MODELLING OF IDEALIZED CONCRETE USING MULTIPLE LEVEL-SET WITHIN XFEM

Tran Anh Binh[1*]

***Summary**: When modelling concrete with high volume fractions, complex microstructures and nearby inclusions, the classical level-set/XFEM method induces some actefacts, even for extremely fine background meshes. It leads to significant errors in the effective thermal conductivity and poor convergence of the solution with respect to the mesh size. We proposed in previous works a method using multiple level-sets within the XFEM method to overcome these issues. In this method, each inclusion interface is associated with a different level-set function and related to a different enrichment strategy. In this paper, we extend this method to estimate effective thermal conductivity of idealized concrete. The proposed approach is demonstrated through the numerical results.*

***Keywords**: XFEM/level-set; multiple level-set; effective conductivity.*

Received: July 6th, 2016, Revised: July 20th, 2016, accepted: October 13th, 2016

1. Introduction

Concrete is known as a high complex material with nearby inclusion. Many studies have been published in the literature for predicting effective thermal conductivity of such material. Analytical methods are often based on a simplification of inclusion shapes, potential theory and spherical harmonic functions... Many exact and approximate closed-form solutions have been derived by such methods for materials having a linear behavior [1-3]. However, its limitations are shown when the microstructure is known in all of its complexity. Upper and lower bounds on the possible values of the effective conductivities [4-6] are not very useful in the case of high contrast of matrix-inclusion conductivities. Some simple approximations [7-9] are available for estimating the effective thermal conductivity but they are not efficient for complex microstructures. The numerical methods can overcome these issues, but the computational cost is a big concern. Finite element method (FEM), boundary element method (BEM) and fast Fourier transform method (FFT) are widely used for homogenization problems. These methods have been reported in numerous works [10-16]. More recently, the use of the Extended Finite Element Method (XFEM) [17-19] has been proposed for modelling and computing the overall properties of complex microstructures. However, it does not well describe the local fields and the convergence is slow when the microstructure contains the nearby inclusions. To overcome these limitations, we use the modified XFEM/Level-set technique [20] which involves multiple level-set functions for describing of the interfaces and introduces additional degrees of freedom (DOF) for nodes associated with element cut by more than one interface. This approach allows modeling the concrete with arbitrary inclusion shape. However, the study area of this paper is limited to modelling of the idealized concrete associated with spherical inclusions embedded in a continuous matrix. More complex concrete shall be the subject of our following study. The layout of this paper is as follows.

Firstly, the XFEM/level-set method is summarized in Section 2. In the next section, the proposed approach is presented. The numerical examples are shown in the Section 4. Some conclusions are finally pointed out in the last section.

2. Quick recall the Level-set/XFEM method

In order to model a multi phasic domain, the Finite Element Method (FEM) requires an explicit meshing of all interfaces, which must conform to the volume mesh. This operation can be highly challenging for complex three-dimensional microstructures. In contrast, the XFEM uses an implicit description of the discontinuities that do not need to coincide with the mesh and an enriched approximation to model the jumps through the surface

[1]*Dr, Faculty of Information Technology. National University of Civil Engineering (NUCE).*
** Corresponding author. E-mail: anh-binh.tran@nuce.edu.vn.*

discontinuities (cracks or interfaces). Sukumar et al. [17] were the first ones to combine the XFEM with a level-set description of the interface. Let Γ^I be an interface between two neighboring domains, which is taken to be a smooth 2D or 3D surface. In this context, Γ^I is defined as the zero level-set of a function $\phi : \mathbf{R}^d \to \mathbf{R}$:

$$\Gamma^I = \left\{ \mathbf{x} \in \mathbf{R}^d \,\middle|\, \phi(\mathbf{x}) = 0 \right\} \tag{1}$$

where d is the dimension of the space under consideration. An important example is the signed distance function:

$$\phi(\mathbf{x}) = \min_{k=1,2,\ldots,m} \left(\left\| \mathbf{x} - \mathbf{x}_{\Gamma^k} \right\| sign\left(\mathbf{n}^k \cdot (\mathbf{x} - \mathbf{x}_{\Gamma^k}) \right) \right), \tag{2}$$

where $\mathbf{x}_{\Gamma^k}$ is the normal projection of $\mathbf{x}$ on Γ^k, $\mathbf{n}^k$ is the unit normal vector as illustrated in Figure 1 and m is the number of inclusions.

