-group, steady-state, neutron transport equation in slab geometry [3],

$$
\left(\mu \frac{\mathrm{d}}{\mathrm{d}x} + \Sigma_t^g(x) \right) \psi^g(x, \mu) = \sum_{g'=1}^{G} \int_{-1}^{1} \Sigma_s^{gg'}(x, \mu_0) \psi^{g'}(x, \mu') \mathrm{d}\mu'
$$

$$
+ \frac{1}{k_{\mathrm{eff}}} \sum_{g'=1}^{G} \frac{\chi^g(x)}{2} \nu \Sigma_f^{g'}(x) \int_{-1}^{1} \psi^{g'}(x, \mu') \mathrm{d}\mu', \tag{1}
$$

$$
g = 1, \ldots, G, \qquad x \in [0, L_t]
$$

where G is the number of energy groups considered, θ is the angle between the direction of travel of the neutron and the x axis, $\mu = cos(\theta)$, θ_0 is the change of directions due to scattering collisions, $\mu_0 = cos(\theta_0)$. $\Sigma_t^g(x)$, $\nu \Sigma_f^g(x)$, $\Sigma_s^{gg'}(x, \mu_0)$ are the total, production and scattering cross sections for energy group g, and $\chi^g(x)$ is the fission spectrum. The dominant eigenvalue of the problem (1), k_{eff}, is the multiplicative factor of the system and measures the reactor criticality. The corresponding eigenvector, $\psi^g(x, \mu)$, is the stationary angular flux distribution in the reactor.

The spherical harmonics approximation to the neutron transport equation in slab geometry assumes that the angular dependence of both the neutron flux distribution and the scattering cross-section can be expanded in terms of $N + 1$ Legendre polynomials,

$$
\psi^g(x, \mu) = \sum_{n=0}^{N} \frac{2n+1}{2} \phi_n^g(x) P_n(\mu), \tag{2}
$$

$$
\Sigma_s^{gg'}(x, \mu_0) = \sum_{n=0}^{N} \frac{2n+1}{2} \Sigma_{sn}^{gg'}(x) P_n(\mu_0). \tag{3}
$$

Inserting equations (2) and (3) in equation (1) and using the Legendre polynomials orthogonality, the one dimensional P_N equations are obtained, which can be expressed in matrix notation [7] as

$$
\frac{\mathrm{d}\,\Phi_1}{\mathrm{d}x} + \boldsymbol{\Sigma_0}\Phi_0 = \frac{1}{k_{\mathrm{eff}}}\mathbf{F}\Phi_0, \tag{4}
$$

$$
\frac{\mathrm{d}}{\mathrm{d}x}\left(\frac{n}{2n+1}\Phi_{n-1} + \frac{n+1}{2n+1}\Phi_{n+1} \right) + \boldsymbol{\Sigma_n}\Phi_n = 0, \tag{5}
$$

$$
\text{for } n = 1, \ldots, N,
$$

where,

$$\mathbf{\Sigma_n} = \begin{pmatrix} \Sigma_t^1 - \Sigma_{sn}^{11} & -\Sigma_{sn}^{12} & \ldots & -\Sigma_{sn}^{1G} \\ \vdots & \vdots & \ddots & \vdots \\ -\Sigma_{sn}^{G1} & -\Sigma_{sn}^{G2} & \ldots & \Sigma_t^G - \Sigma_{sn}^{GG} \end{pmatrix},$$

$$\mathbf{F} = \begin{pmatrix} \chi^1\nu\Sigma_f^1 & \chi^1\nu\Sigma_f^2 & \ldots & \chi^1\nu\Sigma_f^G \\ \vdots & \vdots & \ddots & \vdots \\ \chi^G\nu\Sigma_f^1 & \chi^G\nu\Sigma_f^2 & \ldots & \chi^G\nu\Sigma_f^G \end{pmatrix}, \quad \Phi_n = \begin{pmatrix} \phi_n^1 \\ \vdots \\ \phi_n^G \end{pmatrix}.$$

It must be noted that in many nuclear applications, as usual steady-state reactor calculations, the scattering cross section, Σ_s, is supposed isotropic [7]. Thus, $\mathbf{\Sigma_n}$ is a diagonal matrix for $n > 0$.

