## Fictitious Domain with Least-Squares Spectral Element Method to Explore Geometric Uncertainties by Non-Intrusive Polynomial Chaos Method

L. Parussini $^1$  and V. Pediroda $^2$ 

Abstract: In this paper the Non-Intrusive Polynomial Chaos Method coupled to a Fictitious Domain approach has been applied to one- and twodimensional elliptic problems with geometric uncertainties, in order to demonstrate the accuracy and convergence of the methodology. The main advantage of non-intrusive formulation is that existing deterministic solvers can be used. A new Least-Squares Spectral Element method has been employed for the analysis of deterministic differential problems obtained by Non-Intrusive Polynomial Chaos. This algorithm employs a Fictitious Domain approach and for this reason its main advantage lies in the fact that only a Cartesian mesh needs to be generated. Excellent accuracy properties of method are demonstrated by numerical experiments.

**Keyword:** Non-Intrusive Polynomial Chaos, Fictitious Domain, Lagrange multipliers, Least-Squares Spectral Element Method.

## 1 Introduction

There is an increasing interest in uncertainty analysis applied to computational physics, since the influence of inherent physical and geometric uncertain parameters can no longer be neglected. In fact in order to obtain reliable results, uncertainty quantification is necessary.

Recent research effort has been focusing on developing methods for uncertainty quantification, which can be divided into two categories: nonintrusive, or statistical, (as Monte Carlo [Blith and Pozrikidis (2003)], Stochastic Collocation [Mathelin and Hussaini (2003)], Chaos Collocation [Loeven, Witteveen, and Bijl (2006)]) and intrusive, or non-statistical (as Chaos Polynomials [Xiu and Karniadakis (2003b); Xiu and Tartakovsky (2006)]).

Usually the topology of domain boundaries are described in deterministic terms, without taking in account of their stochastic nature, whereas the effort is focused on exploring random material properties or random boundary conditions (Fig. 1). In literature there are several examples of numerical methods to face such kind of problems. In [Xiu and Karniadakis (2002); Xiu and Karniadakis (2003b); Xiu and Karniadakis (2003a); Wan and Karniadakis (2006); Loeven, Witteveen, and Bijl (2007)] we find applications of these methodologies to thermo-fluid dynamics.

In this work we consider a different problem: we want to solve deterministic problems on random domains (Fig. 2), with geometric uncertainty given by shape tolerance. Actually there are really few examples of numerical methods for geometric uncertainty.

In [Lin, Su, and Karniadakis (2006); Xiu and Tar-



Figure 1: Differential problem with stochastic material properties and random boundary conditions, where  $\theta$  is uncertainty.

<sup>&</sup>lt;sup>1</sup> Researcher, Mechanical Engineering Department, University of Trieste, Trieste, ITALY.

<sup>&</sup>lt;sup>2</sup> Assistant Professor, Mechanical Engineering Department, University of Trieste, Trieste, ITALY.



Figure 2: Differential problem with stochastic definition domain, where  $\theta$  is uncertainty.

takovsky (2006)], geometric uncertainty pertains to roughness, which is an important thermo-fluid dynamic parameter. In particular [Lin, Su, and Karniadakis (2006)] presents an analytical model to study the roughness in supersonic flow and the analytical results are compared with several Polynomial Chaos methodologies, such as mapping, Stochastic Collocation and Sparse Grid. In [Xiu and Tartakovsky (2006)] the fluid dynamics in rough channels is studied using a mapping methodology. The obtained results confirm Chaos methods are suitable to study geometry uncertainty given roughness.

Another interesting point is the study of shape tolerance and its interaction with the state problem (thermal, fluid dynamic, thermo-fluid dynamic). In [Hosder, Walters, and Perez (2006)] the influence of geometric tolerance on fluid dynamic field is shown, referring to an angle. A Chaos methodology is used to explore the random domain, in particular a non-intrusive approach. In [Canuto and Kozubek (2007)] a method is presented for the numerical realization of elliptic PDEs in domains depending on random variables, where the key feature is the combination of a Fictitious Domain approach and a Polynomial Chaos expansion. A (generalized) Wiener expansion is invoked to convert such a stochastic problem into a deterministic one. Discretization is accomplished by standard mixed finite elements in the physical variables and a Galerkin projection method with numerical integration in the stochastic variables.

In this work we present a method to face geomet-

ric tolerance problems, which allows to avoid the limitations of previous referred methodologies, in particular both the difficulty of mapping space variables into a deterministic domain and the need to remesh the geometry of domain. Our method is similar to [Canuto and Kozubek (2007)], but with a non-intrusive approach for solving stochastic problem.

Pursuing this purpose, we present a new method based on the coupling of a Non-Intrusive Polynomial Chaos method and a Fictitious Domain approach. According to Polynomial Chaos theory, a stochastic process can be expressed as a spectral expansion based on suitable orthogonal polynomial with weights associated with a particular density. For non-intrusive approach, a Collocation projection is applied in the random dimension and the resulting system of deterministic equations is then solved to obtain the solution for each random node of nodal approximation. The important advantage of using a non-intrusive method is there is no need to modify the solver of deterministic equations, simplifying the management of computational process.

To solve the deterministic problem Least Squares Spectral Element Method is used [Pontaza and Reddy (2003); Pontaza and Reddy (2004); Pontaza (2007); Proot and Gerritsma (2002); Proot and Gerritsma (2005); Gerritsma and Maerschalck (2006)]. Moreover a Fictitious Domain approach is adopted, introducing more benefits to methodology.

Fictitious Domain methods allow problems formulated on an intricate domain  $\Omega$  to be solved on a simpler domain  $\Pi$  containing  $\Omega$ . The extension of original problem to fictitious region  $\Pi/\Omega$  must be chosen so that the solution of extended problem restricted to  $\Omega$  coincides with the solution of original problem. There are several approaches to implement Fictitious Domain: Elimination method [Zienkiewicz and Taylor (2000)], Penalty method [Zienkiewicz and Taylor (2000); Ramiere, Angot, and Belliard (2005)], Distributed Lagrangian method [Haslinger, Maitre, and Tomas (2001); Glowinski, Pan, Hesla, and Joseph (1999); Glowinski, Pan, Hesla, Joseph, and Periaux (2000)], Boundary

Lagrangian method [Stenberg (1995); Joly and Rhaouti (1999)], Fat Boundary method [Maury (2001)]. A technique which is popular, given its efficiency, is to enforce the boundary conditions by Lagrange multipliers, which is the method we propose in this paper.

The main motivation for Fictitious Domain approach is that, defining the extended problem on a simple domain, enables the use of efficient discretization methods on simple structured grids. In this way the solution of state problem is independent by small variations of domain  $\Omega$  subject to uncertainty and contained into computational domain  $\Pi$ , which is independent by random geometric parameters. Thereby an evident further advantage of the method is that remeshing of computational domain for each random node solution has no more to be performed.

The excellent accuracy of proposed methodology, Non-Intrusive Polynomial Chaos method and Fictitious Domain with Least-Squares Spectral Element approximation, is demonstrated by numerical experiments.

The paper is organized as follows. In Section 2 some details are given about uncertainty quantification methods. In Section 3 the effectiveness of Non-Intrusive Chaos Polynomial approach to solve problems with geometric tolerance is demonstrated, comparing it to the analytic solution and Monte Carlo method. In Section 4 the Fictitious Domain approach is illustrated and good accuracy properties of the method are demonstrated by numerical experiments. In Section 5 the formulation of Non-Intrusive Polynomial Chaos Method with Fictitious Domain approach is explained and in Section 6 some numerical examples to validate the Non-Intrusive Polynomial Chaos Method with Fictitious Domain approach are shown. In Section 7 we give some concluding remarks.

#### 2 Uncertainty quantification methods

## 2.1 Setting of the problem: stochastic differential equation

In this section the Non-Intrusive Generalized Polynomial Chaos is explained in order to solve the following stochastic differential equation:

$$L(\mathbf{x}, t, \theta; \phi) = f(\mathbf{x}, t, \theta)$$
(1)

where *L* is a differential operator which contains space and time differentiation and can be non linear and depended on random parameters  $\theta$ ;  $\phi(\mathbf{x}, t, \theta)$  is the solution and function of the space  $\mathbf{x} \in \Re^d$ , time *t* and random parameters  $\theta$ ;  $f(\mathbf{x}, t, \theta)$  is a space, time and random parameters dependent source term.

## 2.2 The Generalized Polynomial Chaos

Under specific conditions [Schoutens (2000)], a stochastic process can be expressed as a spectral expansion based on suitable orthogonal polynomial with weights associated with a particular density. The first study in this field is the Wiener process [Wiener (1938); Wiener (1958)], which can be written as a spectral expansion in terms of Hermite polynomials with normal distributed input parameters.

