Chapter 2
PGD Solution of the Poisson Equation

Abstract This chapter describes the main features of the PGD technique, in particular the one related to the construction of a separated representation of the unknown field involved in a partial differential equation. For this purpose, we consider the solution of the two-dimensional Poisson equation in a square domain. The solution is sought as a finite sum of terms, each one involving the product of functions of each coordinate. The solution is then calculated by means of a sequence of one-dimensional problems. The chapter starts with the simplest case, that is later extended to cover more complex problems: non-constant source terms, non-homogeneous Dirichlet and Neumann boundary conditions, and high-dimensional problems. Carefully solved numerical examples are discussed to illustrate the theoretical developments.

Keywords Multidimensional model · Poisson's problem · Proper Generalized Decomposition

It is now time to detail the inner workings of the PGD. We begin with a simple but illustrative case study, which we shall progressively make more complex.

Consider the solution of the Poisson equation

$$\Delta u(x, y) = f(x, y), \tag{2.1}$$

in a two-dimensional rectangular domain $\Omega = \Omega_x \times \Omega_y = (0, L) \times (0, H)$.

We specify homogeneous Dirichlet boundary conditions for the unknown field $u(x, y)$, i.e. $u(x, y)$ vanishes at the domain boundary Γ. Furthermore, we assume that the source term f is constant over the domain Ω.

For all suitable test functions u^*, the weighted residual form of (2.1) reads

$$\int_{\Omega_x \times \Omega_y} u^* \cdot (\Delta u - f) \; dx \cdot dy \; = \; 0, \tag{2.2}$$

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or more explicitly

$$\int_{\Omega_x \times \Omega_y} u^* \cdot \left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} - f \right) dx \cdot dy \; = \; 0. \tag{2.3}$$

Our goal is to obtain a PGD approximate solution to (2.1) in the separated form

$$u(x, y) = \sum_{i=1}^{N} X_i(x) \cdot Y_i(y). \tag{2.4}$$

We shall do so by computing each term of the expansion one at a time, thus enriching the PGD approximation until a suitable convergence criterion is satisfied.

2.1 Progressive Construction of the Separated Representation

At each enrichment step n ($n \geq 1$), we have already computed the $n-1$ first terms of the PGD approximation (2.4):

$$u^{n-1}(x, y) = \sum_{i=1}^{n-1} X_i(x) \cdot Y_i(y). \tag{2.5}$$

We now wish to compute the next term $X_n(x) \cdot Y_n(y)$ to obtain the enriched PGD solution

$$u^n(x, y) = u^{n-1}(x, y) + X_n(x) \cdot Y_n(y) = \sum_{i=1}^{n-1} X_i(x) \cdot Y_i(y) + X_n(x) \cdot Y_n(y). \tag{2.6}$$

Both functions $X_n(x)$ and $Y_n(y)$ are unknown at the current enrichment step n, and they appear in the form of a product. The resulting problem is thus non-linear and a suitable iterative scheme is required. We shall use the index p to denote a particular iteration.

At enrichment step n, the PGD approximation $u^{n,p}$ obtained at iteration p thus reads

$$u^{n,p}(x, y) = u^{n-1}(x, y) + X_n^p(x) \cdot Y_n^p(y). \tag{2.7}$$

The simplest iterative scheme is an alternating direction strategy that computes $X_n^p(x)$ from $Y_n^{p-1}(y)$, and then $Y_n^p(x)$ from $X_n^p(x)$. An arbitrary initial guess $Y_n^0(y)$ is specified to start the iterative process. The non-linear iterations proceed until reaching a fixed point within a user-specified tolerance ϵ, i.e.

$$\frac{\|X_n^p(x) \cdot Y_n^p(y) - X_n^{p-1}(x) \cdot Y_n^{p-1}(y)\|}{\|X_n^{p-1}(x) \cdot Y_n^{p-1}(y)\|} < \epsilon, \tag{2.8}$$

where $\| \cdot \|$ is a suitable norm.

The enrichment step n thus ends with the assignments $X_n(x) \leftarrow X_n^p(x)$ and $Y_n(y) \leftarrow Y_n^p(y)$.

The enrichment process itself stops when an appropriate measure of error $\mathcal{E}(n)$ becomes small enough, i.e $\mathcal{E}(n) < \tilde{\epsilon}$. Several stopping criteria are available, as we shall discuss later. We now describe in more detail one particular alternating direction iteration at a given enrichment step.

2.1.1 Alternating Direction Strategy

Each iteration of the alternating direction scheme consists in the following two steps:

- Calculating $X_n^p(x)$ from $Y_n^{p-1}(y)$

  In this case, the approximation reads

$$u^{n,p}(x, y) = \sum_{i=1}^{n-1} X_i(x) \cdot Y_i(y) + X_n^p(x) \cdot Y_n^{p-1}(y), \tag{2.9}$$

  where all functions are known except $X_n^p(x)$.

  The simplest choice for the weight function u^* in the weighted residual formulation (2.3) is

$$u^*(x, y) = X_n^*(x) \cdot Y_n^{p-1}(y), \tag{2.10}$$

  which amounts to select the Galerkin weighted residual form of the Poisson equation.

  Injecting (2.9) and (2.10) into (2.3), we obtain

$$\begin{aligned} &\int_{\Omega_x \times \Omega_y} X_n^* \cdot Y_n^{p-1} \cdot \left(\frac{d^2 X_n^p}{dx^2} \cdot Y_n^{p-1} + X_n^p \cdot \frac{d^2 Y_n^{p-1}}{dy^2} \right) dx \cdot dy \\ &= -\int_{\Omega_x \times \Omega_y} X_n^* \cdot Y_n^{p-1} \cdot \sum_{i=1}^{n-1} \left(\frac{d^2 X_i}{dx^2} \cdot Y_i + X_i \cdot \frac{d^2 Y_i}{dy^2} \right) dx \cdot dy \\ &\quad + \int_{\Omega_x \times \Omega_y} X_n^* \cdot Y_n^{p-1} \cdot f \, dx \cdot dy. \end{aligned} \tag{2.11}$$

Here comes a crucial point: since all functions of y are known in the above expression, we can compute the following one-dimensional integrals over Ω_y:

$$\left\{\begin{array}{l} \alpha^x = \int_{\Omega_y} \left(Y_n^{p-1}(y)\right)^2 \, dy \\ \beta^x = \int_{\Omega_y} Y_n^{p-1}(y) \cdot \dfrac{d^2 Y_n^{p-1}(y)}{dy^2} \, dy \\ \gamma_i^x = \int_{\Omega_y} Y_n^{p-1}(y) \cdot Y_i(y) \, dy \\ \delta_i^x = \int_{\Omega_y} Y_n^{p-1}(y) \cdot \dfrac{d^2 Y_i(y)}{dy^2} \, dy \\ \xi^x = \int_{\Omega_y} Y_n^{p-1}(y) \cdot f \, dy \end{array}\right. . \tag{2.12}$$