For multidimensional problems the simplified P_N approximation is obtained substituting the x derivatives by the corresponding two- or three-dimensional gradient operator in equation (9). The resulting equations are,

$$\vec{\nabla}\Phi_1 + \mathbf{\Sigma_0}\Phi_0 = \frac{1}{k_{\text{eff}}}\mathbf{F}\Phi_0\,, \tag{6}$$

$$\vec{\nabla}\left(\frac{n}{2n+1}\Phi_{n-1} + \frac{n+1}{2n+1}\Phi_{n+1}\right) + \mathbf{\Sigma_n}\Phi_n = 0\,, \tag{7}$$

$$\text{for } n = 1,\, ...,\, N\,. \tag{8}$$

This approximation may seem a bit ad-hoc but its theoretical basis is explained in [2]. Equations (8 are much simpler than the multidimensional P_N equations and can be easily implemented using numerical methods suited for diffusive equations.

Using a linear change of variables, equations (6) and (7) can be expressed as a system of second order elliptic diffusive-like equation for the even moments. In the simplified spherical harmonics method, odd order approximations have found a broader acceptance than even-order approximations because nuclear cross sections are usually available for odd order approximations [2].

Thus, we focus our study in diffusion theory (SP_1) and the SP_3 approximation. For example, the set of SP_3 equations is expressed as

$$-\vec{\nabla}\left(\mathbf{D}\,\vec{\nabla}U\right) + \mathbf{A}U = \frac{1}{k_{\text{eff}}}\mathbf{M}U\,, \tag{9}$$

where the effective diffusion matrix, $\mathbf{D}$, the absorption matrix, $\mathbf{A}$, and the fission matrix, $\mathbf{M}$, are given by

$$\mathbf{D} = \begin{pmatrix} \frac{1}{3}\mathbf{\Sigma_1}^{-1} & 0 \\ 0 & \frac{1}{5}\mathbf{\Sigma_3}^{-1} \end{pmatrix} = \begin{pmatrix} \mathbf{D_0} & 0 \\ 0 & \mathbf{D_1} \end{pmatrix},$$

$$A_{ij} = \sum_{n=1}^{3} c_{ij}^{(n)}\mathbf{\Sigma_n}\,, \quad M_{ij} = c_{ij}^{(1)}\mathbf{F}\,,$$

and the following linear change of variables has been applied,

$$U = \begin{pmatrix} u_0 \\ u_2 \end{pmatrix} = \begin{pmatrix} \Phi_0 + 2\Phi_2 \\ 3\Phi_0 + 4\Phi_2 \end{pmatrix} . \tag{10}$$

Finally, the coefficients matrix, $\mathbf{c^{(m)}}$ is defined as,

$$\mathbf{c^{(1)}} = \begin{pmatrix} 1 & -\frac{2}{3} \\ -\frac{2}{3} & \frac{4}{9} \end{pmatrix}, \quad \mathbf{c^{(2)}} = \begin{pmatrix} 0 & 0 \\ 0 & \frac{5}{9} \end{pmatrix} . \tag{11}$$

In order to find how to implement vacuum boundary condition and other boundary conditions in the simplified spherical harmonics equation the reader is referred to [7].

3 FINITE ELEMENT DISCRETIZATION

As it was reviewed in the last section the SP_N approximation consist of a set of diffusion-like equations for which simultaneous solution for the unknown fluxes moments is required. Thus, the finite element discretization (FEM) that were developed for the diffusion equation in [4] can be applied without major changes. In this work the `deal.II` library [13] has been used to implement the FEM code.

A Galerkin finite element discretization has been applied to equation (9) leading to an algebraic generalized eigenvalue problem. To discretize the problem the reactor domain, Ω, has been partitioned into cells Ω_k, $k = 1, 2, \dots, K$, where the nuclear cross sections are assumed to be constant. In the same way, Γ_k is the set of the corresponding cell surfaces which are part or the external reactor boundary, Γ.