The basic idea is to project the variables of the problem onto a stochastic space spanned by a set of complete orthogonal polynomials  $\Psi$  that are functions of random variables  $\xi(\theta)$ , where  $\theta$  is a random event. For example, the variable  $\phi$  has the following spectral finite dimensional representation:

$$\phi(\mathbf{x},t,\theta) = \sum_{i=0}^{\infty} \phi_i(\mathbf{x},t) \Psi_i(\xi(\theta))$$
(2)

In practical terms the Eq. 2 divides the random variable  $\phi(\mathbf{x}, t, \theta)$  into a deterministic part, the coefficient  $\phi_i(\mathbf{x},t)$  and a stochastic part, the polynomial chaos  $\Psi_i(\xi(\theta))$ . The basis  $\{\Psi_i\}$  is a set of orthogonal polynomials with respect to the probability density function of the input parameters. Following the Askey scheme [Askey and Wilson (1985)], it is possible to introduce the Generalized Polynomial Chaos [Xiu and Karniadakis (2003a)]. Thanks to this theory, known also as Askey-chaos, for certain input parameter distribution there exists the best representation in terms of convergence rate. For example, for Gaussian random input, we have the Hermite Polynomial Chaos representation, for Gamma distribution the Laguerre representation, for Beta distribution the

Jacoby representation, for Uniform distribution the Legendre representation, etc.

In this paper we focus mainly on the Gaussian random input, so we represent the variable  $\phi(\mathbf{x}, t, \theta)$  in terms of Hermite (see Appendix A: Hermite Polynomials) spectral representation, following the Askey scheme:

$$\phi(\mathbf{x},t,\theta) = \phi_0(\mathbf{x},t)H_0 + \sum_{i_1=1}^{\infty} \phi_{i_1}(\mathbf{x},t)H_1(\xi_{i_1}(\theta)) + \sum_{i_1=1}^{\infty} \sum_{i_2=1}^{i_1} \phi_{i_1i_2}(\mathbf{x},t)H_2(\xi_{i_1}(\theta),\xi_{i_2}(\theta)) + \sum_{i_1=1i_2=1}^{\infty} \sum_{i_3=1}^{i_2} \phi_{i_1i_2i_3}(\mathbf{x},t)H_3(\xi_{i_1}(\theta),\xi_{i_2}(\theta),\xi_{i_3}(\theta)) + \dots$$
(3)

where  $H_p(\xi_{i_1},...,\xi_{i_p})$  is the Hermite polynomial of order p in terms of a *n*-dimensional Gaussian random variable  $\xi = (\xi_1,...,\xi_n)$  distributed as N(0,1). The Hermite polynomial is expressed in general form by:

$$H_p\left(\xi_{i_1},\ldots,\xi_{i_p}\right) = e^{\frac{1}{2}\xi^T\xi} \left(-1\right)^p \frac{\partial^p}{\partial\xi_{i_1}\ldots\partial\xi_{i_p}} e^{\frac{1}{2}\xi^T\xi}$$
(4)

and for one-dimensional case:

$$H_0 = 1, H_1 = \xi, H_2 = \xi^2 - 1, H_3 = \xi^3 - 3\xi, \dots$$
(5)

For practical cases, the series has to be truncated to a finite numbers of terms, here denoted with *N*. So the form Eq. 2, using the one-to-one correspondence between the function  $H_p(\xi_{i_1}, \ldots, \xi_{i_p})$ and  $\Psi_p(\xi)$ , as demonstrated in [Xiu and Karniadakis (2002)] for Gaussian random input, becomes:

$$\phi(\mathbf{x},t,\theta) = \sum_{i=0}^{N} \phi_i(\mathbf{x},t) H_i(\xi)$$
(6)

The number of total terms of the series is determined by:

$$N+1 = \frac{(n+p)!}{n!p!}$$
(7)

where n is the uncertainties dimensionality and p is the order of the expansion.

As an example, for a second order twodimensional Hermite polynomial expression, we get the following form:

$$\phi(\mathbf{x},t,\theta) = \phi_0(\mathbf{x},t) + \phi_1(\mathbf{x},t)\xi_1(\theta) + \phi_2(\mathbf{x},t)\xi_2(\theta) + \phi_3(\mathbf{x},t) \left(\xi_1^2(\theta) - 1\right) + \phi_4(\mathbf{x},t) \left(\xi_2^2(\theta) - 1\right) + \phi_5(\mathbf{x},t)\xi_1(\theta)\xi_2(\theta)$$
(8)

where  $\xi_1(\theta)$  and  $\xi_2(\theta)$  are the two random independent variables.

## 2.3 Intrusive and Non-Intrusive Polynomial Chaos

Substituting the Polynomial Chaos series, given in Eq. 6 for Gaussian random input, into the stochastic differential Eq. 1 we obtain:

$$L\left(\mathbf{x},t,\theta;\sum_{i=0}^{N}\phi_{i}(\mathbf{x},t)\Psi_{i}(\boldsymbol{\xi}(\theta))\right) \cong f(\mathbf{x},t,\theta) \quad (9)$$

The method of Weighted Residuals is adopted to solve this equation. The coefficients  $\phi_i(\mathbf{x}, t)$  are obtained imposing the inner product of the residual with respect to a weight function is equal to zero.

If the weight functions are chosen to be the same as the expansion functions  $\Psi_i$  we produce Galerkin method. Performing the Galerkin projection on both sides of the equation, the form becomes:

$$\left\langle L\left(\mathbf{x},t,\boldsymbol{\theta};\sum_{i=0}^{N}\phi_{i}(\mathbf{x},t)\Psi_{i}\right),\Psi_{j}\right\rangle =\left\langle f(\mathbf{x},t,\boldsymbol{\theta}),\Psi_{j}\right\rangle$$
(10)

where j = 0, ..., N. If the operator *L* is non linear, the deterministic set of N + 1 equation is coupled and this form is called *Intrusive Chaos Polynomial*.

If we employ Dirac delta function as weight function we produce Collocation method. Using a collocation projection on both sides of Eq. 9, we obtain:

$$L(\mathbf{x},t,\boldsymbol{\theta}_j;\boldsymbol{\phi}) = f(\mathbf{x},t,\boldsymbol{\theta}_j) \quad j = 0,\dots,N.$$
(11)

This formulation is a linear system equivalent to solving a deterministic problem at each grid point; this form is called *Non-Intrusive Chaos Polynomial*.

To reconstruct the stochastic solution  $\phi(\mathbf{x}, t, \theta)$ , the Eq. 2 is used:

$$E_{PC}(\phi) = \mu_{\phi} = \phi_0(\mathbf{x}, t, \theta) \tag{12}$$

$$Var_{PC}(\phi) = \sigma_{\phi}^{2} = \sum_{i=1}^{N} \left[ \phi_{i}^{2}(\mathbf{x}, t, \theta) \left\langle \Psi_{i}^{2} \right\rangle \right].$$
(13)

Here

where  $\delta_{ij}$  is the Kroneker operator.

The two approaches are based on the same theory, but gives different numerical representations. In practice intrusive method consists in resolution of a coupled system of deterministic equations, non-intrusive method consists in resolution of a decoupled system of deterministic equations. It is evident the difficulty to design an efficient intrusive solver, both because of computational cost and because of the obvious handicap to imply an internal modification of the deterministic solver [Lin, Wan, Su, and Karniadakis (2007)]. The non-intrusive methodology has a simpler computational management. A remarkable advantage of this approach is the deterministic solver represents a black-box and there is no need to modify it. This means the non-intrusive method is more versatile than intrusive method.

A still open problem of non-intrusive approach [Loeven, Witteveen, and Bijl (2007)] is the difficulty to select collocation points: with multi dimensional uncertainties the choice is not unique [Hosder, Walters, and Perez (2006)]. This problem does not exist for one stochastic parameter, because collocation points are the roots of polynomial of order p + 1.

In this paper we focus on geometric tolerances using Fictitious Domain approach and Non-Intrusive Polynomial Chaos method. As the goal is a better comprehension of the problem, for sake of simplicity we will just consider one uncertain parameter with Gaussian distribution using Hermite polynomials for expansion. In this way we avoid the difficulty of arbitrary choice of collocation points for Non-Intrusive Polynomial Chaos method.