Equation (2.11) becomes

$$\int_{\Omega_x} X_n^* \cdot \left(\alpha^x \cdot \frac{d^2 X_n^p}{dx^2} + \beta^x \cdot X_n^p\right) dx$$

$$= - \int_{\Omega_x} X_n^* \cdot \sum_{i=1}^{n-1} \left(\gamma_i^x \cdot \frac{d^2 X_i}{dx^2} + \delta_i^x \cdot X_i\right) dx \; + \int_{\Omega_x} X_n^* \cdot \xi^x \, dx. \tag{2.13}$$

We have thus obtained the weighted residual form of a one-dimensional problem defined over Ω_x that can be solved (e.g. by the finite element method) to obtain the function X_n^p we are looking for. Alternatively, we can return to the corresponding strong formulation

$$\alpha^x \cdot \frac{d^2 X_n^p}{dx^2} + \beta^x \cdot X_n^p \; = - \sum_{i=1}^{n-1} \left(\gamma_i^x \cdot \frac{d^2 X_i}{dx^2} + \delta_i^x \cdot X_i\right) \; + \; \xi^x, \tag{2.14}$$

and solve it numerically by means of any suitable numerical method (e.g. finite differences, pseudo-spectral techniques, ...). The strong form (2.14) is a second-order ordinary differential equation for X_n^p. This is due to the fact that the original Poisson equation involves a second-order x-derivative of the unknown field u.

With either the weighted residual or strong formulations, the homogeneous Dirichlet boundary conditions $X_n^p(x=0) = X_n^p(x=L) = 0$ are readily specified.

Having thus computed $X_n^p(x)$, we are now ready to proceed with the second step of iteration p.

- Calculating $Y_n^p(y)$ from the just-computed $X_n^p(x)$

  The procedure exactly mirrors what we have done above. Indeed, we simply exchange the roles played by all relevant functions of x and y.

The current PGD approximation reads

$$u^{n,p}(x, y) = \sum_{i=1}^{n-1} X_i(x) \cdot Y_i(y) + X_n^p(x) \cdot Y_n^p(y), \tag{2.15}$$

where all functions are known except $Y_n^p(y)$.

The Galerkin formulation of (2.3) is obtained with the particular choice

$$u^*(x, y) = X_n^p(x) \cdot Y_n^*(y). \tag{2.16}$$

Then, by introducing (2.15) and (2.16) into (2.3), we get

$$\begin{aligned}
&\int_{\Omega_x \times \Omega_y} X_n^p \cdot Y_n^* \cdot \left(\frac{d^2 X_n^p}{dx^2} \cdot Y_n^p + X_n^p \cdot \frac{d^2 Y_n^p}{dy^2} \right) dx \cdot dy \\
&= - \int_{\Omega_x \times \Omega_y} X_n^p \cdot Y_n^* \cdot \sum_{i=1}^{n-1} \left(\frac{d^2 X_i}{dx^2} \cdot Y_i + X_i \cdot \frac{d^2 Y_i}{dy^2} \right) dx \cdot dy \\
&\quad + \int_{\Omega_x \times \Omega_y} X_n^p \cdot Y_n^* \cdot f \, dx \cdot dy.
\end{aligned} \tag{2.17}$$

As all functions of x are known, the integrals over Ω_x can be computed to obtain

$$\begin{cases}
\alpha^y = \int_{\Omega_x} \left(X_n^p(x) \right)^2 \, dx \\
\beta^y = \int_{\Omega_x} X_n^p(x) \cdot \dfrac{d^2 X_n^p(x)}{dx^2} \, dx \\
\gamma_i^y = \int_{\Omega_x} X_n^p(x) \cdot X_i(x) \, dx \\
\delta_i^y = \int_{\Omega_x} X_n^p(x) \cdot \dfrac{d^2 X_i(x)}{dx^2} \, dx \\
\xi^y = \int_{\Omega_x} X_n^p(x) \cdot f \, dx
\end{cases}. \tag{2.18}$$

Equation (2.17) becomes

$$\begin{aligned}
&\int_{\Omega_y} Y_n^* \cdot \left(\alpha^y \cdot \frac{d^2 Y_n^p}{dy^2} + \beta^y \cdot Y_n^p \right) dy \\
&= - \int_{\Omega_y} Y_n^* \cdot \sum_{i=1}^{n-1} \left(\gamma_i^y \cdot \frac{d^2 Y_i}{dy^2} + \delta_i^y \cdot Y_i \right) dy \; + \int_{\Omega_y} Y_n^* \cdot \xi^y \, dy.
\end{aligned} \tag{2.19}$$

As before, we have thus obtained the weighted residual form of an elliptic problem defined over Ω_y whose solution is the function $Y_n^p(y)$. Alternatively, the corresponding strong formulation of this one-dimensional problem reads

$$\alpha^y \cdot \frac{d^2 Y_n^p}{dy^2} + \beta^y \cdot Y_n^p = - \sum_{i=1}^{n-1} \left(\gamma_i^y \cdot \frac{d^2 Y_i}{dy^2} + \delta_i^y \cdot Y_i \right) + \xi^y. \tag{2.20}$$

This again is an ordinary differential equation of the second order, due to the fact that the original Poisson equation involves second-order derivatives of the unknown field with respect to y. With both the weighted residual and strong formulations, the homogeneous Dirichlet boundary conditions $Y_n^p(y = 0) = Y_n^p(y = L) = 0$ are readily specified.

We have thus completed iteration p at enrichment step n.

It is important to realize that the original two-dimensional Poisson equation defined over $\Omega = \Omega_x \times \Omega_y$ has been transformed within the PGD framework into a series of *decoupled one-dimensional problems* formulated in Ω_x and Ω_y.

As we shall detail later, should we consider the Poisson equation defined over a domain of dimension D, i.e. $\Omega_1 \times \Omega_2 \times \cdots \times \Omega_D$, then its PGD solution would similarly involve a series of decoupled one-dimensional problems formulated in each Ω_i. This of course explains why the PGD solution of high-dimensional problems is feasible at all.

2.1.2 Stopping Criterion for the Enrichment Process

The enrichment process itself ends when an appropriate measure of error $\mathcal{E}(n)$ becomes small enough, i.e $\mathcal{E}(n) < \tilde{\epsilon}$. Several stopping criteria are suitable.

