# A POD-based reduction approach for multiscale nonlinear structural design

# \*Liang Xia, and Piotr Breitkopf

Laboratoire Roberval, UMR 7337 UTC-CNRS, Université de Technologie de Compiègne, Centre de Recherches de Royallieu, CS 60319, 60203, Compiègne Cedex, France

\*Corresponding author: liang.xia@utc.fr

# Abstract

This paper presents POD-based reduction approach for structural optimization design considering microscopic material nonlinear microstructures. This work introduces Reduced Order Model (ROM) to alleviate the heavy computational demand of nonlinear nested multiscale procedures, particularly in an optimization framework which requires multiple loops involving similar computations. The surrogate model constructed using Proper Orthogonal Decomposition (POD) and Diffuse Approximation reduces the computational effort for solving the microscopic boundary value problems. Multiscale analysis model (FE<sup>2</sup>) is applied to link structure and microstructures in the two scales. Maximum stiffness design of the macroscopic structure is realized using a discrete level-set topology optimization model. It is shown by means of numerical tests that the reduced multiscale model provides reasonable designs as compared to those obtained by the unreduced model while with a significantly reduced computational effort.

Keywords: Model reduction, Diffuse Approximation, Multiscale analysis, Topology optimization

# Introduction

Optimization techniques for structural size, shape, topology designs have been widely developed and employed in engineering applications. One of its most prominent applications is designing lightweight structures for aircrafts. An increasing number of optimized structures, parts and components appear in the latest models of Airbus and Boeing. Most of present optimization algorithms are developed within frameworks of numerical analysis with the assumption that the considered structure is constituted by one-scale linear elastic materials. However, due to the fast development made in the field of material science, advanced fiber-reinforced composites are increasingly used in both aerospace and military applications. More advanced structural analysis models are required such that the structural influences from microscopic heterogeneities can be considered. As a response, multiscale incremental homogenization approaches or the so called  $FE^2$ approach have been proposed and largely developed in the last decade [Feyel and Chaboche (2000), Kouznetsova et al. (2001)]. Generally speaking, this type of approach solves two nested boundary value problems, one at the macroscopic scale and another at the microscopic scale. The  $FE^2$ approach is able to evaluate the macroscopic responses of heterogeneous material with an accurate account for micro characteristics and evolution of the morphology. The challenges of the  $FE^2$ approach are due to high computational effort. Therefore, there is an increasing research demand of bridging structural optimization models and  $FE^2$ -type analysis models.

This paper introduces Reduced Order Model (ROM) to perform multiscale topological optimization design. The multiscale analysis model  $FE^2$  [Feyel and Chaboche (2000)] is applied to link the macroscopic structure and the corresponding RVE microstructures in the microscopic level. The optimization process requires multiple design loops involving similar or even repeated computations of the RVE which perfectly suits the ROM learning process. In the present work the considered RVE is assumed to be the same for all marcoscopic integration points. Maximum stiffness design of the macroscopic structure is performed using a discrete level-set topology

optimization model [Challis (2010)]. The reduction is performed in an adaptive non-intrusive manner which is an alternative to the intrusive approach [Yvonnet and He (2007)}]. The reduced basis is extracted using Proper Orthogonal Decomposition (POD) and the surrogate model is constructed using Diffuse Approximation [Nayroles et al. (1992)}, variant of Moving Least Squares [Lancaster and Salkauskas (1981)].

The remainder of this paper is organized in the following manner: firstly the  $FE^2$  approach is briefly reviewed which links the macroscopic structure and microscopic microstructure RVE; secondly, the discrete level-set model for structural topology optimization design is presented; thirdly, a bi-level reduced surrogate model is developed for microscopic RVE solution using POD and Diffuse Approximation; the presented model is then showcased by one numerical test example; finally, the paper ends with concluding comments and suggestions for future work.



Figure 1. Illustration of the selection of a typical 2D representative volume element (RVE).