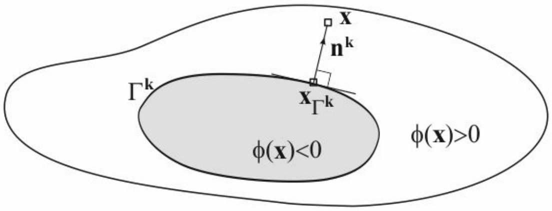


Figure 1. *Level-set function* $\phi(\mathrm{x})$ *related to interface* Γ_k.

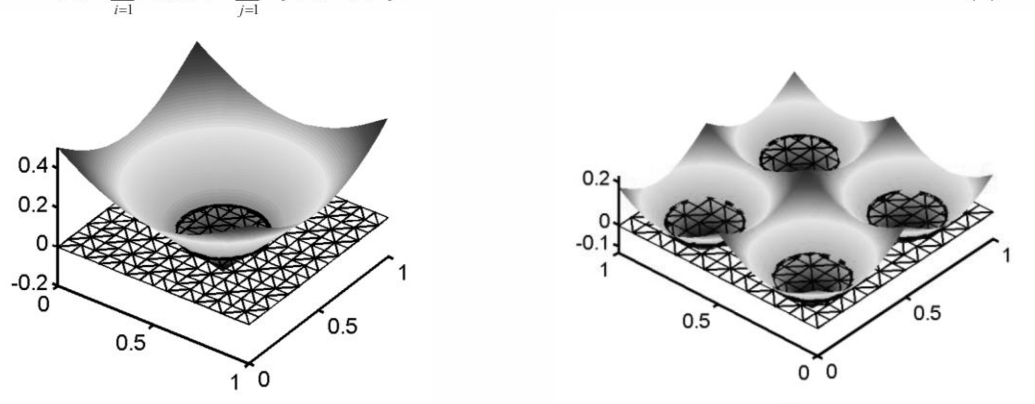
In the case of spherical (circular) inclusions, Eq (2) leads to:

$$\phi(\mathbf{x}) = \min_{k=1,2,\ldots,n_c} \left\{ \left\| \mathbf{x} - \mathbf{x}_c^k \right\| - r^k \right\}, \tag{3}$$

where n_c is number of spherical inclusions; $\mathbf{x}_c^k$ is the center of inclusion k; and r^k is radius of inclusion k. Graphical illustrations of such function are shown in Figure 2.

To introduce discontinuities within elements cut by the interface, the XFEM approximation is employed, assuming the following form for displacement formulation:

$$T^h(\mathbf{x}) = \sum_{i=1}^{n} N_i(\mathbf{x}) T_i + \sum_{j=1}^{m} N_j(\mathbf{x}) F(\mathbf{x}) a_j \,, \tag{4}$$



a) b)

Figure 2. *Level-set function of (a) a circular inclusion; (b) four circular inclusions*

where N_i are the standard shape functions, N_j are the shape functions related to nodes of elements whose support is cut by the interface. The additional DOF a_j are only added to nodes for which support is cut by the interfaces. In the present work, only perfect interfaces are considered, assuming the continuity of both displacements and normal forces through the interfaces. Thus we utilize the enriched function $F(\mathbf{x})$ proposed in [17]:

$$F(\mathbf{x}) = \sum_i |\phi_i| N_i(\mathbf{x}) - \left| \sum_i \phi_i N_i(\mathbf{x}) \right|. \tag{5}$$