A first stopping criterion is associated with the relative weight of the newly-computed term within the PGD expansion. Thus, $\mathcal{E}(n)$ is given by

$$\mathcal{E}(n) = \frac{\|X_n(x) \cdot Y_n(y)\|}{\|u^n(x, y)\|} = \frac{\|X_n(x) \cdot Y_n(y)\|}{\left\| \sum_{i=1}^{n} X_i(x) \cdot Y_i(y) \right\|}. \tag{2.21}$$

Selecting for example the L^2-norm, we have

$$\begin{aligned} \|X_n(x) \cdot Y_n(y)\|_2 &= \left(\int_{\Omega_x \times \Omega_y} (X_n(x))^2 \cdot (Y_n(y))^2 \, dx \cdot dy \right)^{\frac{1}{2}} \\ &= \left(\int_{\Omega_x} (X_n(x))^2 \, dx \right)^{\frac{1}{2}} \cdot \left(\int_{\Omega_y} (Y_n(y))^2 \, dy \right)^{\frac{1}{2}}. \end{aligned} \tag{2.22}$$

Since $u^n(x, y)$ is expressed in a separated form, its square will be also expressed in a separated form having $\frac{n\cdot(n+1)}{2}$ terms:

$$(u^n)^2 = \sum_{i=1}^{\frac{n\cdot(n+1)}{2}} S_i^x(x) \cdot S_i^y(y). \tag{2.23}$$

The corresponding L^2-norm is then readily evaluated as follows

$$\|u^n\|_2 = \left(\int_{\Omega_x \times \Omega_y} \sum_{i=1}^{\frac{n\cdot(n+1)}{2}} S_i^x(x) \cdot S_i^y(y)\, dx \cdot dy \right)^{\frac{1}{2}} \tag{2.24}$$

$$= \left(\sum_{i=1}^{\frac{n\cdot(n+1)}{2}} \left(\int_{\Omega_x} S_i^x(x)\, dx \cdot \int_{\Omega_y} S_i^y(y)\, dy \right) \right)^{\frac{1}{2}}. \tag{2.25}$$

The above stopping criterion involves the evaluation of $2 + n \cdot (n + 1)$ one-dimensional integrals. A similar but less expensive criterion is based on the norm of mode n with respect to the norm of the first mode, i.e.

$$\mathcal{E}(n) = \frac{\|X_n(x) \cdot Y_n(y)\|}{\|X_1(x) \cdot Y_1(y)\|}. \tag{2.26}$$

This second criterion requires the computation of only two one-dimensional integrals.

More appropriate error estimators can be associated to the residual $R(n)$ obtained by inserting the PGD approximation $u^n(x, y)$ into the Poisson equation:

$$R(n) = \sum_{i=1}^{n} \left(\frac{\partial^2 X_i}{\partial x^2} \cdot Y_i(y) + X_i(x) \cdot \frac{\partial^2 Y_i}{\partial y^2} \right) - f. \tag{2.27}$$

Selecting $\mathcal{E}(n) = \|R(n)\|_2$ as error estimator again leads to the computation of one-dimensional integrals as with the previous criteria.

Other error estimators based on quantities of interest in the study of a particular problem are proposed in [1, 2].

2.1.3 Numerical Example

Let us consider the Poisson Eq. (2.1) on a two-dimensional rectangular domain $\Omega = \Omega_x \times \Omega_y = (0, 2) \times (0, 1)$ for which we seek a solution using the procedure described above. The source term f is set to $f = 1$, in which case we obtain analytically the following exact solution for $u(x, y)$:

$$u_{\mathrm{ex}}(x, y) = \sum_{m,n\ \mathrm{odd}} \frac{64}{\pi^4 \left(4n^2 + m^2\right)} \cdot \sin\left(\frac{m\pi x}{2}\right) \cdot \sin\left(n\pi y\right). \qquad (2.28)$$

The unknown functions $X_i(x)$ and $Y_i(y)$ are sought on a uniform grid with M points. All one-dimensional differential problems arising in the solution procedure are solved using second-order finite differences, while the integrals are evaluated numerically using the trapezoidal rule. The chosen stopping criteria for the fixed point iterations and the enrichment process are those described by (2.8) and (2.26), respectively.

In Figs. 2.1 and 2.2 the normalized functions $X_i(x)$ and $Y_i(y)$ are illustrated for $i = 1, \ldots, 4$ and $M = 101$. One can observe that, as i increases, $X_i(x)$ and $Y_i(y)$ both account for a higher frequency content of the numerical solution.

In Fig. 2.3, we show the 2D reconstructed PGD solution together with the normalized functions $X_i(x)$ and $Y_i(y)$. For clarity reasons the 2D solution is shown on a coarser grid.

In the sequel we illustrate the convergence of the PGD solution towards the analytical solution as a function of both the discretization and the number of enrichment steps. For this purpose we define the following quadratic error between the analytical solution $u_{\mathrm{ex}}(x, y)$ and a numerical PGD solution $u_M^N(x, y)$ with N enrichment steps and M discretization points for each coordinate:

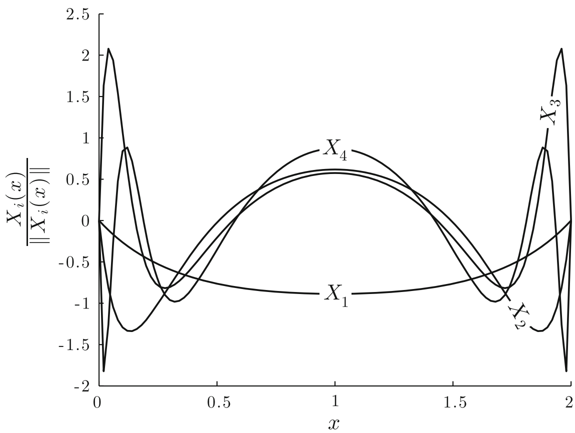


Fig. 2.1 Normalized functions $X_i(x)$ for $i = 1, \ldots, 4$ produced by the PGD solution of (2.1)

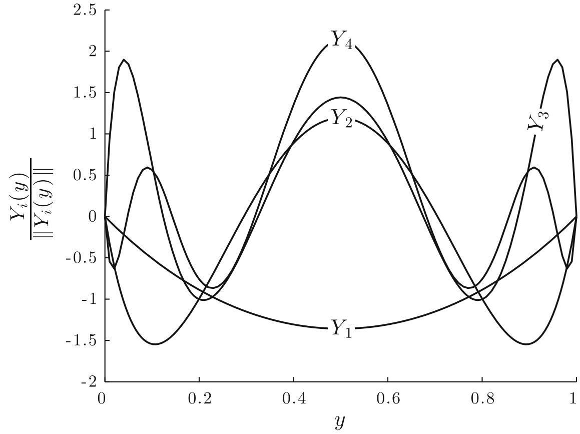


Fig. 2.2 Normalized functions $Y_i(y)$ for $i = 1, \ldots, 4$ produced by the PGD solution of (2.1)