# FE<sup>2</sup> approach

The  $FE^2$  approach [Feyel and Chaboche (2000)] is chosen here to bridge the macroscopic structure and the corresponding microscopic RVE to perform structural topology optimization. The key hypothesis of  $FE^2$  consists in the separation of macroscopic and microscopic scales. It is assumed that the microscopic length scale is large enough to be considered in the framework of continuum mechanics, and at the same time much smaller than the macroscopic length scale considered in terms of periodically ordered pattern [Kouznetsova et al. (2001)], as illustrated in Fig. 1.

The principal concept of the  $FE^2$  approach assumes that each macroscopic material point is attributed with a RVE so that the macroscopic stress and strain for the considered point can be estimated by averaging the corresponding stress and strain fields of the RVE. Thereafter, there is no need to specify the macroscopic constitutive behavior and we only need to define the constitutive behavior for each material phase of the RVE. Let x and y denote the position of a point at the macroscopic and microscopic scales, respectively. At the macroscopic scale, stress and strain fields are denoted by  $\Sigma(x)$  and E(x), which are evaluated as the average of the corresponding microscopic fields  $\sigma(x, y)$  and  $\varepsilon(x, y)$  over the RVE of region  $\Omega_x$  corresponding to the material point x. The FE<sup>2</sup> performs the following steps:

- evaluate the macroscopic strain field E(x) with an initially defined elastic tensor  $C_0$ ;
- define boundary conditions on the RVE at material point x upon the value of E(x);
- evaluate the stress field  $\sigma(x, y)$  through periodic homogenization analysis on the RVE;
- compute the macroscopic stress tensor  $\Sigma(x)$  at material point x via averaging  $\sigma(x, y)$ ;
- update the structural displacement field u(x) using iterative Newton-Raphson method;
- repeat above procedures until the macroscopic force equilibrium is achieved.



Figure 2. Illustration of the implementation of  $FE^2$  in the framework of FEA.

A schematic view of the  $FE^2$  algorithm is depicted in Fig. 2, where each Gauss integration point is attributed with an RVE within the context of finite element analysis (FEA). In case of nonlinear elasticity, the displacement solution at the macroscopic scale is solved using the iterative Newton-Raphson method.

### Nonlinear structural design using level-set method

In order to avoid defining a pseudo-relationship between the intermediate values and the considered RVE, we choose to use the discrete version of level-set topology optimization model [Challis (2010)] to straightforwardly link RVEs to the solid region of the structure. An initial level-set function  $\psi(x, t_0)$  is constructed as a signed distance function upon the discretized initial structural topology following

$$\begin{cases} \psi(\mathbf{x}_e, t_0) < 0 & \text{if } \rho_e = 1 \\ \psi(\mathbf{x}_e, t_0) > 0 & \text{if } \rho_e = 0 \end{cases}$$
 (1)

where  $\mathbf{x}_e$  denotes the center of the *e*th element and  $\rho_e$  is its pseudo-density. The initialized level-set function  $\psi(\mathbf{x}_e, t_0)$  is then be updated to  $\psi(\mathbf{x}_e, t)$  corresponding a new structural topology by solving the ``Hamilton-Jacobi'' evolution equation

$$\frac{\partial \psi(x,t)}{\partial t} + v_n \left| \nabla \psi(x,t) \right| = 0$$
<sup>(2)</sup>

where *t* is a pseudo-time defined corresponding to different optimization iterations. The normal velocity field  $v_n$  determines geometric motion of the boundary of the structure and is chosen based on the shape derivative of the design objective. Within the context of multiscale analysis, the optimization objective corresponding to stiffness maximization or compliance minimization can be written in terms of  $\rho(\psi)$ 

$$\begin{array}{ll}
\min_{\substack{\rho(\psi)\\s.t.:} & \mathbf{R}(\mathbf{u}, \boldsymbol{\rho}(\psi)) = \mathbf{0}\\ & V(\boldsymbol{\rho}(\psi)) = \sum_{e=1}^{N} \rho_e = V_{req}\\ & \rho_e = 0 \text{ or } \mathbf{1}, \forall e = 1, \dots, N, \end{array}$$
(3)