#### **3** Geometric uncertainties

The uncertainty we want to examine is due to geometric tolerance. In this case the geometry of definition domain is a stochastic phenomenon. The problem under study, as defined in [Xiu and Tartakovsky (2006)], writes:

Let  $\theta \in \Theta$  be a random realization drawn from a complete probability space  $(\Theta, A, P)$ , whose event space  $\Theta$  generates its  $\sigma$ -algebra  $A \subset 2^{\Theta}$  and is characterized by a probability measure P. For all  $\theta \in \Theta$ , let  $\Omega(\theta) \subset \Re^d$  be a *d*-dimensional random domain bounded by boundary  $\partial \Omega(\theta)$ . We consider the following stochastic boundary value problem: for *P*-almost everywhere in  $\Theta$ , given  $f: \Omega(\theta) \to \Re$  and  $g: \partial \Omega(\theta) \to \Re$ , find a stochastic solution  $v: \overline{\Omega}(\theta) \to \Re$  such that:

$$A(\mathbf{x}; v) = f(\mathbf{x}) \qquad \text{in } \Omega(\theta) \qquad (15)$$

$$B(\mathbf{x}; v) = g(\mathbf{x})$$
 on  $\partial \Omega(\theta)$  (16)

where  $\mathbf{x} = (x_1, \dots, x_d)$ , *A* is a differential operator and *B* is a boundary operator.

Except for a few studies, random domain problems have not been systematically analyzed. The most complete work on these topics is presented in [Xiu and Tartakovsky (2006)], where a mapping methodology is introduced to transform the original problem defined in a random domain into a stochastic problem defined in a deterministic domain. In particular a one-to-one mapping function and its inverse are established:  $\xi = \xi(\mathbf{x}, \theta)$ ,  $\mathbf{x} = \mathbf{x}(\xi, \theta)$ , which transforms the random domain  $\Omega(\theta) \subset \Re^d$  into a deterministic domain  $\omega \subset \Re^d$ , whose coordinates are denoted as  $\xi =$  $(\xi_1, \dots, \xi_d)$ . I.e., for *P*-almost everywhere  $\theta \in \Theta$ ,  $\mathbf{x} \in \Omega(\theta) \leftrightarrow \xi \in \omega$ .

The stochastic mapping transforms the deterministic differential operators A and B into their stochastic counterparts  $\mathscr{A}$  and  $\mathscr{B}$ , respectively, and the random domain problem into the following stochastic boundary-value problem. For  $\mathscr{P}$ almost everywhere  $\theta \in \Theta$ , given  $\mathscr{F} : \omega \times \Theta \to \Re$ and  $\mathscr{G} : \partial \omega \times \Theta \to \Re$ , find a stochastic solution  $u : \overline{\omega} \times \Theta \to \Re$  such that

$$\mathscr{A}(\boldsymbol{\xi}, \boldsymbol{\theta}; \boldsymbol{u}) = \mathscr{F}(\boldsymbol{\xi}, \boldsymbol{\theta}) \quad \text{in } \boldsymbol{\omega} \quad (17)$$

$$\mathscr{B}(\xi, \theta; u) = \mathscr{G}(\xi, \theta)$$
 on  $\partial \omega$  (18)

where  $\mathscr{F}$  and  $\mathscr{G}$  are the transformed functions of f and g, respectively.

Let us consider this problem as example:

$$\frac{d^2\phi}{dx^2} + k\phi = 0 \quad \text{in } [0, L]$$
  
with  $\left. \frac{d\phi}{dx} \right|_{x=0} = q_0 \quad \text{and} \quad \left. \frac{d\phi}{dx} \right|_{x=L} = k\phi(L)$   
(19)  
 $k = -10^{-5}, \quad q_0 = 0.001, \quad L = N(100, 1),$ 

Eq. 19 is a stochastic domain problem where the length L of domain has a normal distribution with mean equal to 100 and variance equal to 1.

In Fig. 3 is shown the mapping presented in [Xiu and Tartakovsky (2006)], referred to problem Eq. 19.

The stochastic mapping of  $\Omega(\theta) = [0, L]$  onto  $\omega = [0, 1]$  is constructed via solution of Laplace



Figure 3: Mapping technique presented in [Xiu and Tartakovsky (2006)], referred to problem Eq. 19.

equations:

$$\frac{\partial^2 x}{\partial \xi^2} = 0 \quad \text{in } \omega$$
  

$$x(0) = 0 \qquad (20)$$
  

$$x(1) = L.$$

The new stochastic problem defined on a deterministic domain, thanks to this mapping, can be solved by already existing Polynomial Chaos techniques.

The methodology illustrated above has been efficiently implemented to solve two diffusion problems: in a channel with rough surface and in double-connected domains with rough exclusion. The Polynomial Chaos methodology is demonstrated to be more accurate than Monte Carlo method and with lower computational cost. The drawback of the presented method is the difficulty of mapping. In fact this process is simple for connected domains, but it is computationally challenging for complex non-connected domains.

To ride over this problem, the mapping of complex domains, in this work we present the coupling of Fictitious Domain approach with Non-Intrusive Polynomial Chaos for geometric uncertainties. The idea is to avoid the mapping of stochastic domain onto a deterministic domain and to use absolute coordinates. In Fig. 4 is shown how this works.

Geometric uncertainty, represented by probabilistic distribution P(L) of domain length L, becomes an uncertainty on the position of boundary condition. Therefore there is no need of mapping the stochastic domain onto a deterministic domain, as every point of domain is studied in absolute coordinates. The solution of the problem has a probability distribution  $pdf(\phi)$  associated to each point of domain in absolute coordinates. This probability distribution of the solution depends on the position of boundary condition in x = L, which is a stochastic phenomenon. In Fig. 4 it is show the probability P(x) of a point of belonging to domain, which depends on the probabilistic distribution of L in problem Eq. 19.

Referring to definition of Non-Intrusive Polynomial Chaos given in Eq. 11 for solving problem



Figure 4: Stochastic domain problem Eq.(19) in absolute coordinates with normal distribution of length L.

defined in Eq. 19, we have to solve N distinct deterministic problems defined on different lengths of domain.

#### 3.1 Numerical example

To validate the proposed methodology, we consider problem given in Eq. 19. The analytic solution of this problem, if the length L of domain is a deterministic variable, writes as:

$$\phi(x) = \frac{\phi_0}{\sqrt{k}} \frac{\left(1 + \sqrt{k}\right) e^{\sqrt{kL}} e^{-\sqrt{kx}} + \left(1 - \sqrt{k}\right) e^{-\sqrt{kL}} e^{\sqrt{kx}}}{\left(1 + \sqrt{k}\right) e^{\sqrt{kL}} - \left(1 - \sqrt{k}\right) e^{-\sqrt{kL}}}$$

$$(21)$$

As we know the analytic function, we can compare the proposed methodology with the analytic distribution. Given the uncertainty on the length *L*, to compute  $pdf(\phi)$  we can use the formulation [Rotondi, Pedroni, and Pievatolo (2001)]:

Z = f(X) *X* random variable with  $p_X(x)$  (22)  $p_Z(z) = \frac{p_X(x_1)}{|f'(x_1)|} + \frac{p_X(x_2)}{|f'(x_2)|} + \dots + \frac{p_X(x_n)}{|f'(x_n)|}$  where x is the random variable (with distribution  $p_X(x)$ ), Z is the random output variable, and  $x_1, \ldots, x_n$  are the inverse of  $Z(x = f^{-1}(z))$ .

We have compared Polynomial Chaos and Monte Carlo method, too. In fact Monte Carlo is the methodology mainly used for uncertainties, as shown in [Xiu and Karniadakis (2003a); Xiu and Tartakovsky (2006)].

In Fig. 5 the mean and standard deviation of problem given in Eq. 19 are shown, comparing the Polynomial Chaos methodology and two Monte Carlo examples (with 250,000 and 1,000,000 points). Monte Carlo method is accurate to compute mean value, in fact the plots of expected value can not be distinguished, but to get accurate values of standard deviation the number of simulations has to be high (till  $10^6$ ). Increasing the number of simulations we obtain stability and the results become closer to that obtained by Polynomial Chaos.

Let us notice that, for one-dimensional random space, if the polynomial has order P, Polynomial Chaos needs of P + 1 deterministic simulations, equal in number to roots of one order higher polynomial. In Fig. 5 the case with polynomial order equal to 3 is shown. It has been verified that increasing the order further on P = 3 there is not a remarkable improvement of accuracy. This observation means that with only 4 deterministic simulations we can get a really accurate result, in general better than that one obtained by Monte Carlo method with a considerable higher number of simulations.

A better comparison between Polynomial Chaos and Monte Carlo methods can be performed referring to probability density function  $pdf(\phi)$  in three different points of domain,  $x_1 = 0.0$ ,  $x_2 =$ 45.0,  $x_3 = 90.0$ .

