A computational 3D model for the multiscale analysis of nuclear reactors assembly

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Abstract. In this work we propose a multiscale model for the evaluation of the temperature field in a nuclear assembly. In particular the zone where the coolant flows is represented as a three dimensional (3D) domain while the fuel rods are taken into account as one-dimensional (1D) inclusion. In this framework the 3D domain is not conformal with the complex fuel rod grid resulting in a small computational cost of the problem. An interesting aspect of this multiscale approach is, as we show in the numerical results section, that by a proper average of the solution we can retrieve the results obtained with the homogeneous model.

1. Introduction

Numerical simulation of nuclear reactors is a key technology in the quest for improvements in efficiency, safety, and reliability of both existing and future reactor designs. Nuclear reactors are archetypal multiscale, multiphysics systems. Atomistic reactions ultimately drive very large-scale energy generation processes through micro and mesoscale phenomena [1]. Across the range of scales, a lot of physical processes impact the system: nucleate boiling, heat transfer, neutronics, fluid flow, and others. Traditionally, domain-specific software has been developed to tackle individual pieces of this problem and, simulation of an entire reactor, was accomplished by linking together, with a flexible coupling capability, multiple existing codes [2]. Among all the different physics involved in this complex problem, the heat exchange in the assemblies is one of the most challenging and complex aspect from a computational point of view. The importance of the effective modeling and simulation of the heat exchange between the coolant and the fuel rods drove the work of several authors, see for example [3, 4, 5, 6, 7, 8]. In this work we focus the attention on a multi scale assembly model and propose to represent the assembly in its three-dimensional form while all the fuel rods are taken into account as one-dimensional inclusions. In this framework the computational grid that represents the assembly is not conformal to the 1D inclusion resulting in a computational problem with a small amount of degrees of freedom. The coupling between a three and mono-dimensional problem is not trivial and has been investigated and applied by several author in different fields, see for example [9, 12, 10]. The final goal of the project is to develop a detailed and efficient computational model of the nuclear assembly to evaluate the homogenized properties to be used in the macro scale model of the full reactor core. More precisely, the idea is to perform several simulations of different representative assemblies of the reactor and use these results to evaluate the homogenized properties for the
complete simulation of the core. The work is organized as follows. In section 2 we describe the mathematical model used to represent the nuclear assembly in a multidimensional framework. In section 3 we investigate the capability of the multidimensional approach by comparing the results obtained through the new model and the one obtained with a homogenized model of the assembly. Finally in section 4 we give some preliminary conclusions and we draw line for future works.

2. Mathematical model

In this section we describe the mathematical multiscale model of the problem. For the sake of simplicity we consider a simplified assembly with a single fuel rod but the model can be easily extended for any lattice grid configuration.

2.1. Problem set up

The cross section of a simplified assembly is shown in Figure 1. \( \Omega_c \) marks the part of the assembly where the coolant flows while \( \Omega_f \) marks the fuel rod. \( \Gamma \) is the intersection surface between \( \Omega_c \) and \( \Omega_f \). We consider a steady state system, a constant coolant velocity field and that all the thermal power is produced in the fuel rod. We also assume that the fuel cladding thickness is small so that can be taken into account as a lumped model on the interface \( \Gamma \). The steady state internal energy balance in the coolant region reads

\[
\rho_c c_c u \cdot \nabla T_c - \nabla \cdot (K_c \nabla T_c) = 0, \quad \text{in } \Omega_c
\]

where \( T_c \) is the temperature field, \( u \) is the coolant velocity, \( K_c \) is the thermal conductivity of the coolant material, \( \rho_c \) is the coolant density and \( c_c \) is the coolant specific heat. The steady state internal energy balance in the fuel rod region reads

\[
- \nabla \cdot (K_f \nabla T_f) = q_f, \quad \text{in } \Omega_f, \tag{2}
\]

where \( T_f \), \( K_f \) and \( q_f \) are the temperature the thermal conductivity and the volumetric heat power generated inside the fuel rod, respectively. The continuity of the heat flux between the coolant and the fuel regions leads to the following relations between \( T_c \) and \( T_f \) on \( \Gamma_{cf} \)

\[
K_c \nabla T_c \cdot n_c = K_f \nabla T_f \cdot n_f, \quad \text{on } \Gamma_{cf}, \tag{3}
\]

where \( n_c \) and \( n_f \) are the outward unit normal of the coolant and fuel domain, respectively. \( K_f \) is the equivalent thermal conductivity of the fuel cladding that, in the case of cylindrical fuel pin