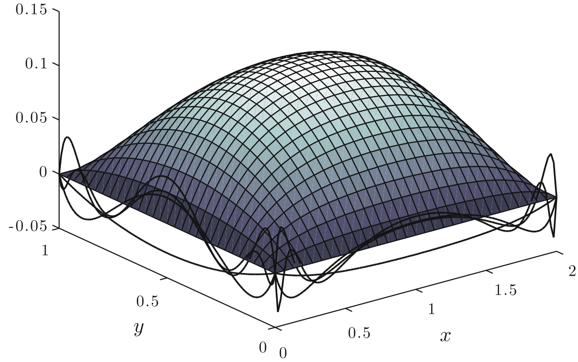


Fig. 2.3 Reconstructed 2D PGD solution of (2.1) and normalized functions $X_i(x)$ and $Y_i(y)$. The 2D solution is shown on a coarser grid

$$E_M(u_M^N) = \tilde{\int_0^1} \tilde{\int_0^2} \Big(u_{\text{ex}}(x, y) - u_M^N(x, y)\Big)^2 \; dx \cdot dy. \tag{2.29}$$

Here, the symbol $\tilde{\int}$ refers to a numerical integration carried out with the trapezoidal rule on the nodal values. We first illustrate the pointwise convergence of the PGD solution towards the exact solution in Fig. 2.4 where we plot $u_{\text{ex}} - u_M^N$ for $M = 41$ and different values of N. For clarity reasons the 2D error is shown on a coarser grid.

We further illustrate the convergence of the PGD solution by showing $E_M(u_M^N)$ as a function of N and as a function of M in Figs. 2.5 and 2.6 respectively. One can immediately notice that, for this problem, only a few enrichment steps are necessary for the PGD to converge to the analytical solution.

In the next example, we compute the first 10 enrichment steps on a coarse mesh ($M = 21$). We then interpolate the computed functions $X_i(x)$ and $Y_i(y)$ on a finer mesh ($M = 41$) using a natural spline interpolation, before computing another 10 enrichment steps on the fine mesh. The error $E_M(u_M^N)$ is shown in Fig. 2.7. This illustrates that after a few enrichment steps the error is mostly a discretization error.

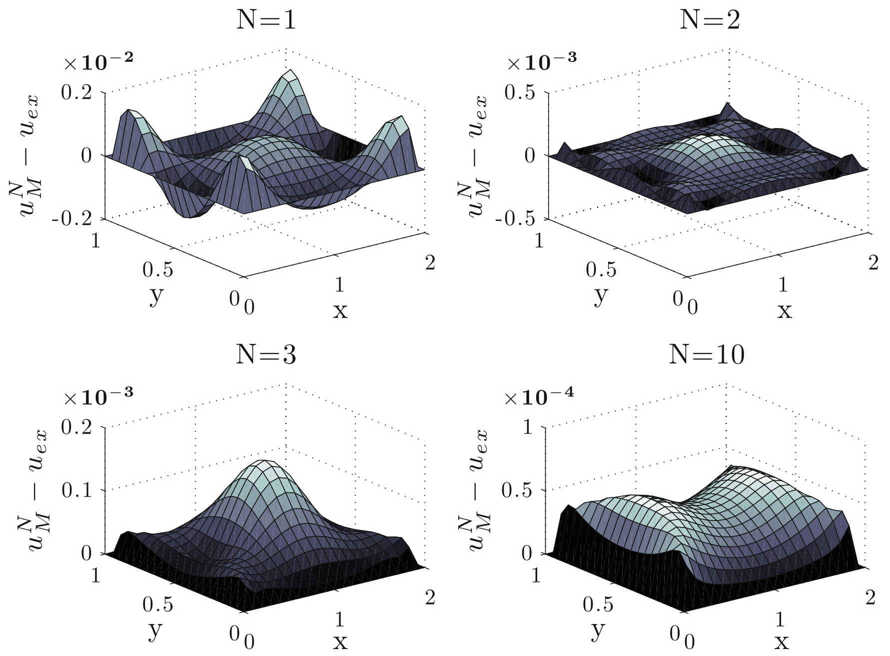


Fig. 2.4 $u_{\text{ex}} - u_M^N$ for $M = 41$ and different values of N

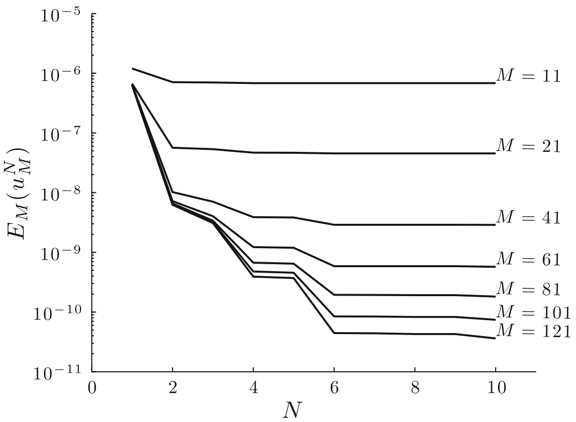


Fig. 2.5 PGD error $E_M(u_M^N)$ as a function of the number of enrichment steps N for different numbers M of discretization points

2.2 Taking into Account Neumann Boundary Conditions

In the sequel, we still consider the Poisson equation (2.1) with a constant source term defined in the domain $\Omega = \Omega_x \times \Omega_y$. The boundary conditions are somewhat different, however. We indeed specify a flux or Neumann condition along part of the domain boundary:

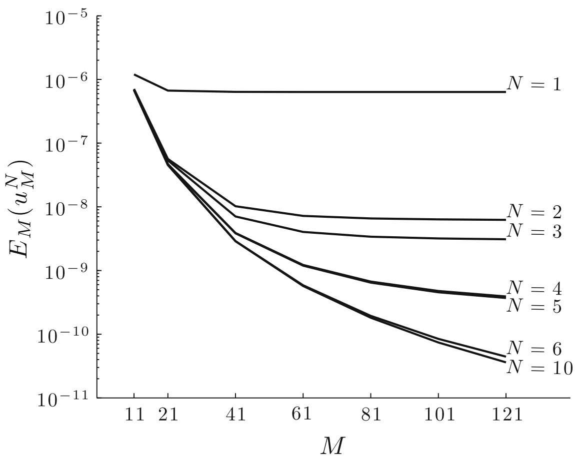


Fig. 2.6 PGD error $E_M(u_M^N)$ as a function of the number of grid points M for different numbers N of enrichment steps

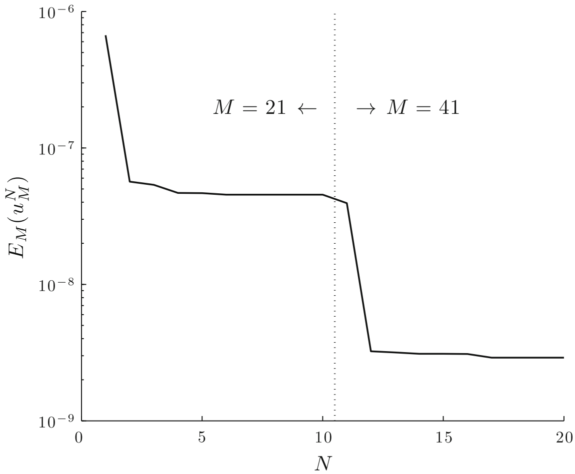


Fig. 2.7 PGD error $E_M(u_M^N)$ as a function of the number of enrichment steps. The first 10 enrichment steps have been computed on a coarse mesh with $M = 21$. The following enrichment steps have been computed on a finer mesh with $M = 41$

$$\begin{cases} u(x=0,y)=0 \\ u(x=L,y)=0 \\ u(x,y=0)=0 \\ \dfrac{\partial u}{\partial y}\Big|_{x,y=H}=q \end{cases} . \tag{2.30}$$