where  $\rho = (\rho_1, ..., \rho_N)$  is the vector of the element pseudo-densities. In the following, we will denote  $\rho(\psi)$  by  $\rho$  to alleviate the notation. The objective  $c(\rho(\psi))$  is twice of the strain energy. The macroscopic structural stiffness is maximized in terms of minimizing the global strain energy.  $V(\rho)$  is the total number of solid elements and  $V_{req}$  is the required number of solid elements. **u** is the final converged displacement solution. **R**(**u**,  $\rho$ ) stands for the force residual at the macroscopic scale

$$\mathbf{R}(\mathbf{u},\boldsymbol{\rho}) = \mathbf{f}_{ext} - \sum_{e=1}^{N} \int_{\Omega_e} \mathbf{B}^T \boldsymbol{\rho}_e \left\langle \boldsymbol{\sigma}(\mathbf{x},\mathbf{y}) \right\rangle \mathrm{d}\Omega_e.$$
(4)

An augmented Lagrangian method is applied to convert the original constrained optimization problem Eq. (3) into an unconstrained problem as presented in [Belytschko et al. (2003)].

#### **Bi-level reduced surrogate model**

A bi-level reduced surrogate model is constructed coupling the POD and Diffuse Approximation procedures. The first level of reduction is achieved by Proper Orthogonal Decomposition (POD), allowing to expand a displacement field as a linear combination of the truncated modes. Secondly, the surrogate model based on Diffuse Approximation is built to express the POD projection coefficients as functions of the average micro strain tensors.

#### Proper Orthogonal Decomposition of RVE displacement field

We consider a *D*-dimensional (D = 2 or 3) RVE of *N* points subjected to a time-dependent loading  $\mathbf{E}(t) = \langle \boldsymbol{\varepsilon} \rangle(t)$  during a time interval I = [0, T] discretized by *M* instants  $\{t_1, t_2, \dots, t_M\}$ . Let  $\mathbf{u}_i \in \mathbb{R}^{DN}$  denote the *DN* -dimensional nodal displacement vector recorded at the instant  $t_i$ . The reduced order displacement vector  $\mathbf{u}^R(t) \in \mathbb{R}^{DN}$  may be written

$$\mathbf{u}^{R}(t) = \mathbf{u}_{0} + \sum_{i=1}^{m} \phi_{i} \alpha_{i} (\langle \boldsymbol{\varepsilon} \rangle(t)), \qquad (5)$$

where  $m \ll \min(M, DN)$ ,  $\mathbf{u}_0 = 1/M \sum_{i=1}^M \mathbf{u}_i \ \phi_i \in \mathbb{R}^{DN}$  are constant vectors and coefficients  $\alpha_i(\langle \boldsymbol{\varepsilon} \rangle(t))$  are scalar functions of pseudo-time *t*.  $\phi_i$  are the eigenvectors of the eigenvalue problem

$$\mathbf{C}_{u}\phi_{i}=\lambda_{i}\phi_{i},\tag{6}$$

where  $\mathbf{C}_{u}$  is the covariance matrix

$$\mathbf{C}_{u} = \sum_{i=1}^{M} (\mathbf{u}_{i} - \mathbf{u}_{0}) (\mathbf{u}_{i} - \mathbf{u}_{0})^{T}$$
(7)

The size of the truncated basis *m* is chosen in consideration of the projection error  $\epsilon$  induced by the POD procedure

$$\epsilon = 1 - \frac{\sum_{i=1}^{m} \lambda_i}{\sum_{j=1}^{M} \lambda_j} < \delta,$$
(8)

where  $\delta$  is a prescribed tolerance.

## Diffuse Approximation of the projection coefficients

The surrogate model of the projection coefficients  $\alpha_i$ , i = 1, ..., m, with respect to average stain  $\langle \varepsilon \rangle$  in Eq. (15) is constructed using the method of Diffuse Approximation

$$\widetilde{\alpha}(\langle \boldsymbol{\varepsilon} \rangle) = \mathbf{p}^T \mathbf{a},\tag{9}$$

where  $\mathbf{p} = [p_1, p_2, ...]^T$  is the polynomial basis vector. In 2D case, the polynomial basis vector expressed in terms of the average strain in 2D case is

$$\mathbf{p} = \left[1, \left\langle \mathcal{E} \right\rangle_{11}, \left\langle \mathcal{E} \right\rangle_{22}, \left\langle \mathcal{E} \right\rangle_{12}, \ldots\right]^T, \tag{10}$$



Figure 3. Illustration of the approximation procedure of the surrogate model.