In this case we can represent analytically  $pdf(\phi)$ , using Eq. 22, and we can get the errors of Monte Carlo (pt = 1,000,000) and Polynomial Chaos (P = 3) referring to analytical  $pdf(\phi)$ . In Fig. 6, Fig. 7 and Fig. 8 it is evident there is a different magnitude order of errors. The Polynomial Chaos solution has a lower error than Monte Carlo method. A substantive difference of com-



Figure 5: Mean and standard deviation of problem given in Eq. 19, comparing the Polynomial Chas methodology and two Monte Carlo examples (with 250,000 and 1,000,000 points).



Figure 7: Solution of problem given in Eq. 19: analytical  $pdf(\phi)$  and comparison of error respect to analytical  $pdf(\phi)$  of Non-Intrusive Polynomial Chaos and Monte Carlo  $pdf(\phi)$  in  $x_2 = 45.0$ .



Figure 6: Solution of problem given in Eq. 19: analytical  $pdf(\phi)$  and comparison of error respect to analytical  $pdf(\phi)$  of Non-Intrusive Polynomial Chaos and Monte Carlo  $pdf(\phi)$  in  $x_1 = 0.0$ .



Figure 8: Solution of problem given in Eq. 19: analytical  $pdf(\phi)$  and comparison of error respect to analytical  $pdf(\phi)$  of Non-Intrusive Polynomial Chaos and Monte Carlo  $pdf(\phi)$  in  $x_3 = 90.0$ .

putational effort has to be remarked, too. We can notice  $pdf(\phi)$  is not completely symmetric, demonstrating the need of using a polynomial order equal to 2 at least. Let us notice Hermite polynomial of order 1 is linear, giving simply a Gaussian representation.

With this example we have demonstrated that the proposed approach, Non-Intrusive Polynomial Chaos without mapping, can be accurate. The drawback of this method is the need to modify the computational domain of every different simulation. So if we can not solve analytically the differential equations, we have to remesh the computational domain for each new simulation. It is evident the difficulty to have an accurate grid for every geometry. To avoid this problem we introduce Fictitious Domain methodology. In this way the stochastic domain does not coincide with the computational domain, which is the same for all simulations. The geometric position of Lagrange multipliers, which enforce the boundary conditions immersed in the computational domain, has just to be modified for the new geometries.

## 4 Fictitious Domain via Lagrange Multipliers with Least-Squares Spectral Element Method

#### 4.1 Fictitious Domain approach

Fictitious domain approach allows to solve easily differential problems defined on domain changing in time and space, i.e. in general structural elastic problems, fluid dynamics problems with moving rigid bodies, shape optimization problems, and so on. This means the same problem is solved on different domains.

In general to front these problems the boundary variation technique is used, based on a sequence of domain (Fig. 9). Using a method based on domain discretization, such as finite element method, spectral elements, finite volumes, after the shape variation the computational domain has to be remeshed, the data of state problem have to be recompute and the update problem has to be solved. It is evident this requires high computing time. Moreover it is difficult to find a partition of domain such that grid quality is good for every domain.

In this case it is useful to consider a Fictitious Domain approach (Fig. 10), where the computational domain is not the same of the definition domain of problem, but it contains that one, so when the definition domain changes the computational domain does not change with evident advantages. The need of such kind of tool is confirmed by experience.



Figure 9: Classical approach based on the boundary variation technique to solve differential problems defined on domain changing in time and space.



Figure 10: Fictitious Domain approach to solve differential problems defined on domain changing in time and space.

Several variants of fictitious domain method exist: the basic idea is to extend the operator and the domain into a larger simple shaped domain. The most important ways to do this are algebraic and functional analytic approaches. In algebraic fictitious domain methods the problem is extended typically at algebraic level in such a way that the solution of original problem is obtained directly as a restriction of the solution of extended problem without any additional constraint. There are several variants of such an approach [Rossi and Toivanen (1999); Makinen, Rossi, and Toivanen (2000)] and they can be rather efficient, but typically they are restricted to quite a narrow class of problems.

More flexibility and better efficiency can be obtained by using a functional analytic approach where the use of constraints ensures that the solution of extended problem coincides with the solution of original problem. In our implementation we enforce constraints by Lagrange multipliers [Parussini (2007)].

The physical aspects of the problem can always be stated in a variational principle form. A variational principle specifies a scalar quantity, the functional J, which is defined by an integral form

$$J = \int_{\Omega} F\left(\phi, \frac{\partial \phi}{\partial x}, \frac{\partial \phi}{\partial y}, ..., x, y, ...\right) d\Omega + \int_{\Gamma} E\left(\phi, \frac{\partial \phi}{\partial x}, \frac{\partial \phi}{\partial y}, ..., x, y, ...\right) d\Gamma$$
(23)

in which  $\Gamma = \partial \Omega$ ,  $\phi$  is the unknown function and *F* and *E* are specified operators. The solution to the continuum problem is a function  $\phi$  which make *J* stationary with respect to small changes  $\delta \phi$ ; thus, for a solution to the continuum problem, the variation is  $\delta J = 0$ .

To implement the Fictitious Domain approach we have to extend the operator F and the domain  $\Omega$  into a larger simple shaped domain  $\Pi$  and to constrain the functional on  $\Gamma = \partial \Omega$  (Fig. 11). To treat such problems Lagrangian multipliers are introduced, so that the problem is now equivalent to find the stationary point of J', where

$$J' = \int_{\Pi} F\left(\phi, \frac{\partial\phi}{\partial x}, \frac{\partial\phi}{\partial y}, ..., x, y, ...\right) d\Omega + \int_{\Gamma} \lambda(\mathbf{x}) E\left(\phi, \frac{\partial\phi}{\partial x}, \frac{\partial\phi}{\partial y}, ..., x, y, ...\right) d\Gamma.$$
(24)

Here  $\lambda(\mathbf{x})$  is an undetermined multiplier which is in general a function of position, because the local condition must be satisfied at every point of  $\Gamma$ , rather than being a global restriction.

New approach, we present in this paper, is



Figure 11: Example of a fictitious rectangular domain  $\Pi$  containing the original domain  $\Omega$ .

the coupling of Fictitious Domain together with an high order method. To discretize the problem under study we use the Least Squares Spectral Element Method, based on higher order functions, locally defined over finite size parts of domain. The Least Squares Spectral Element Method (LSQSEM) combines the least squares formulation with a spectral element approximation. This provides several advantages. The method produces symmetric positive definite linear systems for every type of partial differential equation, i.e. elliptic, parabolic and hyperbolic equations. No compatibility requirements need to be imposed between approximating function spaces for mixed problems. The method converges just as fast with hp refinement than conventional Galerkin methods. Furthermore, no stabilization is required for convection dominated flows. Moreover using Fictitious Domain approach, where extended problem is defined on a simple domain, enables the use of efficient computational grids, in our case just simple Cartesian grids.

Good accuracy properties of the method are demonstrated by numerical experiments.

## 4.2 Least Squares variational principle

Let  $\overline{\Omega}$  be the closure of an open bounded region  $\Omega$  in  $\Re^d$ , where *d* represents the number of space

dimensions, and let  $\mathbf{x} = (x_1, ..., x_d)$  be a point in  $\overline{\Omega} = \Omega \bigcup \partial \Omega$ , where  $\partial \Omega = \Gamma$  is the boundary of  $\Omega$ . We consider the model problem stated as follows: Find  $\phi(\mathbf{x})$  such that

 $-\triangle \phi = f \qquad \text{in } \Omega \qquad (25)$ 

 $\phi = \phi^s \qquad \text{on} \quad \Gamma \qquad (26)$ 

where f is the source term and  $\phi^s$  is the prescribed value of  $\phi$  on boundary  $\Gamma$ . This problem is chosen only for notational simplicity; our statements are also valid for every type of deterministic differential problem, i.e. elliptic, parabolic and hyperbolic equations.