In order to simplify the notation, in this Section only one group of energy is considered. Thus, the discretization of SP_3 equations can be written as the generalized algebraic eigenvalue problem,

$$\begin{pmatrix} \mathbf{L_{00}} & \mathbf{L_{01}} \\ \mathbf{L_{10}} & \mathbf{L_{11}} \end{pmatrix} \begin{pmatrix} \tilde{u}_0 \\ \tilde{u}_2 \end{pmatrix} = \frac{1}{k_{\text{eff}}} \begin{pmatrix} \mathbf{S_{00}} & \mathbf{S_{01}} \\ \mathbf{S_{10}} & \mathbf{S_{11}} \end{pmatrix} \begin{pmatrix} \tilde{u}_0 \\ \tilde{u}_2 \end{pmatrix}, \tag{12}$$

where $\tilde{u}_0$ and $\tilde{u}_2$ are the algebraic vectors representing u_0 and u_2 and the matrix blocks are

constructed as,

$$
(\mathbf{L_{00}})_{ij} = \sum_{k=1}^{K} D_0(\vec{\nabla} N_i, \ \vec{\nabla} N_j)_{\Omega_k} - D_0(\vec{\nabla} N_i, \ N_j)_{\Gamma_k} + A_{00}(N_i, \ N_j)_{\Omega_k},
$$

$$
(\mathbf{L_{01}})_{ij} = \sum_{k=1}^{K} A_{01}(N_i, \ N_j)_{\Omega_k}, \qquad (\mathbf{L_{10}})_{ij} = \sum_{k=1}^{K} A_{10}(N_i, \ N_j)_{\Omega_k},
$$

$$
(\mathbf{L_{11}})_{ij} = \sum_{k=1}^{K} D_1(\vec{\nabla} N_i, \ \vec{\nabla} N_j)_{\Omega_k} - D_1(\vec{\nabla} N_i, \ N_j)_{\Gamma_k} + \Sigma_1(N_i, \ N_j)_{\Omega_k},
$$

$$
(\mathbf{S_{00}})_{ij} = \sum_{k=1}^{K} M_{00}(N_i, \ N_j)_{\Omega_k}, \qquad (\mathbf{S_{01}})_{ij} = \sum_{k=1}^{K} M_{01}(N_i, \ N_j)_{\Omega_k},
$$

$$
(\mathbf{S_{10}})_{ij} = \sum_{k=1}^{K} M_{10}(N_i, \ N_j)_{\Omega_k}, \qquad (\mathbf{S_{11}})_{ij} = \sum_{k=1}^{K} M_{11}(N_i, \ N_j)_{\Omega_k},
$$

where the common notation for the scalar product, $(a, \ b)_\Omega = \int_\Omega a \, b \, \mathrm{d}V$ has been used. N_i is the prescribed shape function associated with the i-th degree of freedom or support point. The shape functions used are part of the Lagrange finite elements [4].

To solve the algebraic eigenvalue problem (12) for the dominant eigenvalue k_{eff} and its corresponding eigenvector, the power iteration method is used. As initial guess of the solution in refined meshes the method uses k_{eff}, u_0 and u_2 obtained in the coarser meshes.

Finally, the solution fluxes must be normalized using some arbitrary criteria as all eigenvalue problems. Usually, it is forced that the average neutronic power, P, is equal to 1 in the whole reactor core,

$$
1 = \frac{1}{V} \int_\Omega P \, \mathrm{d}V = \frac{1}{V} \sum_{g=1}^{G} \int_\Omega \Sigma_{fg} \phi_0^g \, \mathrm{d}V. \tag{13}
$$

4 ERROR ESTIMATORS

After the problem is solved, it is convenient to estimate if the obtained solution has enough accuracy and if this is not the case, to refine the mesh accordingly. In this way, three types of refinement strategies are considered, a uniform refinement, where all cells are refined, and two adaptive mesh refinements (AMR), where only a part of the cells are refined. To choose which cells are refined two error indicators are used, a gradient recovery based method proposed by Kelly et al. [11] and a goal oriented error estimator to reduce the error in the desired assembly. Even though, these error estimator were developed for linear problems of the form

$$
a(b, U) = s(b) \qquad \forall \, b \in V \,, \tag{14}
$$

where $a(\cdot, \cdot)$ is the bilinear form and $s(\cdot)$ is the linear form associated with the right hand side, these estimators are good refinement indicators for generalized eigenvalue problems [4].