To carry out numerical integration, elements cut by the interfaces must be subdivided [17]. The approximated interface can be constructed through a linear approximation of nodal values of level-set function. Let ϕ_i and ϕ_j denoting nodal value of level-set functions values at two vertices $\mathbf{x}_i$ and $\mathbf{x}_j$ of an element. An element edge is cut by the zero level-set if $\phi_i \phi_j < 0$. The intersection is then found by:

$$\mathbf{x_p} = \mathbf{x_i} + \xi(\mathbf{x_j} - \mathbf{x_i}),\ \xi = -\frac{\phi_i}{\phi_j - \phi_i}, \tag{6}$$

where $\mathbf{x_p}$ is the intersection point.

When the XFEM/Level-set method is used to model a basic cell containing nearby inclusions, different artefacts are observed [20]. The first one is artificial percolation. When the distance between two inclusions is smaller than the local element size, or when a single element is cut by more than one interface, the level-set method is not capable to describe accurately the local topology of the interfaces. It results in an artificial connexion between two inclusions. The second one is due to the fact that when a single node is contained between two interfaces, the kinematical fields cannot be reproduced accurately due to a lack of degrees of freedom. The third one is the incapability of the level-set method to accurately describe nearby interfaces with a single level-set function, when single nodes are contained between two interfaces. The consequences of these issues are strongly oscillating and slow convergence of solution and of effective properties with respect to the mesh size when applying linear homogenization. The objective of this paper is to present a modified version of the XFEM/level-set to avoid to aforementioned difficulties.

3. XFEM/multiple Level-sets method

This section presents a modified version of the level-set/XFEM method where each inclusion interface is described by a level-set function and is associated with an individual enrichment. In that framework the approximation scheme is given by:

$$T^h(\mathbf{x}) = \sum_{i=1}^{n} N_i(\mathbf{x}) T_i + \sum_{k\in N_{inter}} \sum_{j=1}^{m} N_j(\mathbf{x}) F^k(\phi^k(\mathbf{x})) a_j^k , \quad (7)$$

where n is the number of nodes of the element, m is the number of enriched nodes of the element, and N_{inter} is the set of nodes whose support is cut by an interface. The functions $N_i(\mathbf{x})$ and $N_j(\mathbf{x})$ are the classical FEM shape functions and $F^k(\phi^k(\mathbf{x}))$ is an enrichment function constructed via the level-set function ϕ^k of an individual inclusion k with boundary Γ^k. The general form of level-set function ϕ^k is such as

$$\Gamma^k = \left\{ \mathbf{x}\in \mathbf{R}^d \,\middle|\, \phi^k(\mathbf{x}) = 0 \right\}. \quad (8)$$

In the case of the signed distance, we obtain:

$$\phi^k(\mathbf{x}) = \left\| \mathbf{x} - \mathbf{x}_{\Gamma^k} \right\| sign\left(\mathbf{n}^k.(\mathbf{x} - \mathbf{x}_{\Gamma^k})\right). \quad (9)$$

For a spherical (circular) inclusion, it yields:

$$\phi^k(\mathbf{x}) = \left\{ \left\| \mathbf{x} - \mathbf{x}_c^k \right\| - r^k \right\}. \quad (10)$$

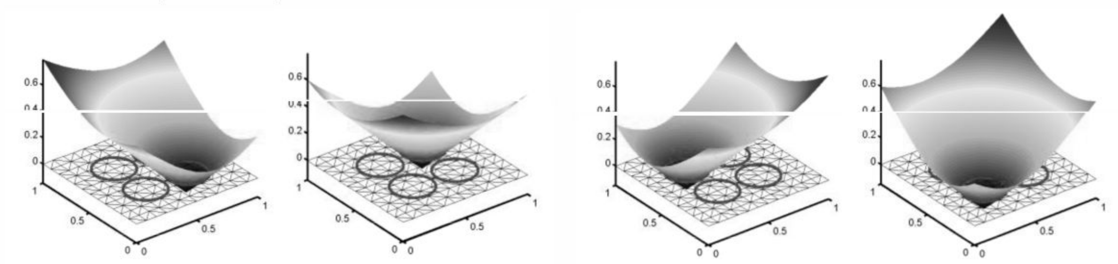


Figure 3. *Level-set function of four circular inclusions*

Using (7) allows to represent several discontinuities in a single element. It also removes all the numerical artefacts due by nearby inclusions.