Although direct application of the least squares variational principles to Eq. 25 is possible, it will result in an impractical least squares finite element model, as these have associated with them the requirement of higher regularity of the finite element spaces. The degree of necessary smoothness is dictated by the differentiability requirements of the governing equation under consideration. Moreover, the resulting condition number of the corresponding discrete problem would be much higher compared with the condition number resulting from application of the weak form Galerkin method to the same problem. To reduce the higher regularity requirements, the governing equations are first transformed into an equivalent first-order system. Transformation of the governing equations to an equivalent first-order system necessarily implies that additional independent variables need be introduced, implying an increase in cost. However, the auxiliary variables may be argued to be beneficial as they may represent physically meaningful variables, e.g. fluxes, and will be directly approximated in the model. We proceed by replacing the problem, Eq. 25-Eq. 26, with its first-order equivalent system: Find  $\phi(\mathbf{x})$  and  $\mathbf{q}(\mathbf{x})$  such that

 $-\nabla \cdot \mathbf{q} = f \qquad \text{in } \Omega \qquad (27)$ 

 $\nabla \phi - \mathbf{q} = 0 \qquad \text{in } \Omega \qquad (28)$ 

 $\nabla \times \mathbf{q} = 0$  in  $\Omega$  (29)

 $\phi = \phi^s \qquad \text{on} \quad \Gamma \qquad (30)$ 

where **q** is a vector valued function whose components are the fluxes of scalar function  $\phi$ , as defined in Eq.(28). Eq. 29 is a curl constraint to ensure  $H^1$ -coercivity of the system.

For  $s \ge 0$ , we use the standard notation and definition for the Sobolev spaces  $H^s(\Omega)$  and  $H^s(\Gamma)$  with corresponding inner products denoted by  $(\cdot, \cdot)_{s,\Omega}$ and  $\langle \cdot, \cdot \rangle_{s,\Gamma}$  and norms by  $\|\cdot\|_{s,\Omega}$  and  $\|\cdot\|_{s,\Gamma}$ , respectively. We denote the  $L_2(\Omega)$  and  $L_2(\Gamma)$  inner products by  $(\cdot, \cdot)_{\Omega}$  and  $\langle \cdot, \cdot \rangle_{\Gamma}$ , respectively. By  $\mathbf{H}^s(\Omega)$  we denote the product space  $[H^s(\Omega)]^n$ . In the least-squares approach, the variational problem is such that the function  $\phi$  and its flux

**q** minimize the sum of the squares of the residuals of the governing equations measured in the  $L^2$ norm. The associated functional is given by

$$J(\boldsymbol{\phi}, \mathbf{q}; f) = \frac{1}{2} \| -\nabla \cdot \mathbf{q} - f \|_{0,\Omega}^{2}$$

$$+ \frac{1}{2} \| \nabla \boldsymbol{\phi} - \mathbf{q} \|_{0,\Omega}^{2} + \frac{1}{2} \| \nabla \times \mathbf{q} \|_{0,\Omega}^{2}.$$
(31)

According to Fictitious Domain methodology the problem will be extended to a simple shaped domain  $\Pi \supset \Omega$  with immersed constraints enforced via Lagrange multipliers. So the new functional associated with the equivalent Fictitious Domain transport problem will be:

$$J(\phi, \mathbf{q}, \lambda; f, \phi^{s})$$

$$= \frac{1}{2} \| -\nabla \cdot \mathbf{q} - f \|_{0,\Pi}^{2}$$

$$+ \frac{1}{2} \| \nabla \phi - \mathbf{q} \|_{0,\Pi}^{2} + \frac{1}{2} \| \nabla \times \mathbf{q} \|_{0,\Pi}^{2}$$

$$+ \| \lambda (\phi - \phi^{s}) \|_{0,\Gamma}$$
(32)

where the Lagrange multiplier defined on  $\Gamma$  is denoted by  $\lambda$ , with  $\mu$  the associated weight function. The least squares principles for functional Eq. 32 can be stated as:

Find  $(\phi, \mathbf{q}, \lambda) \in \mathbf{X} \times M$  such that for all  $(\psi, \mathbf{p}, \mu) \in \mathbf{X} \times M$ 

$$J(\phi, \mathbf{q}, \lambda; f, \phi^s) \le J(\psi, \mathbf{p}, \mu; f, \phi^s), \tag{33}$$

where we use the spaces  $\mathbf{X} = \{(\phi, \mathbf{q}) \in H^1(\Pi) \times \mathbf{H}^1(\Pi)\}$  and  $M = \{\lambda \in H^{-1/2}(\Gamma)\}.$ 

This yields:

Find 
$$(\phi, \mathbf{q}, \lambda) \in \mathbf{X} \times M$$
 such that  
 $a((\phi, \mathbf{q}), (\psi, \mathbf{p})) + b((\psi, \mathbf{p}), \lambda) = l((\psi, \mathbf{p}))$   
 $\forall (\psi, \mathbf{p}) \in \mathbf{X}$   
 $b((\phi, \mathbf{q}), \mu) = g(\mu) \quad \forall \mu \in M$ 
(34)

where

$$a((\phi, \mathbf{q}), (\psi, \mathbf{p})) = ((-\nabla \cdot \mathbf{q}), (-\nabla \cdot \mathbf{p})) + ((\nabla \phi - \mathbf{q}), (\nabla \psi - \mathbf{p})) + ((\nabla \times \mathbf{q}), (\nabla \times \mathbf{p}))$$
(35)

$$b\left((\boldsymbol{\psi}, \mathbf{p}), \boldsymbol{\lambda}\right) = \langle \boldsymbol{\psi}, \boldsymbol{\lambda} \rangle \tag{36}$$

$$l((\boldsymbol{\psi}, \mathbf{p})) = (f, (-\nabla \cdot \mathbf{p})) \tag{37}$$

$$g(\mu) = \langle \phi^s, \mu \rangle. \tag{38}$$

The solution of problem, Eq. 25-Eq. 26, will be the restriction to  $\Omega$  of the minimum, defined on domain  $\Pi$ , of functional Eq. 33.

#### 4.3 Spectral Element approximation

The problem Eq. 36 can not be solved analytically and therefore it is necessary to use a numerical method to get approximated solution.

The spectral hp element method is a numerical technique for solving partial differential equations based on variational formulation of boundary and initial value problems which is employed in several fieds: fluid dynamics [Karniadakis and Sherwin (1999); Pontaza and Reddy (2003); Gerritsma and Maerschalck (2006)], structural analysis [Wu, Liu, Scarpas, and Ge (2006); Wu, Al-Khoury, Kasbergen, Liu, and Scarpas (2007); Mitra and Gopalakrishnan (2006)], geophysics [Komatitsch and Vilotte (1998); Komatitsch, Vilotte, Vai, Castillo-Covarrubias, and Sánchez-Sesma (1999)], acoustics [Lin (1998)]. The solution is represented by a finite number of basis functions. Spectral hp element method is based on higher order functions, which are locally defined over finite size parts of domain. The advantage of such kind of method respect to traditional finite element method is its exponential convergence property with the increasing of polynomial order *p*.

We proceed to define a discrete problem by choosing appropriate finite element subspaces for  $\phi$ , each of the components of the vector valued function **q** and Lagrange multipliers  $\lambda$ .

There are no restrictive compatibility conditions on the discrete spaces of the primary variables  $\phi$ and **q**, so we choose the same finite element subspace for each one. The only requirement on approximating spaces is that we choose continuous piecewise polynomials that are at least bi-linear in two dimensions or tri-linear in three dimensions.

Consider the two-dimensional case and let  $\mathscr{P}_h$  be a family of quadrilateral finite elements  $\overline{\Omega}_e$  that make up the connected model  $\overline{\Omega}_h$ . We map  $\overline{\Omega}_e$ to a bi-unit square  $\hat{\Omega}_e = [-1,1] \times [-1,1]$ , where  $(\xi,\eta)$  is a point in  $\hat{\Omega}_e$ . Over a typical element  $\hat{\Omega}_e$ , we approximate  $\phi$  by the expression

$$\phi(\xi,\eta) = \sum_{i=1}^{q} \tilde{\phi}_i \varphi_i(\xi,\eta) \quad \text{in}\,\hat{\Omega}_e. \tag{39}$$

In modal expansion,  $\varphi_i$  are tensor products of the one-dimensional  $C^0$  p-type hierarchical basis

$$\psi_{p} = \begin{cases} \frac{1-\xi}{2} & \text{for } p = 0\\ \frac{1-\xi}{2} \frac{1+\xi}{2} P_{p-1}^{\alpha,\beta} & \text{for } 0 (40)$$

and  $\tilde{\phi}_i$  are coefficients associated with each of the modes of hierarchical basis. In Eq. 40  $P_p^{\alpha,\beta}$  are the Jacobi polynomials (Appendix B: Jacobi Polynomials) of order p, in particular ultraspheric polynomials corresponding to the choice  $\alpha = \beta$  with  $\alpha = \beta = 1$ . This choice is due to the considerations about the sparsity of the matrices we obtain discretizing the problem presented by [Karniadakis and Sherwin (1999)]. We approximate the components of the vector valued function  $\mathbf{q}$  on  $\hat{\Omega}_e$  in similar manner as we did for  $\phi$  in Eq. 39.