However, [12] describes techniques how to extend goal-oriented methodology to eigenvalue problems. Such methods could be used to efficiently and accurately compute the eigenvalue of the problem k_{eff}.

4.1 Kelly Error Estimator

A modified version of the error estimator proposed by Kelly et al. [11] is used. This error indicator tries to approximate the error per cell by integration of the jump of the gradient of the solution along the faces of each cell. It can be understood as a gradient recovery estimator, see the book [9] for a complete discussion. This estimator, η_k, is extended for non-constant diffusion coefficients and generalized for a multigroup approximation as

$$\eta_k = \sqrt{\frac{h_e}{24}} \sum_{g=1}^{G} \sum_{n=0,2,\ldots}^{N} \left(\Sigma_{fg} \int_{\mathcal{T}_e} \left(D_g \vec{\nabla} \phi_n^g \right) \mathrm{d}\vec{S} \right) = \sum_{g=1}^{G} \sum_{n=0,2,\ldots}^{N} \Sigma_{fg} \, \kappa(\phi_n^g), \qquad (15)$$

where $\mathcal{T}_k$ denotes all interior boundaries of the element k and h_k is the adimensional cell size. In other words, we are using the jump in the net current weighted by the fission cross sections as the error estimator in the neutronic power. The operation of adding the jump of the gradient through the cell boundary is defined as $\kappa(\phi)$. Even though, this is an error estimator for the Poisson's equation, i.e. $\nabla^2 \varphi = f$, this indicator is widely used as a heuristic refinement indicator and it is considered a good choice in the absence of actual estimators for a particular equation.

4.2 Goal Oriented Error Estimator

Goal oriented error estimators are used because they indicate which cells have the majority of error in order to compute a functional derived from the solution. This kind of refinement indicators are composed of both the local error as well as a quantity that describes how important the accuracy of the solution on a given cell is toward the goal of the computation [6]. In this way a large error can be tolerated on a cell far away from the region of interest, and conversely, a cell with a relatively small error may still require further refinement if this cell is important for the goal.

Let us assume that we are not interested in the solution U of a given problem but in a functional $I(U)$ of this solution. For simplicity, it is assumed that I is a linear functional though the methodology can be extended to non linear goal functionals as well [10].

Our main objective is the to accurately compute $I(U)$ but all we have is available is $I(U_h)$, computed from the finite element discretization on our current mesh. Therefore, the error in the quantity of interest $|I(U) - I(U_h)| = |I(e)|$ where the error is defined as $e = U - U_h$. In order to estimate this error in the quantity of interest, let $\hat{U}$ be the solution of the adjoint problem defined by

$$a(\hat{U}, b) = \hat{a}(b, \hat{U}) = I(b), \qquad \forall \, b \in V, \qquad (16)$$

where $a(\cdot, \cdot)$ is the primal formulation of the L matrix of equation (12) and $\hat{a}(\cdot, \cdot)$ is the adjoint source operator of this matrix. Using the Galerkin orthogonality property it can be seen that,

$$I(U) - I(U_h) = a(\hat{U}, e) - a(\hat{U}_h, e) = a(\hat{e}, e), \qquad (17)$$

where the dual error is defined as $\hat{e} = \hat{U} - \hat{U}_h$.