The classical way of accounting for Neumann conditions is to integrate by parts the weighted residual form (2.3) and implement the flux condition as a so-called natural boundary condition:

$$-\int_{\Omega_x \times \Omega_y} \nabla u^* \cdot \nabla u \, dx \cdot dy \; = \; \int_{\Omega_x \times \Omega_y} u^* \cdot f \; dx \cdot dy - \int_{\Omega_x} u^*(x, y = H) \cdot q \; dx, \tag{2.31}$$

or more explicitly

$$\int_{\Omega_x \times \Omega_y} \left(\frac{\partial u^*}{\partial x} \cdot \frac{\partial u}{\partial x} + \frac{\partial u^*}{\partial y} \cdot \frac{\partial u}{\partial y} \right) dx \cdot dy$$

$$= -\int_{\Omega_x \times \Omega_y} u^* \cdot f \; dx \cdot dy + \int_{\Omega_x} u^*(x, y = H) \cdot q \; dx. \tag{2.32}$$

This is the starting point from which a PGD solution can be sought in the separated form

$$u(x, y) = \sum_{i=1}^{N} X_i(x) \cdot Y_i(y). \tag{2.33}$$

The PGD solution procedure then readily follows as described in the first case study. At enrichment step n, one iteration p of the alternating direction strategy amounts to the following computations:

- Calculating $X_n^p(x)$ from $Y_n^{p-1}(y)$

  At this stage, the PGD approximation is given by

$$u^{n,p}(x, y) = \sum_{i=1}^{n-1} X_i(x) \cdot Y_i(y) + X_n^p(x) \cdot Y_n^{p-1}(y), \tag{2.34}$$

  where $X_n^p(x)$ is the only unknown function.

  Using Galerkin's method, we select the following weight function

$$u^*(x, y) = X_n^*(x) \cdot Y_n^{p-1}(y). \tag{2.35}$$

  Inserting (2.34) and (2.35) into (2.32), we obtain

$$\int_{\Omega_x \times \Omega_y} \left(\frac{dX_n^*}{dx} \cdot \frac{dX_n^p}{dx} \cdot \left(Y_n^{p-1} \right)^2 + X_n^* \cdot X_n^p \cdot \left(\frac{dY_n^{p-1}}{dy} \right)^2 \right) dx \cdot dy$$

$$= -\int_{\Omega_x \times \Omega_y} \sum_{i=1}^{n-1} \left(\frac{dX_n^*}{dx} \cdot \frac{dX_i}{dx} \cdot Y_n^{p-1} \cdot Y_i + X_n^* \cdot X_i \cdot \frac{dY_n^{p-1}}{dy} \cdot \frac{dY_i}{dy} \right) dx \cdot dy$$

$$-\int_{\Omega_x \times \Omega_y} X_n^* \cdot Y_n^{p-1} \cdot f \; dx \cdot dy + \int_{\Omega_x} X_n^* \cdot Y_n^{p-1}(y = H) \cdot q \; dx. \tag{2.36}$$

In the above expression, all functions of the coordinate y are known, and we can evaluate the corresponding one-dimensional integrals:

$$\begin{cases} \alpha^x = \int_{\Omega_y} \left(Y_n^{p-1}(y) \right)^2 \, dy \\ \beta^x = \int_{\Omega_y} \left(\dfrac{dY_n^{p-1}(y)}{dy} \right)^2 \, dy \\ \gamma_i^x = \int_{\Omega_y} Y_n^{p-1}(y) \cdot Y_i(y) \, dy \\ \delta_i^x = \int_{\Omega_y} \dfrac{dY_n^{p-1}(y)}{dy} \cdot \dfrac{dY_i(y)}{dy} \, dy \\ \xi^x = \int_{\Omega_y} Y_n^{p-1}(y) \cdot f \, dy \\ \mu^x = Y_n^{p-1}(y = H) \cdot q \end{cases}. \tag{2.37}$$

We thus obtain the weighted residual form of an elliptic problem for $X_n^p(x)$ defined over Ω_x:

$$\int_{\Omega_x} \left(\frac{dX_n^*}{dx} \cdot \frac{dX_n^p}{dx} \cdot \alpha^x + X_n^* \cdot X_n^p \cdot \beta^x \right) dx$$

$$= -\int_{\Omega_x} \sum_{i=1}^{n-1} \left(\frac{dX_n^*}{dx} \cdot \frac{dX_i}{dx} \cdot \gamma_i^x + X_n^* \cdot X_i \cdot \delta_i^x \right) dx$$

$$-\int_{\Omega_x} X_n^* \cdot \xi^x \, dx + \int_{\Omega_x} X_n^* \cdot \mu^x \, dx. \tag{2.38}$$

The finite element method, for example, can then be used to discretize this one-dimensional problem, with the remaining Dirichlet condition $X_n^p(x = 0) = X_n^p(x = L) = 0$.

- Calculating $Y_n^p(y)$ from the just computed $X_n^p(x)$

Here again, the second step of iteration p simply mirrors the first one with an exchange of role between x and y coordinates.

The current PGD approximation reads

$$u^{n,p}(x, y) = \sum_{i=1}^{n-1} X_i(x) \cdot Y_i(y) + X_n^p(x) \cdot Y_n^p(y), \tag{2.39}$$

where $Y_n^p(y)$ is the only unknown function.