The vector of coefficients  $\mathbf{a} = [a_1, a_2, ...]^T$  are the minimizers of functional defined by

$$J(\mathbf{a}) = \frac{1}{2} \sum_{k=1}^{M} w_k (\mathbf{p}^T \mathbf{a} - \alpha(\langle \boldsymbol{\varepsilon} \rangle_k))^2, \qquad (11)$$

in which  $w_k$  are the weights of Euclidean distance defined following [Breitkopf et al. (2004)].

### Bi-level reduced model

An illustrative flowchart of the approximation procedure is given in Fig. 3. With a given admissible value of average micro strain  $\langle \varepsilon \rangle^*$ , the corresponding approximated POD projection coefficients from  $\alpha_1$  to  $\alpha_m$  are locally interpolated using Diffuse Approximation. Thereafter, we have the reduced order solution of the displacement filed

$$\mathbf{u}^{R} = \mathbf{u}_{0} + \mathbf{\Phi} \alpha \left( \langle \boldsymbol{\varepsilon} \rangle^{*} \right), \tag{14}$$

where  $\Phi = \{\phi_1, \dots, \phi_m\}$  is the reduced basis obtained through POD of RVE displacement fields.

The surrogate model is applied to replace full FEA in microscopic analysis. Computations during the first time step of the first optimization iteration are performed using full FEA to initialize the surrogate model. The surrogate model is then used to replace full FEA in solving the micro problem in the following computations when there are enough neighboring points to perform the approximation. When there is no enough points within the local influence zone, the micro problem is solved using full FEA and the results are used to update the POD basis  $\Phi$  and enrich the surrogate.

### Numerical example

The benchmark cantilever problem is considered with anisotropic material defined at microscopic scale. As illustrated in Fig. 4, the macroscopic structure is discretized into  $32 \times 20$  four-node plane strain elements where each element has four Gauss integration points. Each Gauss point in the macroscopic structure corresponds to a considered RVE in the microscopic scale. The material property of the solid phase in the RVE is assumed to be isotropic with a nonlinear elastic constitutive behavior as shown in Fig. 4. Conventional unreduced FE<sup>2</sup> approach requires  $32 \times 20 \times 4$  independent RVE analysis in the microscopic scale for one time evaluation at the macroscopic scale. For the sake of simplicity, the initial elastic stiffness matrix have been kept during the Newton-Raphson iterative resolution procedure. In order to perform sensitivity analysis, tangent stiffness matrix is evaluated using the perturbation method at the converged moment of each design iteration.



Figure 4. Illustration of the test example.



Figure 5. Resultant tractions of the first 7 POD modes after the optimization.

The external loading force is set to 1.5 N and the considered volume ratio constraint is set to 32%. The tolerance error in Eq. (8) is set as in the previous case of  $\delta = 10^{-6}$ . The extracted POD modes vary adaptively during the optimization procedure and the size of the reduced basis is 6 after the first iterations and then increase to 7 during the following iterations until the end. The resultant tractions of the first 7 of the final POD modes are shown in Fig. 5 together with their associated normalized eigenvalues.

The structural topological evolution in the macroscopic scale is given in Fig. 6. The convergence histories of the strain energy and the volume ratio are demonstrated in Figs. 7(a) and (b), respectively. During the loading phase of the first optimization iteration, the periodic homogenizations of the RVE in the microscopic scale are performed using full FEA. Since the second optimization iteration, both FEA and the surrogate model are used for the microscopic analysis. Fig. 7(c) gives the percentage of FEA usage in each optimization iteration. It can be seen that less than 4% microscopic analysis require full FEA except a jump from 2% in iteration 20 to 17% in iteration 21. It can be seen that a branch of the structure splits in iteration 21. Such a severe topological variation results in a large variation of the structural physical response and hence the surrogate built according to the previous calculations is no longer accurate enough. Therefore, an increased number of full FEA is required to recompute the set of the reduced basis. The surrogate model is updated thereafter and the usage ratio of FEA drops back below 4% and decreases to 0% in the following iterations as the structural topology converges, meaning that all computations are performed with the surrogate.