4. Numerical examples

The field equations of thermo-static problem are given by:

$$\nabla \cdot \mathbf{q}(\mathbf{x}) - r(\mathbf{x}) = 0 \ \text{ in } \ \Omega, \quad (11)$$

$$\mathbf{q}(\mathbf{x}) = -c(\mathbf{x}) \nabla T(\mathbf{x}). \quad (12)$$

Above, $\mathbf{q}(\mathbf{x})$ denotes the heat flux, $r(\mathbf{x})$ is a heat source term and $c(\mathbf{x})$ the thermal conductivity. Using XFEM/Level-set or XFEM/multiple level-set procedure, one finds the discrete system of linear ordinary equations:

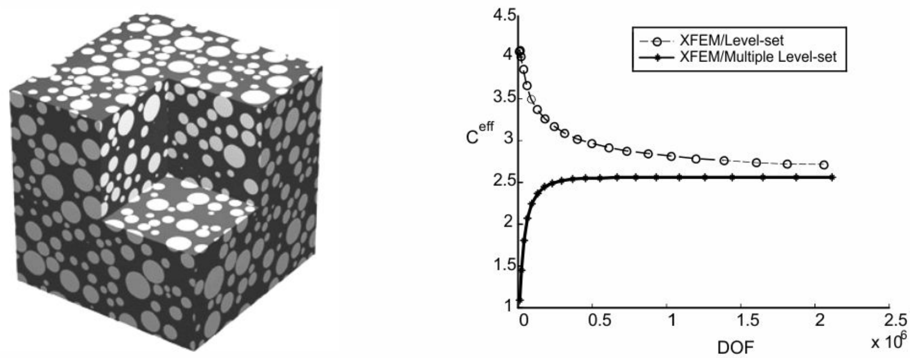
$$\mathbf{K}\,\mathbf{D} = \mathbf{Q}, \ \mathbf{D} = \{\mathbf{T} \quad \mathbf{a}\}^{\mathrm{T}}, \quad (13)$$

where $\mathbf{D}$ are nodal unknowns and $\mathbf{K}$ and $\mathbf{Q}$ are the global stiffness matrix and external flux, respectively. More precisely, the matrix $\mathbf{K}$ and vector $\mathbf{Q}$ are defined by

$$\mathbf{K} = \int_\Omega \mathbf{B}^T c(\mathbf{x}) \mathbf{B} d\Omega, \ \mathbf{Q} = \int_\Omega \mathbf{N}^{\mathrm{T}} r d\Omega, \quad (14)$$

where $\mathbf{B}$ and $\mathbf{N}$ are the matrices of shape function derivatives and shape functions associated with the approximation scheme (4,7).

As the first example, we consider a basic cell of idealized concrete which contains 2024 spherical inclusions having thermal conductivity $c(\mathbf{x}) = c_I = 20w/mK$ embedded in a matrix of thermal conductivity $c(\mathbf{x}) = c_M = 0.9w/mK$ (Figure 4). The phase fractions as well as the essential parameters of the geometries are reported in Table 1. We assume the perfect interface between matrix and inclusions and small deformation. The microstructure of idealized concrete is provided by French Electricity (Electricité de France - EDF) [15].



a) b)