![Figure 1. Cross section of a single fuel rod assembly.](image-url)
and annular cladding reads $K_Γ = 2\pi K_{cl}/\ln(r_o/r_i)$, where $K_{cl}$ is the thermal conductivity of the cladding while $r_o$ and $r_i$ are the outer and the internal radius of the annular region, respectively. According to the introduced notation, the steady state temperature in the assembly is described by the following system of equations

\begin{align}
\rho_c c_c c_c u \cdot \nabla T_c - \nabla \cdot (K_c \nabla T_c) &= 0 \quad \text{in } \Omega_c, \quad (4) \\
K_c \nabla T_c \cdot n_c &= K_Γ (T_c - T_f) \quad \text{in } \Omega_c \cup \Gamma_{cf}, \quad (5) \\
-K_f \nabla T_f \cdot n_f &= -K_Γ (T_c - T_f) \quad \text{in } \Omega_f \cup \Gamma_{cf}. \quad (6)
\end{align}

We remark this system of equations must be closed with a proper set of boundary conditions that are discussed in later.

2.2. Dimensional model reduction

The full scale simulation of the fuel assembly requires a fine resolution of the geometry in order to take into account the fuel rods. This approach may results in a huge computational cost of the simulation. Therefore, in this work, we propose a topological model reduction of the fuel rod, namely going from a 3D-3D to a 3D-1D formulation. Such approach has been widely accepted in literature and has been used, for example, for the dimensional reduction of complex geomechanical application, see for example [10, 12] and citations therein. The dimensional model reduction approach is based on the main assumption the diameter of the rod is small if compared to the assembly dimension and the temperature $T_f$, as the coefficient of the fuel problem, have a uniform profile along the cross section of the fuel rod. We consider an arbitrary cylindrical portion ($P$) of the fuel rod bounded by two cross sections perpendicular to the center line of the rod $\Lambda$. Integrating the second equation of the system (7) we obtain

$$
\int_P -\nabla \cdot (K_f \nabla T_f) d\Omega = \int_P q_f d\Omega. \quad (8)
$$

Fuel rods are parametrized by their length $s$, so that the differentiation over the rods is defined by the unit tangent vector $i_t$ as $d_s = i_t \cdot \nabla$. We can show now that Eq. (8) is equivalent to

$$
-\pi r^2 d_s \left( K_f d_s T_f \right) + 2\pi r K_Γ T_f = 2\pi r K_Γ T_c + \pi r^2 q_f \quad \text{on } \Lambda, \quad (9)
$$

where

$$
\overline{T}(s) = (\pi R)^2 (\int_D T d\sigma), \quad \quad \quad \quad \quad T(s) = (2\pi R)^{-1} \int_{\partial D} T d\gamma. \quad (10)
$$

The weak form of Eq. (9) consist in finding $T_f \in H^1(\Lambda)$ such that

$$
\pi r^2 (K_f d_s T_f, d_s V)_\Lambda + 2\pi r (K_Γ T_f, V)_\Lambda = 2\pi r (K_Γ T_c, V)_\Lambda + \pi r^2 (q_f, V)_\Lambda \quad (11)
$$

for all $V \in H^1(\Lambda)$. The interested reader can find in [10, 12] all the details.