The approximation of Lagrange multipliers requires the discretization of the immersed boundary  $\Gamma$  into curvilinear one-dimensional elements  $\overline{\Gamma}_e$ , which are mapped to linear unit elements



Figure 12: Shape of modal expansion modes for a polynomial order of P = 5

 $\hat{\Gamma}_e = [-1, 1]$ . On these elements the function  $\lambda$  is approximated by the expression

$$\lambda(\xi) = \sum_{i=1}^{r} \tilde{\lambda}_{i} \psi_{i}(\xi) \quad \text{on } \hat{\Gamma}_{e}$$
(41)

where  $\psi_i$  are defined in Eq. 39 and  $\tilde{\lambda}_i$  are the coefficients associated with expansion modes of function  $\lambda$ . In this way we proceed to generate a system of linear algebraic equations at element level. The integrals in these equations are evaluated using Gauss-Legendre quadrature rules.

The choice of Lagrange multipliers discrete space is not independent by the discrete spaces of variables  $\phi$  and **q**. To ensure the convergence of the solution of discretized model to that one of the continuous problem, the Ladyzhenskaja-Babuska-Brezzi(LBB)-condition has to be satisfied:

$$\sup_{\psi_{hp}\in H_{hp}^{1}(\Pi)} \frac{\int_{\Gamma} \mu_{HP} \psi_{hp} ds}{\left\|\psi_{hp}\right\|_{H}^{1}(\Pi)} \geq \overline{\beta} \left\|\mu_{HP}\right\|_{H}^{1/2}(\Gamma),$$
$$\forall \mu_{HP} \in H_{HP}^{1/2}(\Gamma) \quad (42)$$

for some  $\overline{\beta} > 0$  independent of *hp* an *HP*.

The global system of equations is assembled from the element contributions using the direct summation approach. The assembled system of equations can be written as

$$\begin{pmatrix} \mathbf{A} & \mathbf{B}^T \\ \mathbf{B} & \mathbf{0} \end{pmatrix} \begin{pmatrix} \tilde{\mathbf{y}} \\ \tilde{\boldsymbol{\lambda}} \end{pmatrix} = \begin{pmatrix} \mathbf{f} \\ \mathbf{g} \end{pmatrix}$$
(43)

where  $\tilde{\mathbf{y}}$  are the modal unknown coefficients associated with  $\phi$  and  $\mathbf{q}$ ,  $\tilde{\lambda}$  are the modal unknown coefficients associated with  $\lambda$ ,  $\mathbf{A}$  is the least squares matrix,  $\mathbf{B}$  is the matrix coupling the primal variables  $\phi$  and  $\mathbf{q}$  and the Lagrange multipliers  $\lambda$ ,  $\mathbf{f}$  is the load vector and  $\mathbf{g}$  is the constraint vector. To solve the system Eq. 43 we use a direct method. Note that the information on the geometry of domain is encoded only in  $\mathbf{B}$  and  $\mathbf{g}$ , not in  $\mathbf{A}$  or  $\mathbf{f}$ . So if we want to solve the same heat conduction equation on a different domain  $\Omega$  we have just to calculate again the matrix  $\mathbf{B}$  and the vector  $\mathbf{g}$ , because  $\mathbf{A}$  and  $\mathbf{f}$  will not change.

#### 4.4 Numerical example

We solve the convection-diffusion equation

$$-\Delta \phi + \{\mathbf{1}\}^T \cdot \nabla \phi = f(x, y) \tag{44}$$

on pentagonal domain  $\Omega$  shown in Fig. 13. On the boundary  $\Gamma$  Robin constraints have been imposed. The source term f(x,y) and the boundary



Figure 13: Function  $\phi$ , solution of problem Eq. 44.





Figure 14: Numerical grids used for calculations. The model of domain  $\Pi$  consists of four quadrilateral finite elements in the first case, with ten (a) immersed boundary linear elements and fifty (b), and twenty-five in the second one, with ten (c) immersed boundary linear elements and fifty (d).

Figure 15: Convergence of the function  $\phi$  to the exact solution of diffusion problem Eq. 44 in the  $L_2$  – *norm.* (a) Numerical grid of Fig. 14(a); (b) Numerical grid of Fig. 14(b); (c) Numerical grid of Fig. 14(c); (d) Numerical grid of Fig. 14(d).

constraints are such that solution is the function  $\phi : \Re^2 \Longrightarrow \Re$ , so defined:

$$\phi(x, y) = -(x^2 + y^2) + 1 + e^{xy}.$$
(45)

The fictitious domain considered is a square  $\Pi = [-1.1, 1.1] \times [-1.0, 1.2]$ , containing  $\Omega$ . Several numerical grids have been used for calculations, as shown in Fig. 14. Computational domain  $\Pi$  has been divided into four first and twenty-five after quadrilateral finite elements. The immersed boundary  $\Gamma$  has been discretized into ten and fifty linear elements.

In Fig. 15 the convergence of  $\phi$  is shown as function of the expansion order of domain in a linearlogarithmic scale. Each curve corresponds to a different expansion order of Lagrange multipliers. These curves are characterized by a minimum. We can observe if the number of immersed linear elements is low the curves with crescent expansion order move toward lower errors, on the contrary if the number of immersed linear elements is high the curves move toward higher errors. Interpolating the minimum values reached for each expansion order of domain p the convergence to exact solution is spectral. The interpolating curve is pretty the same if we consider an identical discretization of domain  $\Pi$ , modifying just the Lagrange multiplier number of elements. Another remark is that the convergence of the interpolating curve is faster refining the discretized model of computational domain  $\Pi$ .

# 5 The deterministic formulation of the stochastic Fictitious Domain problem

Let  $\theta \in \Theta$  be a random realization drawn from a complete probability space  $(\Theta, A, P)$ , whose event space  $\Theta$  generates its  $\sigma$ -algebra  $A \subset 2^{\Theta}$  and is characterized by a probability measure P. For all  $\theta \in \Theta$ , let  $\Omega(\theta) \subset \Re^d$  be a d-dimensional random domain bounded by boundary  $\Gamma(\theta)$ . We consider the following stochastic boundary value problem: for P-almost everywhere in  $\Theta$ , find a stochastic solution  $\phi : \overline{\Omega}(\theta) \to \Re$  such that:

Find  $\phi(\mathbf{x}, \theta)$  such that

$$-\triangle \phi = f \qquad \text{in } \Omega(\theta) \qquad (46)$$

$$\phi = \phi^s \qquad \text{on } \Gamma(\theta) \qquad (47)$$

where *f* is the source term and  $\phi^s$  is the prescribed value of  $\phi$  on stochastic boundary  $\Gamma(\theta)$ . This problem is chosen only for notational simplicity. We proceed by replacing the problem, Eq. 46 and Eq. 47, with its first-order equivalent system: Find  $\phi(\mathbf{x}, \theta)$  and  $\mathbf{q}(\mathbf{x}, \theta)$  such that

$$-\nabla \cdot \mathbf{q} = f \qquad \text{in } \Omega(\theta) \qquad (48)$$

$$\nabla \phi - \mathbf{q} = 0 \qquad \text{in } \Omega(\theta) \qquad (49)$$

$$\nabla \times \mathbf{q} = 0 \qquad \text{in } \Omega(\theta) \qquad (50)$$

 $\phi = \phi^s \qquad \text{on } \Gamma(\theta) \qquad (51)$ 

where **q** is the flux of scalar function  $\phi$ .