Selecting the Galerkin method, i.e.

$$u^*(x,y) = X_n^p(x) \cdot Y_n^*(y), \tag{2.40}$$

we introduce (2.39) and (2.40) into (2.32) to obtain

$$\begin{aligned}
&\int_{\Omega_x \times \Omega_y} \left(\left(\frac{dX_n^p}{dx} \right)^2 \cdot Y_n^* \cdot Y_n^p + \left(X_n^p \right)^2 \cdot \frac{dY_n^*}{dy} \cdot \frac{dY_n^p}{dy} \right) dx \cdot dy \\
&= -\int_{\Omega_x \times \Omega_y} \sum_{i=1}^{n-1} \left(\frac{dX_n^p}{dx} \cdot \frac{dX_i}{dx} \cdot Y_n^* \cdot Y_i + X_n^p \cdot X_i \cdot \frac{dY_n^*}{dy} \cdot \frac{dY_i}{dy} \right) dx \cdot dy \\
&\quad - \int_{\Omega_x \times \Omega_y} X_n^p \cdot Y_n^* \cdot f \; dx \cdot dy + \int_{\Omega_x} X_n^p \cdot Y_n^*(y=H) \cdot q \; dx.
\end{aligned} \tag{2.41}$$

Now, all functions of x are known, and we can compute the integrals

$$\left\{ \begin{array}{l}
\alpha^y = \int_{\Omega_x} \left(X_n^p(x) \right)^2 \; dx \\
\beta^y = \int_{\Omega_x} \left(\dfrac{dX_n^p(x)}{dx} \right)^2 \; dx \\
\gamma_i^y = \int_{\Omega_x} X_n^p(x) \cdot X_i(x) \; dx \\
\delta_i^y = \int_{\Omega_x} \dfrac{dX_n^p(x)}{dx} \cdot \dfrac{dX_i(x)}{dx} \; dx \\
\xi^y = \int_{\Omega_x} X_n^p(x) \cdot f \; dx \\
\mu^y = \int_{\Omega_x} X_n^p(x) \cdot q \; dx
\end{array} \right. . \tag{2.42}$$

We thus obtain the weighted residual form of an elliptic problem for $Y_n^p(y)$ defined over Ω_y:

$$\begin{aligned}
&\int_{\Omega_y} \left(\beta^y \cdot Y_n^* \cdot Y_n^p + \alpha^y \cdot \frac{dY_n^*}{dy} \cdot \frac{dY_n^p}{dy} \right) dy \\
&= -\int_{\Omega_y} \sum_{i=1}^{n-1} \left(\delta_i^y \cdot Y_n^* \cdot Y_i + \gamma_i^y \cdot \frac{dY_n^*}{dy} \cdot \frac{dY_i}{dy} \right) dy \\
&\quad - \int_{\Omega_y} \xi^y \cdot Y_n^* \; dy + Y_n^*(y=H) \cdot \mu^y.
\end{aligned} \tag{2.43}$$

Here again, we can use the finite element method to discretize this one-dimensional problem, with the remaining Dirichlet conditions $Y_n^p(y=0) = 0$.

2.3 Increasing the Complexity of the Case Study

2.3.1 Non-Constant Source Term

We have assumed so far a constant source term f. We now extend the PGD strategy to the case of a non-uniform source $f(x, y)$. We shall see in Sect. 3.2 how to obtain a separated representation of f in the form

$$f(x, y) = \sum_{j=1}^{\mathcal{F}} F_j^x(x) \cdot F_j^y(y). \tag{2.44}$$

With the following notation,

$$\xi_j^x = \int_{\Omega_y} Y_n^{p-1}(y) \cdot F_j^y(y)\, dy, \tag{2.45}$$

it is then easy to verify that (2.13) and (2.38) become respectively

$$\int_{\Omega_x} X_n^* \cdot \left(\alpha^x \cdot \frac{d^2 X_n^p}{dx^2} + \beta^x \cdot X_n^p \right) dx$$

$$= - \int_{\Omega_x} X_n^* \cdot \sum_{i=1}^{n-1} \left(\gamma_i^x \cdot \frac{d^2 X_i}{dx^2} + \delta_i^x \cdot X_i \right) dx + \int_{\Omega_x} X_n^* \cdot \left(\sum_{j=1}^{\mathcal{F}} \xi_j^x \cdot F_j^x(x) \right) dx, \tag{2.46}$$

and

$$\int_{\Omega_x} \left(\frac{dX_n^*}{dx} \cdot \frac{dX_n^p}{dx} \cdot \alpha^x + X_n^* \cdot X_n^p \cdot \beta^x \right) dx$$

$$= - \int_{\Omega_x} \sum_{i=1}^{n-1} \left(\frac{dX_n^*}{dx} \cdot \frac{dX_i}{dx} \cdot \gamma_i^x + X_n^* \cdot X_i \cdot \delta_i^x \right) dx$$

$$- \int_{\Omega_x} X_n^* \cdot \left(\sum_{j=1}^{\mathcal{F}} \xi_j^x \cdot F_j^x(x) \right) dx + \int_{\Omega_x} X_n^* \cdot \mu^x \, dx. \tag{2.47}$$

Similarly, with the definition

$$\xi_j^y = \int_{\Omega_x} X_n^p(x) \cdot F_j^x(x)\, dx, \tag{2.48}$$

Equations (2.19) and (2.43) become respectively

$$\int_{\Omega_y} Y_n^* \cdot \left(\alpha^y \cdot \frac{d^2 Y_n^p}{dy^2} + \beta^y \cdot Y_n^p \right) \, dy$$

$$= - \int_{\Omega_y} Y_n^* \cdot \sum_{i=1}^{n-1} \left(\gamma_i^y \cdot \frac{d^2 Y_i}{dy^2} + \delta_i^y \cdot Y_i \right) \, dy \; + \int_{\Omega_y} Y_n^* \cdot \left(\sum_{j=1}^{j=\mathcal{F}} \xi_j^y \cdot F_j^y(y) \right) \, dy \tag{2.49}$$

and

$$\int_{\Omega_y} \left(\beta^y \cdot Y_n^* \cdot Y_n^p + \alpha^y \cdot \frac{dY_n^*}{dy} \cdot \frac{dY_n^p}{dy} \right) \, dy$$

$$= - \int_{\Omega_y} \sum_{i=1}^{n-1} \left(\delta_i^y \cdot Y_n^* \cdot Y_i + \gamma_i^y \cdot \frac{dY_n^*}{dy} \cdot \frac{dY_i}{dy} \right) \, dy$$

$$- \int_{\Omega_y} Y_n^* \cdot \left(\sum_{j=1}^{j=\mathcal{F}} \xi_j^y \cdot F_j^y(y) \right) \, dy + Y_n^*(y = H) \cdot \mu^y. \tag{2.50}$$

The same procedure is used when the problem to be solved has non-constant coefficients.

2.3.2 Non-Homogeneous Dirichlet Boundary Conditions

Let us now specify non-homogeneous Dirichlet conditions along a part Γ_D of the domain boundary Γ: $u(x, y) = \overline{u}(x, y) \neq 0$ for $(x, y) \in \Gamma_D$.

In order to apply the PGD strategy, we simply consider a function $g(x, y)$ regular enough that satisfies the same Dirichlet conditions, i.e. $g(x, y) = \overline{u}(x, y)$ for $(x, y) \in \Gamma_D$, but is otherwise arbitrary [3].