2.3. Reduction of the interface condition

Let us now consider the weak formulation of the first equation of 7 that describes the temperature in the coolant domain. For the sake of simplicity we consider homogeneous Dirichlet boundary condition on the boundary $\partial \Omega_D = \partial \Omega_c \setminus \Gamma$ so that integrating by parts and using boundary and interface conditions we obtain

$$
0 = (K_c \nabla T_c \cdot \nabla v)_\Omega - (K_c \nabla T_c \cdot n_c, v)_\Gamma + (\rho_c u \cdot \nabla T_c, v)_\Omega, \quad (12)
$$
for all \( v \in H^1_{\partial \Omega_D}(\Omega_c) \), where \( H^1_{\partial \Omega_D}(\Omega_c) \) denotes the subspace of \( H^1(\Omega_c) \) with vanishing trace on \( \partial \Omega_D \). The boundary integral is

\[
(K_e \nabla T_e \cdot n_e, v)_\Gamma = (K_\Gamma (T_c - T_f), v)_\Gamma .
\]  

(13)

We can now split the solution and the test function on the surface \( \Gamma \) as their average and a fluctuation, then, identifying the domain \( \Omega_c \) with \( \Omega = \Omega_c \cup \Omega_f \) and assuming that the product of fluctuation can be neglected, we can show that

\[
(K_\Gamma (T_c - T_f), v)_\Gamma = 2\pi r (K_\Gamma T_c, v)_\Lambda - 2\pi r (K_\Gamma T_f, v)_\Lambda .
\]  

(14)

By means of the previous calculation the problem described in Eq. (12) becomes

\[
(K_e \nabla T_e, \nabla v)_\Omega + (\rho_e c_e u \cdot \nabla T_e, v)_\Omega + 2\pi r (K_\Gamma T_c, v)_\Lambda = 2\pi r (K_\Gamma T_f, v)_\Lambda
\]  

(15)

for all \( v \in H^1(\partial \Omega) \), so that the weak formulation of the complete problem reads, find \((T_c, T_f) \in H^1(\partial \Omega) \times H^1(\partial \Lambda) \) such that

\[
(K_e \nabla T_e, \nabla v)_\Omega + (\rho_e c_e u \cdot \nabla T_e, v)_\Omega + 2\pi r (K_\Gamma T_c, v)_\Lambda = 2\pi r (K_\Gamma T_f, v)_\Lambda ,
\]

\[
\pi r^2 (K_f d_s T_f, d_s \varphi)_\Lambda + 2\pi r (K_\Gamma T_f, \varphi)_\Lambda = 2\pi r (K_\Gamma T_c, \varphi)_\Lambda + \pi r^2 (q_f, \varphi)_\Lambda ,
\]

(16)  

(17)

for all \( v \in H^1(\partial \Omega) \) and \( \varphi \in H^1(\partial \Lambda) \).

3. Numerical example

Figure 2. Computational domain composed by three assemblies labeled with different colors (left) and single assembly together with the fuel rods grid (right).

In this section we exploit the capability of the model proposed in the previous section with a preliminary test case in which we investigate the stationary temperature field of several nuclear assemblies under nominal working conditions. The working conditions are the ones typical of lead cooled fast example, see for example [11]. The numerical simulation has been performed with the computational platform GetFEM++, an open source library that aims to offer the most flexible framework for solving coupled systems of linear and nonlinear partial differential equations with the finite element method. In order to investigate the performance of the multidimensional
approach we consider two numerical experiments. In the first case (Test A) the assembly is modeled through a three dimensional homogeneous domain so that the heat generation is taken into account as a homogeneous distributed source term. In the second test case (Test B) the assembly is described through the multidimensional model presented in the previous section and the same heat production of the Test A occurs only in the monodimensional inclusions that represent the fuel rods. We compare the results obtained the multidimensional model with the ones obtained with the classic homogenized model.

We consider a computational domain composed by three simplified closed assemblies of a lead

**Figure 3.** Temperature profile for Test A in the case of homogenized source term (left). Temperature profile of Test B in the multidimensional case (right).