The  $L^2$  least-squares functional associated with first-order equivalent system formulation is given by

$$J(\phi, \mathbf{q}; f) = \frac{1}{2} \| -\nabla \cdot \mathbf{q} - f \|_{0,\Omega(\theta)}^{2}$$

$$+ \frac{1}{2} \| \nabla \phi - \mathbf{q} \|_{0,\Omega(\theta)}^{2} + \frac{1}{2} \| \nabla \times \mathbf{q} \|_{0,\Omega(\theta)}^{2}.$$
(52)

and its Fictitious Domain implementation will be:

$$J(\phi, \mathbf{q}, \lambda; f, \phi^{s})$$

$$= \frac{1}{2} \| -\nabla \cdot \mathbf{q} - f \|_{0,\Pi}^{2}$$

$$+ \frac{1}{2} \| \nabla \phi - \mathbf{q} \|_{0,\Pi}^{2} + \frac{1}{2} \| \nabla \times \mathbf{q} \|_{0,\Pi}^{2}$$

$$+ \| \lambda (\phi - \phi^{s}) \|_{0,\Gamma(\theta)}$$
(53)

where the Lagrange multiplier defined on  $\Gamma$  is denoted by  $\lambda$ , with  $\mu$  the associated weight function. The least squares principles for functional Eq. 53 can be stated as:

Find  $(\phi, \mathbf{q}, \lambda) \in \mathbf{X} \times M(\theta)$  such that for all  $(\psi, \mathbf{p}, \mu) \in \mathbf{X} \times M(\theta)$ 

$$J(\phi, \mathbf{q}, \lambda; f, \phi^s) \le J(\psi, \mathbf{p}, \mu; f, \phi^s), \tag{54}$$

where we use the spaces  $\mathbf{X} = \{(\phi, \mathbf{q}) \in H^1(\Pi) \times \mathbf{H}^1(\Pi)\}$  and  $M(\theta) = \{\lambda \in H^{-1/2}(\Gamma(\theta))\}.$ 

This yields:

$$\begin{cases} \text{Find } (\phi, \mathbf{q}, \lambda) \in \mathbf{X} \times M(\theta) \text{ such that} \\ a((\phi, \mathbf{q}), (\psi, \mathbf{p})) + b((\psi, \mathbf{p}), \lambda) = l((\psi, \mathbf{p})) \\ \forall (\psi, \mathbf{p}) \in \mathbf{X} \\ b((\phi, \mathbf{q}), \mu) = g(\mu) \quad \forall \mu \in M(\theta) \end{cases}$$
(55)

where

$$a((\phi, \mathbf{q}), (\psi, \mathbf{p})) = \int_{\Pi} (-\nabla \cdot \mathbf{q}) (-\nabla \cdot \mathbf{p}) d\Pi$$
$$+ \int_{\Pi} (\nabla \phi - \mathbf{q}) \cdot (\nabla \psi - \mathbf{p}) d\Pi$$
$$+ \int_{\Pi} (\nabla \times \mathbf{q}) , (\nabla \times \mathbf{p}) d\Pi$$
(56)

$$b((\boldsymbol{\psi}, \mathbf{p}), \boldsymbol{\lambda}) = \int_{\Gamma(\boldsymbol{\theta})} \boldsymbol{\psi} \boldsymbol{\lambda} d\Gamma(\boldsymbol{\theta})$$
(57)

$$l((\boldsymbol{\psi}, \mathbf{p})) = \int_{\Pi} f(-\nabla \cdot \mathbf{p}) \, d\Pi \tag{58}$$

$$g(\mu) = \int_{\Gamma(\theta)} \phi^s \mu d\Gamma(\theta).$$
(59)

The solution of problem, Eq. 46-Eq. 47, will be the restriction to  $\Omega(\theta)$  of the minimum, defined on domain  $\Pi$ , of functional Eq. 54.

The saddle point problem Eq. 55 has a stochastic formulation. We assume that the boundary  $\Gamma(\mathbf{x}, \theta)$  of  $\Omega(\mathbf{x}, \theta) \subset \Pi(\mathbf{x})$  depends on  $\theta$  via *n* mutually indipendent real random variables  $\xi(\theta)$ with zero mean and unit variance with respect to a density function  $\rho$  defined on some interval  $I \in \Re$ , so that  $\mathbf{I} = I^n$ . Referring to Eq. 6 we can write the stochastic process as

$$\Gamma(\mathbf{x},\boldsymbol{\theta}) \cong \Gamma^*(\mathbf{x},\boldsymbol{\theta}) = \sum_{i=0}^N \Gamma_i(\mathbf{x}) H_i(\boldsymbol{\xi}).$$
(60)

Substituting the polynomial Chaos series into Eq. 55 we obtain

$$\begin{cases} \text{Find } (\phi^*, \mathbf{q}^*, \lambda^*) \in L^2_{\rho}(\mathbf{I}; \mathbf{X}) \times L^2_{\rho}(\mathbf{I}; M^*) \\ \text{such that} \\ a((\phi^*, \mathbf{q}^*), (\psi^*, \mathbf{p}^*)) + b((\psi^*, \mathbf{p}^*), \lambda^*) \\ = l((\psi^*, \mathbf{p}^*)) \quad \forall (\psi^*, \mathbf{p}^*) \in L^2_{\rho}(\mathbf{I}; \mathbf{X}) \\ b((\phi^*, \mathbf{q}^*), \mu^*) = g(\mu^*) \quad \forall \mu \in L^2_{\rho}(\mathbf{I}; M^*) \end{cases}$$

where

1

$$\phi^*(\mathbf{x}, \theta) = \sum_{i=0}^{N} \phi_i(\mathbf{x}) H_i(\xi)$$
(62)

$$\mathbf{q}^*(\mathbf{x}, \boldsymbol{\theta}) = \sum_{i=0}^{N} \mathbf{q}_i(\mathbf{x}) H_i(\boldsymbol{\xi})$$
(63)

$$\lambda^*(\mathbf{x}, \theta) = \sum_{i=0}^N \lambda_i(\mathbf{x}) H_i(\xi)$$
(64)

and  $M^* = \{\lambda^* \in H^{-1/2}(\Gamma^*)\}$ . In this way we divide the random process into a deterministic part and a stochastic part. To solve Eq. 61 the method of Weighted Residuals is adopted, in particular the collocation projection. This formulation gives a linear system of decoupled equations equivalent to solving a deterministic problem at each grid point:

Find 
$$(\phi_i, \mathbf{q}_i, \lambda_i) \in \mathbf{X} \times M_i$$
 such that  
 $a((\phi_i, \mathbf{q}_i), (\psi_i, \mathbf{p}_i)) + b((\psi_i, \mathbf{p}_i), \lambda_i) = l((\psi_i, \mathbf{p}_i))$   
 $\forall (\psi_i, \mathbf{p}_i) \in \mathbf{X}$   
 $b((\phi_i, \mathbf{q}_i), \mu_i) = g(\mu_i) \quad \forall \mu_i \in M_i$ 
(65)

with i = 0, ..., N where  $M_i = \{\lambda_i \in H^{-1/2}(\Gamma_i)\}$ . To reconstruct the stochastic solution  $\phi(\mathbf{x}, \theta)$  the equations Eq. 12 and Eq. 13 are used.

## 6 Applications of Non-intrusive Polynomial Chaos method with Fictitious Domain approach

#### 6.1 One-dimensional problem

To verify the accuracy of the presented methodology, i.e. the coupling of Non-Intrusive Polynomial Chaos and Fictitious Domain for geometric uncertainties, we consider the problem Eq. 17, comparing the analytical solution in three points  $(x_1 = 0.0, x_2 = 45.0, x_3 = 90.0)$  with the results obtained by Polynomial Chaos and Fictitious Domain method. We have already demonstrated as the Monte Carlo method is not as accurate as Polynomial Chaos approximation, so we will not consider it for comparison.



Figure 16: Solution of problem given in Eq. 19: analytical  $pdf(\phi)$  and comparison of error respect to analytical  $pdf(\phi)$  of Non-Intrusive Polynomial Chaos  $pdf(\phi)$  with different expansion order *P* in  $x_1 = 0.0$ .



Figure 18: Solution of problem given in Eq. 19: analytical  $pdf(\phi)$  and comparison of error respect to analytical  $pdf(\phi)$  of Non-Intrusive Polynomial Chaos  $pdf(\phi)$  with different expansion order *P* in  $x_3 = 90.0$ .



Figure 17: Solution of problem given in Eq. 19: analytical  $pdf(\phi)$  and comparison of error respect to analytical  $pdf(\phi)$  of Non-Intrusive Polynomial Chaos  $pdf(\phi)$  with different expansion order *P* in  $x_2 = 45.0$ .



Figure 19: Mean function  $E(\phi)$  and uncertainty bars  $E(\phi) \pm \sigma$  of problem given in Eq. 19.

In Fig. 16, Fig. 17 and Fig. 18 the behaviour of accuracy of pdf obtained by our approach is shown for increasing polynomial order. It is evident the accuracy is pretty much the same in different points of domain and the accuracy improves visibly increasing the polynomial order from P = 1 to P = 3.

Let us notice as the accuracy obtained for P = 1 is in practice the same of that one obtained by Monte Carlo method with 1,000,000 points in section 3.1, but with great advantage about computational cost.

Another remark is the pdf obtained by Non-Intrusive Polynomial Chaos and Fictitious Domain with P = 3 is pretty the same as the pdfobtained for pure analytical test. This result confirms the efficiency of Fictitious Domain method and the excellent integration between Polynomial Chaos and Fictitious Domain for geometric tolerances.

In Fig. 19 the evolution of temperature is plotted in error bars, with the line centered at the mean value  $E(\phi)$  and the length of uncertainty bars equal to two standard deviations, that is the interval which contains 99% of all possible values. There is an increase of uncertainty bars with growing abscissa and a corresponding decrease of mean value of temperature. This result is consistent with that one obtained for the analytical case (see Fig. 5). This behaviour is due to higher closeness to the uncertain point (L = N(100, 1)) with growing abscissa and a greater influence of uncertainty to points close to that one.