Similarly to [6], the refinement indicator is defined as the product of the primal and dual errors.

$$\tilde{\eta}_k = \sum_{g=1}^{G} \|\nabla e\|_k \|\nabla \hat{e}\|_k \approx \sum_{g=1}^{G} \kappa(u_{0h}^g)\, \kappa(\hat{u}_{0h}^g), \tag{18}$$

where the exact primal and dual error are approximated by the widely used Kelly estimator[11]. $\hat{U}_0^g$ is the solution of the adjoint problem.

$$L_{00}^g\, \hat{u}_0^g = I(U), \tag{19}$$

A practical goal used in nuclear engineering is to describe accurately the power in the hottest assembly denoted by Ω_H. Thus, each component i of the function of interest is defined as

$$(I(U))_i = \frac{\delta_H(x_i)}{V_H} \int_{\Omega_H} \phi_0 \, dV, \qquad \delta_H(x) = \begin{cases} 1 & \text{if } x \in \Omega_H \\ 0 & \text{if } x \notin \Omega_H \end{cases}, \tag{20}$$

where V_H is the volume of the assembly of interest.

5 NUMERICAL RESULTS

To compare the performance of the described error estimators the two-dimensional BIBLIS benchmark has been used. This benchmark is a realistic and highly non-separable two energy group problem representative of an actual operating pressurised water reactor (PWR). This problem is characterized by a chequerboard effect caused by fuel reloading. It presents one quarter symmetry that is used to compute efficiently the critical eigenvalue of the reactor employing zero current boundary conditions to model symmetry. The definitions of the 8 different materials and their cross sections are given in [14].

BIBLIS benchmark has been solved recursively employing three different refinement strategies: a uniform global refinement, the modified version of the Kelly error estimator exposed in equation (15) and the goal oriented error estimator trying to reduce the error in the maximum power cell. For adaptive mesh refinement cases 60% of the cells are refined each step. All meshes are computed using quadratic polynomials in the finite element discretization. Figure 1 shows the grid employed during the first 6 steps of adaptive local refinement using the Kelly error estimator. Similarly, Figure 2 shows the grid employed during the first 6 steps of adaptive local using the goal oriented error estimator. In the last case, the *assembly of interest* where the error indicator leads the AMR to accurately compute the neutronic power is shown with a red cross. It can be seen that around this cross the cells are refined repeatedly while far from this cell the mesh is coarser.

Figure 3a shows the convergence graph of the eigenvalue for the diffusion approximation or SP_1 calculation using the mentioned refinement strategies. The convergence graph compares

the number of the degrees of freedom (DoFs) against the eigenvalue error $\times 10^5$ because it is know that the CPU time to solve this type of eigenvalue problems is dependent of the size of the matrices as the computation of the error estimator is not relevant against the time employed by the eigenvalue solver. Figure 3b displays the convergence of the neutron power in the assembly of interest, also known as the error in the power peaking factor (PPF). From these results it can be seen that the best refinement strategy is the goal oriented because it presents a minimum error for a fixed number of degree of freedom. However, the differences are not relevant for error around 10 pcm for the eigenvalue and 1 % for the PPF, usual accuracy limits for the SP_1 equations.