Then again, as explained in Sect. 3.2, we compute *a priori* the separated representation of the function $g(x, y)$

$$g(x, y) = \sum_{j=1}^{\mathcal{G}} G_j^x(x) \cdot G_j^y(y). \tag{2.51}$$

This expansion can be seen as a (very) approximate solution that satisfies the Dirichlet boundary conditions but does not verify neither the partial differential equation nor the natural boundary conditions. In order to enforce both, it suffices to enrich this approximation to obtain

$$u(x, y) = \sum_{j=1}^{N} X_i(x) \cdot Y_i(y), \tag{2.52}$$

where $X_i(x) = G_i^x(x)$ and $Y_i(y) = G_i^y(y)$, for $i = 1, \ldots, \mathcal{G}$. The remaining functions $X_i(x)$ and $Y_i(y)$, for $i > \mathcal{G}$, are calculated by using the PGD procedure described previously for homogeneous Dirichlet conditions.

2.3.3 Higher Dimensions and Separability of the Computational Domain

The PGD procedure described in this chapter can easily be generalized to models defined in D dimensions as long as the computational domain is *separable*. By this we mean that the domain is the Cartesian product of one-dimensional intervals:

$$\Omega = \Omega_1 \times \Omega_2 \times \cdots \times \Omega_D. \tag{2.53}$$

Thus, the unknown field $u(x_1, \ldots, x_D)$ is sought in the separated form

$$u(x_1, \ldots, x_D) = \sum_{i=1}^{N} X_i^1(x_1) \times \cdots \times X_i^D(x_D). \tag{2.54}$$

For example, should we consider the Poisson equation, then its PGD solution in Ω would involve a series of decoupled one-dimensional problems (second-order ordinary differential equations) formulated in each Ω_i.

For a non-separable domain, one possible approach consists in embedding Ω into a separable domain $\overline{\Omega} = \overline{\Omega}_1 \times \overline{\Omega}_2 \times \cdots \times \overline{\Omega}_D$ such that $\Omega \subset \overline{\Omega}$. One then applies the PGD strategy in $\overline{\Omega}$ together with an appropriate penalty formulation in $\overline{\Omega} \setminus \Omega$ [3].

In many applications, the computational domain is not strictly separable according to our definition, but it is the Cartesian product of multi-dimensional sets. One can then easily apply a PGD strategy by separating the coordinates into the several groups that correspond to these sets. For example, consider a three-dimensional extruded domain $\Omega = \Omega_{(x,y)} \times \Omega_z$. Here, the domain Ω is the extrusion of the non-separable two-dimensional domain $\Omega_{(x,y)}$ along the z axis. In this case, the PGD decomposition reads most naturally

$$u(x, y, z) = \sum_{i=1}^{N} X_i(x, y) \cdot Z_i(z). \tag{2.55}$$

This approach is particularly well suited to problems involving plates, shells or profiled geometries. The PGD calculations thus involve a series of decoupled two-dimensional problems in $\Omega_{(x,y)}$ to compute the functions $X_i(x, y)$, and one-dimensional problems in Ω_z to compute the functions $Z_i(z)$. As a result, the fully-three dimensional PGD simulation has a numerical complexity typical of two-dimensional analyses.

2.4 Numerical Examples

2.4.1 2D Heat Transfer Problem

In this section, we illustrate the developments of the previous sections by comparing the PGD and the finite element solutions of the following problem:

$$\Delta u(x, y) = f(x, y), \tag{2.56}$$

defined in a two-dimensional rectangular domain $\Omega = \Omega_x \times \Omega_y = (0, 2) \times (0, 1)$. The boundary conditions are specified as follows:

$$\begin{cases} u(x = 0, y) = y \cdot (1 - y) \\ u(x = 2, y) = 0 \\ u(x, y = 0) = 0 \\ \dfrac{\partial u}{\partial y}|_{x, y=1} = -1 \end{cases} . \tag{2.57}$$

Thus, we can write (2.51) as:

$$g(x, y) = G_1^x(x) \cdot G_1^y(y) = \frac{2 - x}{2} \cdot y \cdot (1 - y). \tag{2.58}$$

Finally, we consider the following separated representation for the source term $f(x, y)$:

$$f(x, y) = F_1^x(x) \cdot F_1^y(y) = -5e^{-10 \cdot (x-1)^2} \cdot e^{-10 \cdot (y-0.5)^2}. \tag{2.59}$$

The unknown functions $X_i(x)$ and $Y_i(y)$ are sought on a uniform grid with $M = 41$ points. All one-dimensional differential problems and integrals arising in the solution procedure are solved or computed using linear one-dimensional finite elements. The stopping criteria for the fixed point iterations and the enrichment process are those described by (2.8) and (2.26), respectively. Error levels are computed using the following expression:

$$E_M(u_M^N) = \int_0^1 \int_0^2 \Big(u_{\mathrm{FE},M}(x, y) - u_M^N(x, y) \Big)^2 \, dx \cdot dy, \tag{2.60}$$

where $u_{\mathrm{FE},M}(x, y)$ is the corresponding 2D finite element solution on an equivalent mesh.

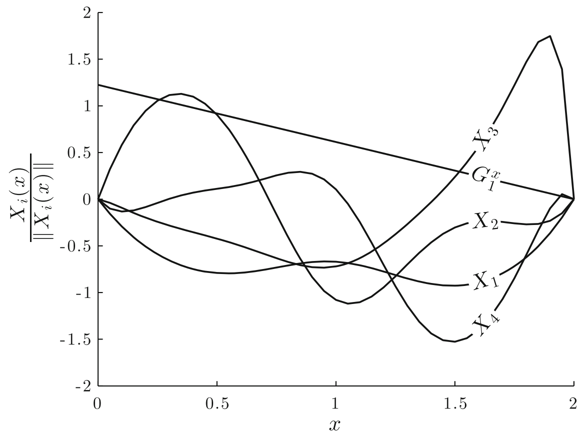


Fig. 2.8 Normalized functions $G_1^x(x)$ and $X_i(x)$ for $i = 1, \ldots, 4$

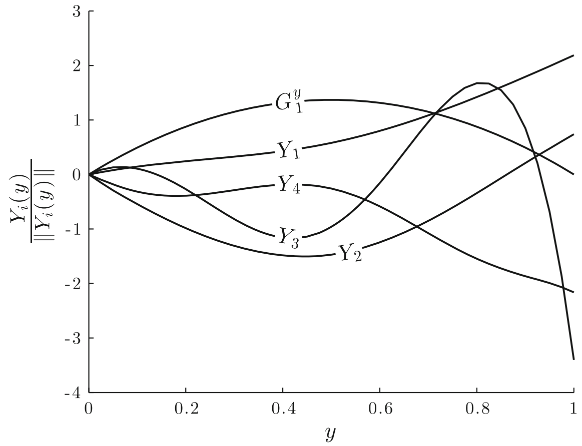


Fig. 2.9 Normalized functions $G_1^y(y)$ and $Y_i(y)$ for $i = 1, \ldots, 4$

In Figs. 2.8 and 2.9, we show the normalized functions $G_1^x(x)$, $X_i(x)$, $G_1^y(y)$ and $Y_i(y)$ for $i = 1, \ldots, 4$. In Fig. 2.8 one can observe that only $G_1^x(x)$ is non-zero for $x = 0$ since all the $X_i(x)$ have to preserve the non-zero Dirichlet condition imposed through $G_1^x(x)$ and $G_1^y(y)$.