**Figure 4.** Temperature profile for Test A in different transversal sections of the domain (left). Temperature profile for Test B in the multidimensional case in several transversal slices of the domain together with 1D inclusion overview (left).
cooled nuclear reactor. Every assembly has a squared cross section with a characteristic length of 0.1\text{m} and a height of 1\text{m}, a sketch of the computational domain is shown in the left part of Figure 2. We consider that in every assembly there are 9 fuel rods disposed on a regular lattice grid as shown in the right part of Figure 2. Every rod is a cylinder characterized by a radius of 0.01\text{m} and a height of 1\text{m}. The cladding thickness is 0.75\text{mm}. We consider that the assemblies are cooled by lead that enters the domain in the bottom surface at a constant temperature of 400\text{C}, we further assume that in the inlet section the fuel rods are in thermal equilibrium with the coolant. In particular a Dirichlet boundary condition in the inlet surface of the assembly is considered for both the three and the monodimensional problem and a homogeneous Neuman condition is considered in the remaining part of the domain. We also assume that the coolant flows into the domain with a prescribed constant velocity of 0.5\text{m/s} in the axial direction and that the total heat production per assembly is 0.2\text{MW}. The thermal conductivity of the coolant, the fuel and the cladding are 40, 30 and 25\text{W/m/K}, respectively.

In Figure 3 the temperature profile obtained from Test A on the left and from Test B on the right, is shown. From that Figure we notice that the homogenized model (Test A) results, as expected, in a uniform temperature field that increases only with respect to the axial direction. From the multidimensional model (right part of Figure 3) we notice that the temperature field exhibits large gradient also with respect to the transversal direction resulting in several temperature peaks in correspondence of the one-dimensional inclusion where the heat production is confined. This effect is further appreciable in Figure 4 where the temperature field is shown on several cross sections of the domain. We observe that using the multidimensional model (right part of Figure 4) the temperature field is no longer uniform along the cross section as obtained using the homogenized model (left part of Figure 4). In particular we notice that the temperature field in every cross section highly increases near the mono dimensional inclusion. In Figure 5 the temperature profile along the center line of the cross section at \(z = 0.5\text{m}\) is shown for the different test cases. In particular \(T_A\) and \(T_B\) marks the profiles obtained in the Test case A and B, respectively, while \(T_{B_{avg}}\) is the average of \(T_B\) over the cross section at \(z = 0.5\text{m}\). We remark that by averaging the temperature obtained with the multidimensional model, we retrieve the bulk temperature obtained with the homogenized approach providing an empirical prove of the consistency of the multidimensional approach. Finally in Figure 6 the thermal flux on the interface between two assemblies is shown. We notice that with the homogenized

Figure 5. Temperature profile on the transversal center line of the domain at \(z = 0.5\text{m}\). \(T_A\) and \(T_B\) are the temperature profiles obtained for the Test A and Test B case while \(T_{B_{avg}}\) is the average of \(T_B\) over the cross section.
Figure 6. Thermal flux on the interface between two assemblies for Test A (left) and Test B (right).

model (left part of the figure) there is no thermal flux across the assemblies while using the multidimensional approach (right part of the Figure) the transversal component of the thermal flux is no longer null. This transversal effect is not represented by the homogenized model of the assemblies and should be taken into account in order to better represent the heat exchange dynamics in a reactor core.

4. Conclusions
In this paper we have introduced a mathematical model to represent the heat exchange in a nuclear assembly by means of a multidimensional approach. In particular the assembly is represented through a three dimensional domain in which several mono dimensional inclusion, representing the fuel rods, are immersed. In this framework the heat production is confined in the monodimensional inclusion. The coupling between the three and the mono dimensional problems is obtained through specific terms that depend on the fuel assembly geometry and the cladding material. One of the major advantages of this approach is that the 3D computational grid is not required to be conformal with the 1D inclusion, resulting in an efficient method that allows to easily investigate the performance of different configuration of the fuel rods.

We have tested the performance of the multidimensional approach through a numerical experiment. In particular we have investigated the temperature field of a simplified model of three neighboring assemblies working under nominal conditions. We have performed the simulation using a homogenized model of the assembly and the proposed multidimensional approach and we compared the obtained results. We have shown that the different models produce different temperature field and we have shown that by averaging the temperature field obtained with the multidimensional framework, we retrieve a temperature field in great accordance to the one obtained through the homogenized model. We also have shown that the homogenized model is not able to reproduce the transversal thermal flux obtained with the multidimensional approach.

For future work we plan to validate the multidimensional model by comparing the results obtained within this framework and the one obtained with a full scale simulation of a nuclear assembly. We also aim to use the multi scale simulations of the assembly to evaluate the effective
thermal diffusivity that is used in the homogenize model of the full reactor core.

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