Similarly, Figures 4a and 4b show the eigenvalue convergence and PPF convergence during several cycles of refinements using SP_3 equations. As before, the best refinement strategy to accurately solve the PPF of the reactor is to use the proposed goal oriented strategy. However, the eigenvalue error is converged analogously with the Kelly error estimator and the proposed goal estimator as both error estimator try to reduce the global error.
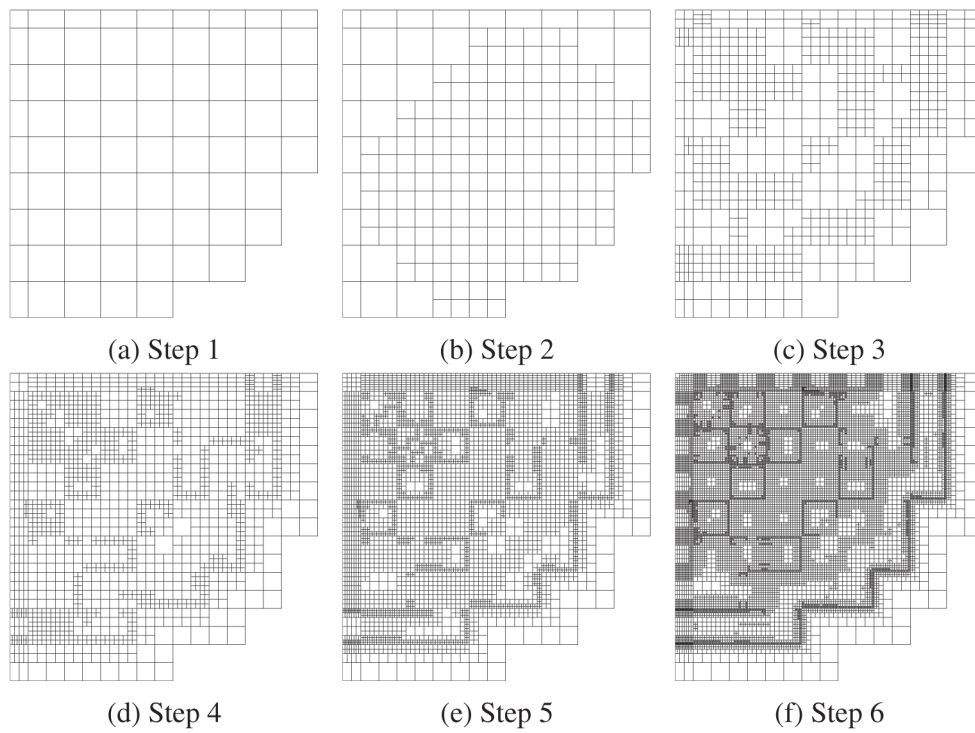
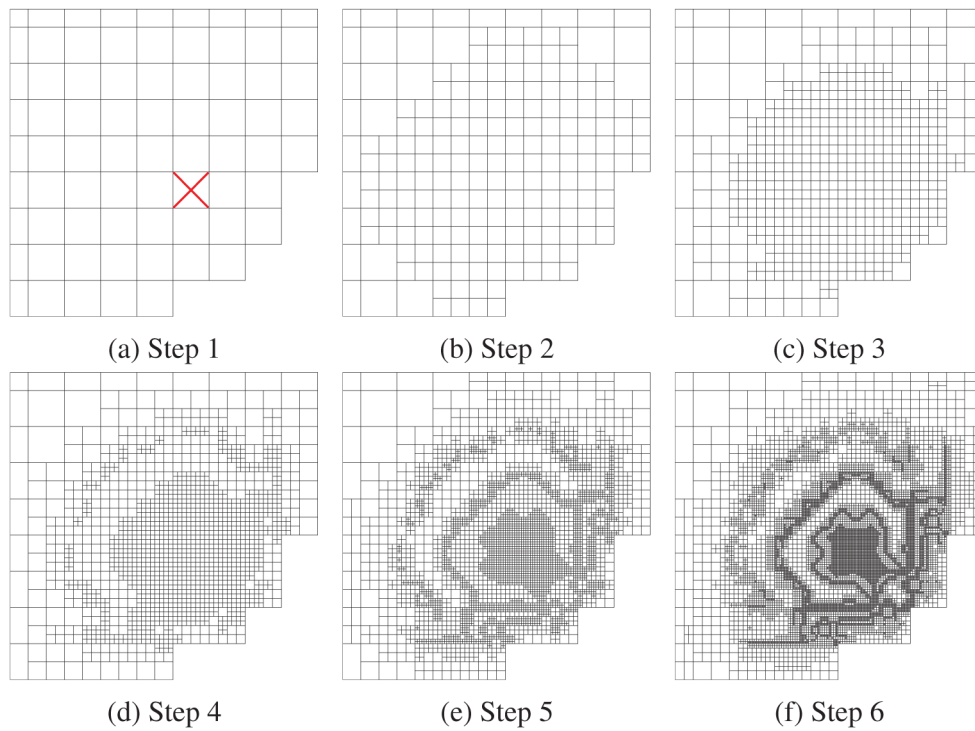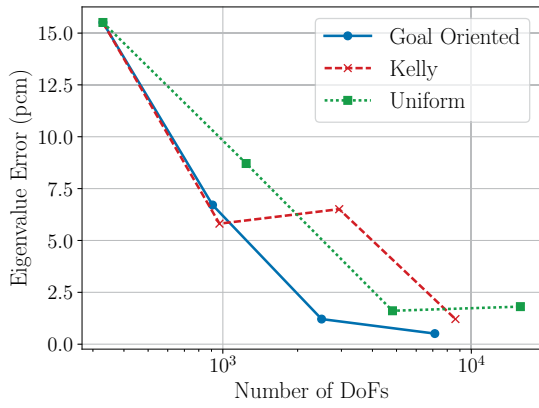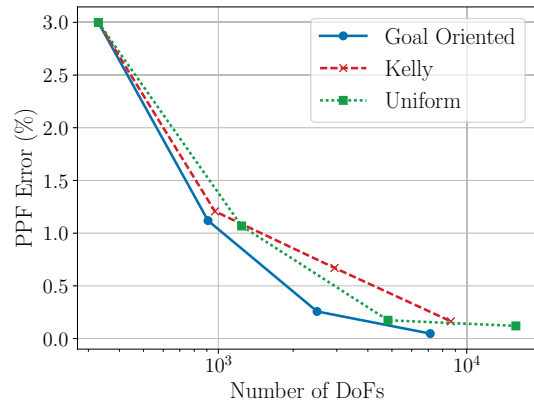Figure 1: Meshes using the gradient recovery error indicator.