This example demonstrates the capability of developed methodology, so we can use it to study a two-dimensional problem with geometric tolerance.

#### 6.2 Two-dimensional problem

In this section we consider the stationary heat conduction in an electronic chip [Xiu and Karniadakis (2003a)], subject to geometric tolerances:

$$-\nabla \cdot (k\nabla T) = f \quad \text{in } \Omega(\theta) \tag{66}$$

with k = 1 and f = 0. The stochastic domain is shown in Fig. 20. The domain dimensions are deterministic parameters except thickness of cavity



Figure 20: Stochastic domain of stationary heat conduction problem in electronic chip under study.



Figure 21: Schematic of the computational fictitious domain of stationary heat conduction problem in electronic chip under study.

*L* which has a normal distribution N(0.6, 0.01). The boundary of domain consists of four segments: the top  $\Gamma_T$ , the bottom  $\Gamma_B$ , the two sides  $\Gamma_S$  and the boundaries of the cavity  $\Gamma_C$ . Adiabatic boundary conditions are prescribed on  $\Gamma_B$  and  $\Gamma_S$ . The cavity boundary  $\Gamma_C$  is exposed to heat flux  $q_b|_{\Gamma_C} = 1$ . On the top  $\Gamma_T$  is maintained at constant temperature T = 0.

Fig. 21 shows the computational domain which differs from chip geometry and in particular contains it, according to Fictitious Domain approach. The fictitious domain has been discretized into 15 spectral elements of order 8.

We are interested in the stochastic solution at the points of domain. Actually we solve the heat conduction problem on all the points of fictitious domain and we associate to each point the probability to belong to chip, as shown in Fig. 22 for the top left corner of the cavity. In this way we have the mean and the standard deviation of temperature due to geometric tolerance even in points which do not really belong to chip, but, as we associate a probability of belonging, the results are



Figure 22: Probability of points of fictitious domain to belong to chip.

still significant.

We verify the behaviour of accuracy of the method varying the polynomial order of Polynomial Chaos approximation. In Fig. 22 and Fig. 23 the comparison of mean solution and variance respectively along the axis of symmetry, which corresponds to section x = 0 (see Fig. 25 and Fig. 26), are shown, obtained with polynomial order P = 1, P = 2, P = 3. The curves of mean coincide, but we have different accuracy of standard deviation with increasing *P*. For values higher of 3 there are no significant variation of solutions so there is no need to increase *P* further more, taking into account of computational cost, too.

Fig. 25 shows the contours of mean field of temperature and Fig. 26 shows the contours of standard deviation. It is evident that the largest output uncertainty, indicated by the standard deviation, occurs near the top of the cavity, whose position is subject to probability distribution. In fact this is the result we expected according to results obtained studying the one-dimensional problem in section 6.1. This behaviour is due to greater influence of uncertainty to points close to that one.

#### 7 Conclusions

In this paper we presented a Non-Intrusive Polynomial Chaos method using a Fictitious Domain approach to study geometric tolerances. In particular the method has been applied to one- and two-dimensional elliptic problems with geometric uncertainties in order to demonstrate the accuracy and convergence of the methodology.

A big advantage of the proposed method is that



Figure 23: Comparison of mean solution along the axis of symmetry obtained by Polynomial Chaos with polynomial order P = 1, P = 2, P = 3.



Figure 24: Comparison of variance along the axis of symmetry obtained by Polynomial Chaos with polynomial order P = 1, P = 2, P = 3.

it is non-intrusive, which means existing deterministic solvers can be used without any internal modification. In this way we get a simplification of computational process management. A new



Figure 25: Contours of temperature distributions in the electronic chip: mean field.



Figure 26: Contours of temperature distributions in the electronic chip: standard deviation field.

Least-Squares Spectral Element method has been employed for the analysis of deterministic differential problems obtained by Collocation projection. To avoid the remeshing of computational domain for the different differential problems, Fictitious Domain approach is introduced. Its main advantage lies in the fact that only one Cartesian mesh, that represents the enclosure, needs to be generated.

Excellent accuracy properties of the method are demonstrated by numerical experiments. We have compared it to analytical solution and Monte Carlo method, considering a one-dimensional elliptic problem with uncertainties on domain length. The algorithm has been finally used to solve a two-dimensional heat conduction problem with random domain.

Several issues need to be addressed:

• comparison between Intrusive and Non-Intrusive Polynomial Chaos methods: in case of multiple uncertain parameters the number of coefficients is lower using an intrusive approach, but it is evident the difficulty to implement it inside the solver; taking in account of both these remarks, it would be interesting evaluate computational benefits of the two approaches;

- problems with multi dimensional stochastic domain by Non-Intrusive Polynomial Chaos: the choice of collocation points in case of multiple uncertain parameters is not unique, so an effective criteria should be given;
- fluid dynamic problems defined on stochastic domain: the Fictitious Domain approach has been implemented just to solve advection-diffusion equation; even if the theory is simple to be extended to fluid dynamic case, the implementation and validation of the methodology has still to be achieved.

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#### **Appendix A: Hermite Polynomials**

In the Sturm-Liouville Boundary Value Problem, there is a special case called Hermite's Differential Equation which arises in the treatment of the harmonic oscillator in quantum mechanics. Hermite's Differential Equation is defined as:

$$H_{n}^{''}(x) - 2xH_{n}^{'}(x) + 2nH_{n} = 0$$

and in Sturm-Liouville form:

$$\frac{d}{dx}\left(e^{-x^2}H_n'\right) + 2ne^{-x^2}H_n = 0$$

where *n* is a real number. For non-negative integer *n*, the solutions of Hermite's Differential Equation are often referred to as Hermite Polynomials  $H_n(x)$ .

The Hermite Polynomials  $H_n(x)$  can be expressed by Rodriguez formula:

$$e^{-x^2}H_n(x) = (-1)^n \frac{d^n}{dx^n} \left(e^{-x^2}\right)$$

These polynomials can be constructed using a recursion relationship:

$$H_{n+1}(x) - 2xH_n(x) + 2nH_{n-1}(x) = 0.$$

Hermite Polynomials  $H_n(x)$ , with n = 0, 1, ..., form a complete orthogonal set on the interval  $-\infty < x < +\infty$  with respect to the weighting function  $e^{-x^2}$ . It can be shown that:

$$\frac{1}{\sqrt{\pi}}\int_{-\infty}^{+\infty}e^{-x^2}H_m(x)H_n(x)dx=2^nn!\delta_{mn}.$$

Let us notice after rescaling x by  $\sqrt{2}$  in weighting function  $e^{-x^2}$ , the weighting function is the same as the probability density function of a standard Gaussian random variable with zero mean and unit variance.

### Appendix B: Jacobi Polynomials

Jacobi polynomials represent a family of polynomial solutions to the singular Sturm-Liouville problem. A significant feature of these polynomials is that they are orthogonal in the interval [-1,1] with respect to the function  $(1-x)^{\alpha} (1-x)^{\beta}$   $(\alpha,\beta>-1)$ .

These polynomials can be constructed using a recursion relationship:

$$\begin{split} P_0^{\alpha,\beta}(x) &= 1 \\ P_1^{\alpha,\beta}(x) &= \frac{1}{2} \left[ \alpha - \beta + (\alpha + \beta + 2) x \right] \\ a_n^1 P_{n+1}^{\alpha,\beta}(x) &= (a_n^2 + a_n^3 x) P_n^{\alpha,\beta}(x) - a_n^4 P_{n-1}^{\alpha,\beta}(x) \\ a_n^1 &= 2(n+1)(n+\alpha+\beta+1)(2n+\alpha+\beta)) \\ a_n^2 &= (2n+\alpha+\beta+1)(\alpha^2-\beta^2) \\ a_n^3 &= (2n+\alpha+\beta)(2n+\alpha+\beta+1)(2n+\alpha+\beta+2) \\ a_n^4 &= 2(n+\alpha)(n+\beta)(2n+\alpha+\beta+2) \end{split}$$

A class of symmetric polynomials, known as ultraspheric polynomials, corresponds to the choice  $\alpha = \beta$ . Well known ultraspheric polynomials are the Legendre polynomial ( $\alpha = \beta = 0$ ) and the Chebychev polynomial ( $\alpha = \beta = -1/2$ ).

Further formulae and properties for Jacobi polynomials can be found in [Abramowitz and Stegun (1972); Karniadakis and Sherwin (1999)].