We first illustrate the pointwise convergence of the PGD solution towards the reference solution in Fig. 2.10 where we plot $u_{\mathrm{FE},M} - u_M^N$ for $M = 41$ and different values of N. For $N = 0$, the solution reduces to $u(x, y) = g(x, y)$. We further illustrate the convergence of the PGD solution in Fig. 2.11 by showing $E_M(u_M^N)$ as a function of N.

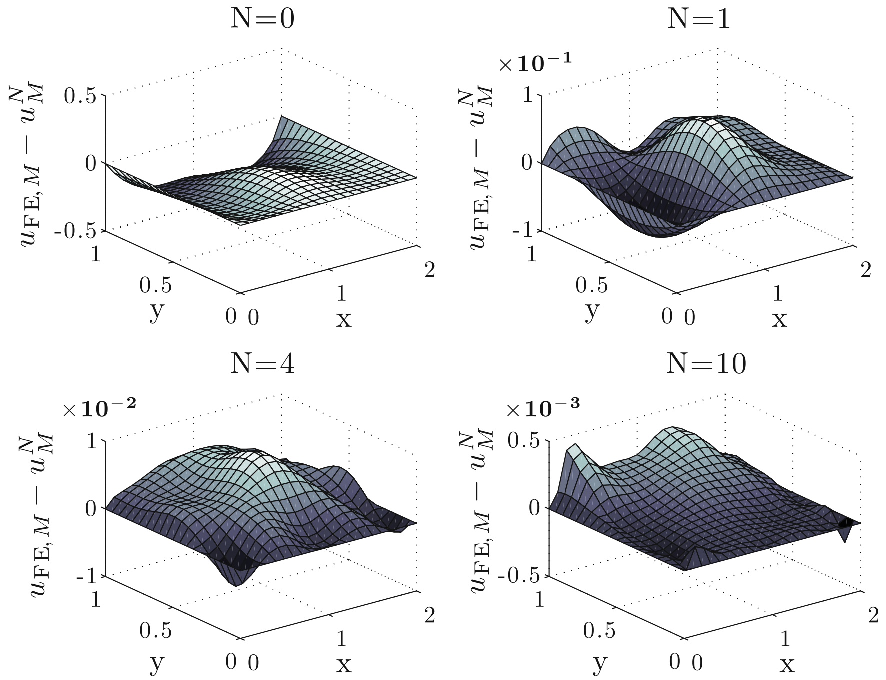
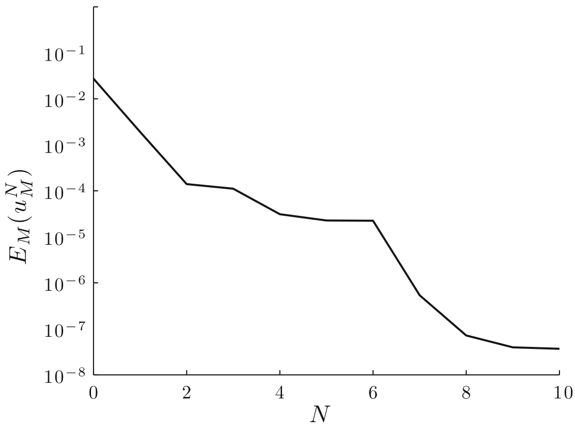


Fig. 2.10 $u_{\mathrm{FE},M} - u_M^N$ for $M = 41$ and different values of N

Fig. 2.11 PGD error $E_M(u_M^N)$ as a function of the number N of enrichment steps for $M = 41$



2.4.2 High-Dimensional Problem

We now focus on the solution of the following high-dimensional problem:

$$\Delta u(x_1, \ldots, x_D) = f(x_1, \ldots, x_D), \tag{2.61}$$

in a D-dimensional hypercube $\Omega = \Omega_1 \times \cdots \times \Omega_D = (-1, 1) \times \cdots \times (-1, 1)$. The boundary conditions are homogeneous on the whole boundary of Ω . The source term $f(x_1, \ldots, x_D)$ is taken such that we have the following 2-term separated solution:

$$u_{\text{ex}}^D = \prod_{d=1}^{D} x_d \cdot \sin(d \cdot \pi \cdot x_d) + \prod_{d=1}^{D} x_d^2 \cdot \sin((D+1-d) \cdot \pi \cdot x_d) . \tag{2.62}$$

Similarly to the previous examples, we seek a N-term PGD solution of the form:

$$u_{M,N}^D = \sum_{i=1}^{N} \prod_{d=1}^{D} X_i^d(x_d), \tag{2.63}$$

where M is the number of finite element nodal values along each dimension. Remember that, using standard grid-based methods, the solution would involve M^D degrees of freedom. Again, the one-dimensional integrals and BVP arising in the PGD solution procedure are computed using linear finite elements. Error levels are computed using the following expression:

$$E_M^D(u_{M,N}^D) = \tilde{\int}_{\Omega_1} \cdots \tilde{\int}_{\Omega_D} \left(u_{\text{ex}}^D - u_{M,N}^D\right)^2 \, dx_1 \cdots dx_D, \tag{2.64}$$

where $\tilde{\int}$ refers to the numerical integration on the finite element mesh. We show in Fig. 2.12, for $M = 101$, the decrease of the normalized error levels for different values of D as we increase the number of terms in the PGD solution. In this particular case, the PGD solution is optimal in the sense that after only two enrichment steps, the relative error is about 10^{-15} and does not decrease upon further enrichment.

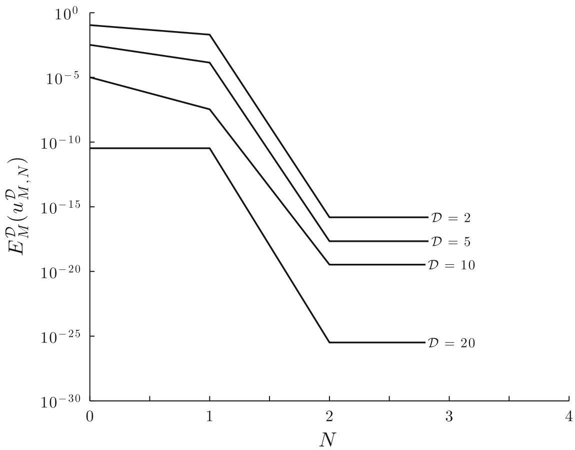


Fig. 2.12 PGD error $E_M^D(u_{M,N}^D)$ as a function of the number N of enrichment steps for different values of D and $M = 101$

For $D = 10$, the PGD solution is computed in a few seconds on a laptop computer. Traditional grid-based methods with the same level of discretization would require more than 10^{20} degrees of freedom, which is far beyond the capabilities of today's computers.

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