Figure 2: Meshes using the goal oriented error indicator. In a red cross it is marked the assembly of interest, where the error indicator aims to reduce it error.
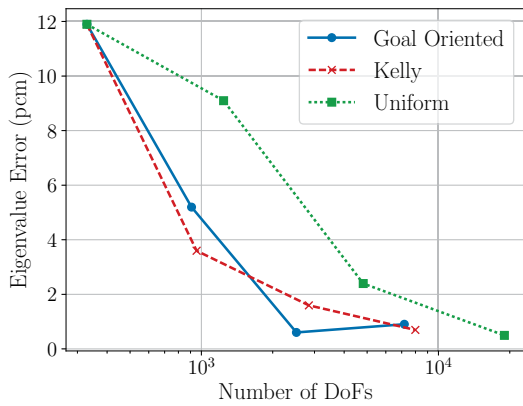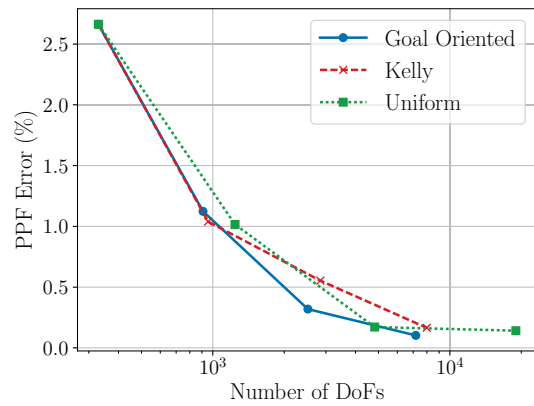
(a) Eigenvalue convergence.

(b) PPF convergence.

Figure 3: Eigenvalue and PPF convergence for SP$_1$ computation.

(a) Eigenvalue Convergence

(b) PPF convergence

Figure 4: Eigenvalue and PPF convergence for SP$_3$ computation.

6 CONCLUSIONS

In this work, an *h*-adaptable finite element method for the simplified harmonics approximation to the neutron transport equation is studied. To chose which cells have most of the error in order to refine them a goal oriented error estimator is presented. The goal oriented or duality based error estimator need to solve an adjoint problem with the a quantity of interest in the right hand side. Goal oriented adaptivity combines the benefits of the standard AMR methods with the knowledge of the end goal of the computation. Hence the AMR method proceeds by refining mesh cells whose errors are large and whose importance towards the computational goal is high. In this work, the quantity of interest is set as the maximum averaged power assembly of the reactor as this is a design constraint. To compare the proposed refinement strategy, goal oriented error estimator is compared with an usual error gradient recovery error estimator and a uniform global refinement. The proposed goal oriented error estimator has been demonstrated to be the most accurate strategy in order to minimize the error in the defined quantity of interest and as much as efficient as standard error estimators to compute the eigenvalue.

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