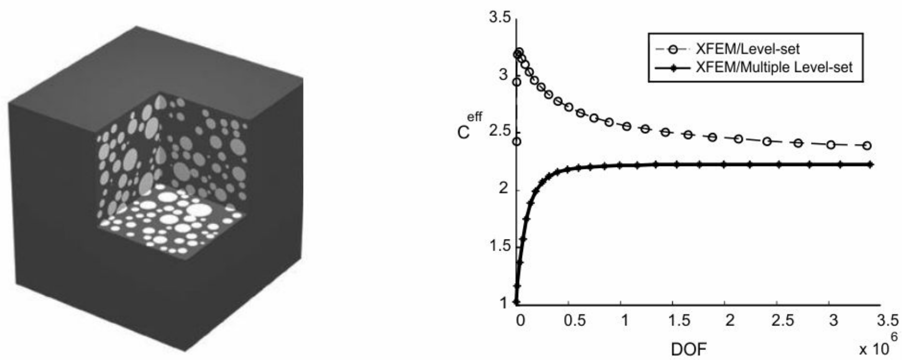
Figure 4. *a) The basic cell contains 2024 spherical inclusions.*
b) Effective thermal conductivity of the basic cell with XFEM/level-set and XFEM/multiple level-sets

We aim to compute the effective thermal conductivity c^{eff} of the basic cell using both XFEM with single level-set function and XFEM with multiple level-set functions. The results are reported in the Figure 4.b. These results are obtained with help a super computer of 400GB RAM and 32 cores. For using the full computational power of your machine, we code the program in MATLAB® with parallel technique to take advantage of multicore and multiprocessor computers. It can be shown that the proposed approach converges faster than XFEM/single level-set method does, as a function of the total number of DOF., by avoiding the artefacts. The method XFEM/multiple level-sets seem to converge at 5.10^5 DOFS. While XFEM/single level-sets do not converge yet at the 5.10^6 DOFS.

The second example, 3200 spherical inclusions are embedded in a continuous matrix as depicted in Figure 6.a. The information about microstructure are presented in the Table 1. We take the material parameter as the same as in previous example. The obtained results are shown in Figure 5.b. Here again, proposed technique converges faster than XFEM/single level-set method. Furthermore, Figure 4 and 5 show that the model containing 3200 spherical inclusions have more inclusions, but have lower effective thermal conductivity than one of 2024 inclusions. This result came from the fact that the volume fraction of 3200 inclusions is smaller than one of 2024 inclusions (see Table 1).

Table 1. *Essential phase information about the microstructures. f_i is the inclusion fraction, ϕ_{min} is the minimum diameter, ϕ_{max} is the maximum diameter and d_{min} is the minimum inter-inclusion distance*

$\mathbf{n}_c$	$\mathbf{f}_i$	ϕ_{min}	ϕ_{max}	$\mathbf{d}_{min}$
2024	0.402	0.043	0.167	1.14×10^{-3}
3200	0.361	0.036	0.125	2.17×10^{-7}



a) b)

Figure 5. *a) The basic cell contains 3200 spherical inclusions.*
b) Effective thermal conductivity of the basic cell with XFEM/level-set and XFEM/multiple level-sets

5. Conclusions

We extended our previous work to treat thermal problem aiming at determining the effective conductivity of concrete. The method allows to model the concretes with arbitrary inclusion shape by changing the form of level-set function. However, the research in this paper is limited in the simple morphology of concretes which contain only spherical inclusions. The concrete associated with complex inclusion shapes shall be the subject of our future study. The code is built in MATLAB® with parallel technique which allows to execute on multicore and multiprocessor of super computer. The big tests of idealized concrete containing 2024 inclusions and 3200 spherical inclusions embedded in continuous matrix have been carried out. XFEM/multiple level-set functions always give a better convergence than XFEM/single level-set function especially in the case of complex microstructure.

Acknowledgement

This research is funded by Vietnam National Foundation for Science and Technology Development (NAFOSTED) under grant number 107.02-2014.08

References

1. Sangani AS, Acrivos A (1983), "The effective conductivity of a periodic array of spheres", *Proceedings of the Royal Society A*, 386: 263–275.