Figure 6. Structural topology variations during the optimization process.



Figure 7. Optimization history: (a) convergence history of the strain energy, (b) convergence history of the volume ratio, (c) the ratio of FEA usage in each iteration.

The same optimization design has also been performed without using the surrogate. The unreduced  $FE^2$  approach gives an exactly the same optimization design result as the reduced model where the relative errors of the objective are less than  $10^{-5}$ . Generally speaking, it requires around two hours of computing for each optimization iteration on a HP Z420 Workstation when using the unreduced sequential  $FE^2$ . In contrast, the reduced  $FE^2$  approach requires only ten minutes of computing on average for each design iteration apart from the first design iteration. More saving in computation can be expected using the reduced approach when larger scale problems are considered.

Fig. 8 depicts the equivalent strain distributions in the microscopic scale at selected points where the nodal displacements are scaled 20 times for the purpose of illustration. One may note that the existence of the holes in the RVE concentrates much higher strains and hence stresses in the microscopic scale than the homogenized macroscopic values. The micro strain distributions clearly manifest the difference of the loading status in different structural branches. The micro strain distributions at points b and c are quite similar because they are located in the same branch of the structure. The higher stress concentration may lead to the initial material failure or crack at the micro scale which cannot be detected when using the conventional one scale fracture analysis.

## Conclusions

In this work, we have proposed a reduced multiscale model for macroscopic structural design considering microscopic material nonlinear microstructures. Several established techniques have been applied: the structural design is realized using a discrete level-set topology optimization model, the multiscale analysis is performed using the  $FE^2$  approach, and the surrogate model is constructed

using POD and Diffuse Approximation. The surrogate model is constructed in an on-line manner: initially built during the first optimization design iteration is then updated in the following design iterations. It has been observed that the surrogate model can significantly reduce the computational cost, particularly when multiple loops involving similar computations are required. Further improvement of the proposed model could be the employment of the advanced models of any of the applied techniques, such as considering nucleation in level-set topology optimization in order to avoid an artificially defined initial topology, considering the size effect in multiscale analysis, and other possible strategies to perform model reduction either in an intrusive manner or non-intrusive manner using different approaches to construct the surrogate.



Figure 8. Equivalent strain distribution at selected points.

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#### References

- Belytschko T., Xiao S., Parimi C. (2003), Topology optimization with implicit functions and regularization, *International Journal for Numerical Methods in Engineering* **57** 1177–1196.
- Challis V. J. (2010), A discrete level-set topology optimization code written in matlab, *Structural and Multidisciplinary Optimization* **41** 453–464.
- Feyel F. and Chaboche J. (2000) FE<sup>2</sup> multiscale approach for modelling the elastoviscoplastic behaviour of long fibre sic/ti composite materials, *Computer Methods in Applied Mechanics and Engineering* **183** 309–330.
- Kouznetsova V., Brekelmans W. A. M., Baaijens F. P. T. (2001), An approach to micro-macro modeling of heterogeneous materials, *Computational Mechanics* 27 37-48.
- Lancaster P., Salkauskas K. (1981), Surfaces generated by moving least squares methods, *Mathematics of Computation* **87** 141–158.
- Nayroles B., Touzot G., Villon P. (1992), Generalizing the finite element method: Diffuse approximation and diffuse elements, *Computational Mechanics* **10** 307–318.
- Breitkopf P., Rassineux A., Savignat J. M., Villon P. (2004), Integration constraint in diffuse element method, *Computer Methods in Applied Mechanics and Engineering* **193** 1203–1220.
- Yvonnet J., He Q. C. (2007), The reduced model multiscale method (r3m) for the non-linear homogenization of hyperelastic media at finite strains, *Journal of Computational Physics* **223** 341–368.