2. Cheng H, Torquato S (1997), "Effective conductivity of periodic arrays of spheres with interfacial resistance", *Proceedings of the Royal Society A*, 453: 145–161.

3. Eshelby JD (1957), "The determination of the elastic field of an ellipsoidal inclusion, and related problems", *Proceedings of the Royal Society A*, 241: 376–396.

4. Pham D.C. (1994), "Bounds for the effective conductivity and elastic moduli of fully-disordered multi-component materials", *Arch Rational Mech Analysis*, 127: 191-198.

5. Pham D.C. (1996), "Bounds for the effective properties of isotropic composite and poly-crystals", *D. Sci*. Thesis.

6. Phan-Thien, N., Pham, D.C. (2000), "Differential multiphase models for polydispersed spheroidal inclusions: thermal conductivity and effective viscosity", I*nternational Journal Engineering Science Technology*, 38:73-88.

7. Pham, D.C. (2008), "Weighted effective medium approximations for conductivity of random composites", *International Journal of Heat and Mass Transfer*, 51:3355-3361.

8. Le Quang, H., Bonnet, G., Pham, D.C. (2011), "Bounds and correlation approximation for the effective conductivity of heterogeneous plates", *Physical Review E*, 84:061153.

9. Pham, D.C., Tran, A.B., Do, Q.H. (2013), "On the effective medium approximations for the properties of isotropic multicomponent matrix-based composites", *International Journal Engineering Science*, 68:75-85.

10. Jae Young Kim, Byung Jun Yoon (1999), "The Effective Conductivities of Composites with Cubic Arrays of Spheroids and Cubes", *Journal of Composite Materials*, 33(14):1344-1362

11. Tao R, Chen Z, Sheng P (1990), "First-principles Fourier approach for the calculation of the effective dielectric constant of periodic composites", *Physical Review B*, 41: 2417–2420.

12. Michel JC, Moulinec H, Suquet P (1999), "Effective properties of composite materials with periodic microstructure: a computational approach", *Computer Methods in Applied Mechanics and Engineering*, 172: 109–143.

13. Monchiet V, Bonnet G (2013), "A polarization-based fast numerical method for computing the effective conductivity of composites", *International Journal of Numerical Methods for Heat & Fluid Flow*, 23(7):1256–1271.

14. Monchiet V, Bonnet G (2012), "A polarization-based FFT iterative scheme for computing the effective properties of elastic composites with arbitrary contrast", *International Journal for Numerical Methods in Engineering*, 89: 1419–1436.

15. B. Bary, S. Brisard, C. Dunant, A. Giorla, C. Péniguel, J. Sanahuja, C. Toulemonde, A.-B. Tran, F. Willot and J.Yvonnet (2013), "A critical comparison of several numerical methods for computing effective properties of highly heterogeneous materials", *Advances in engineering Software*, 58:1-12.

16. T. Wua, I. Temizer, P. Wriggers (2013), "Computational thermal homogenization of concrete", *Cement & Concrete Composites*, 35:59–70.

17. N. Sukumar, DL. Chopp, N. Mo¨es, T. Belytschko (2001), "Modeling holes and inclusions by level-sets in the extended finite-element method", *International Journal of Solids and Structures*, 190:6183-6200.

18. J. Yvonnet, Q-C. He, C. Toulemonde (2008), "Numerical modelling of the effective conductivities of composites with arbitrarily shaped inclusions and highly conducting interface", *Composites Science and Technology*, 68:2825-2828.

19. Soheil Mohammadi (2008), *Extended Finite Element Method*, Blackwell Publishing.

20. A.B. Tran, J. Yvonnet, Q-C. He, C. Toulemonde, J. Sanahuja (2011), "A multiple level set approach to prevent numerical artefacts in complex microstructures with nearby inclusions within XFEM", *International Journal for Numerical Methods in Engineering*, 85:1436-1459.