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Bayesian assimilation of multi-fidelity finite element models

F.A. DiazDelaO *,[1], S. Adhikari [2]

Civil and Computational Engineering Centre, College of Engineering, Swansea University, Singleton Park, Swansea, SA2 8PP, United Kingdom

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ABSTRACT

A complex system can be modeled using various fidelities with the finite element method. A high-fidelity model is expected to be more computationally expensive compared to a low-fidelity model and in general may contain more degrees of freedom and more elements. This paper proposes a novel multi-fidelity approach to solve boundary value problems using the finite element method. A Bayesian approach based on Gaussian process emulators in conjunction with the domain decomposition method is developed. Using this approach one can seamlessly assimilate a low-fidelity model with a more expensive high-fidelity model. The idea is illustrated using elliptic boundary value problems.

1. Introduction

The size of the finite element models has increased significantly over the past decade. For example, in the automotive industry, 2 to 5 million degrees-of-freedom models are quite common nowadays. Such high-resolution models, combined with detailed physics can give good fidelity to experimental results. However, a potential disadvantage is that such large models may be computationally expensive. One alternative to address this problem is to use a low-resolution model. Although such low-resolution models are often used during the design iteration, they are likely to be low-fidelity and may miss some crucial physics. The motivation of this paper is therefore to investigate the possibility of improving the fidelity of a low-fidelity model without completely solving a detailed high-fidelity problem.

A common tool when solving expensive finite element models is the domain decomposition method [1–7], a divide-and-conquer algorithm aimed at solving partial differential equations (PDEs). Its main feature is that a linear system of discretised PDEs is recast as a set of smaller linear systems to be solved separately. A finite element model can thus be parallelized by partitioning the domain Ω in a number of subdomains. This allows an increase in the resolution of the model, along with a reduction in CPU requirements. There is, however, a potential disadvantage with this approach, since in order to obtain the finite element solution for each subdomain, the governing PDEs must be solved in the interface of each pair of subdomains. This paper presents a metamodeling approach, known as *Gaussian process emulation*, in order to approximate the solution to the interface problem. Broadly speaking, a Gaussian process emulator works by treating a set of *training runs* as data, which is in turn used to update some prior beliefs about the output of an expensive *simulator* such as the interface problem. These beliefs are represented by a Gaussian stochastic process prior distribution. As noted by some authors [8], the choice of a Gaussian process is made for much the same reasons that the Gaussian distribution repeatedly appears in statistics: it is analytically tractable, flexible, and quite often realistic. After conditioning on the training runs and updating the prior distribution, the mean of the resulting posterior distribution approximates the output of the simulator at any untried node in the input domain of the interface problem, whereas it reproduces the known output at each input belonging to the training runs. The idea of using a stochastic process to solve domain decomposition problems has been employed in the past [9]. However, the implementation of Gaussian process emulators is relatively simple and flexible. In addition to this, Gaussian process emulators have already been implemented in various scientific fields in order to alleviate the computational burden of expensive simulators with encouraging results. These fields include climate prediction [10,11], environmental science [12], medicine [13–15], structural dynamics [16,17], reservoir forecasting [18], hydrogeology [19], quality control [20], heat transfer [21], and reliability analysis [22], among others.

The paper is organized as follows. Section 2 introduces the concepts of mutli-fidelity modeling in the context of finite element method. A brief overview of domain decomposition and

* Corresponding author. Tel.: +44 01792 602088; fax: +44 01792 295676.
E-mail addresses: f.a.diazdelao@swansea.ac.uk (F.A. DiazDelaO), s.adhikari@swansea.ac.uk (S. Adhikari).
URLs: http://engweb.swan.ac.uk/~diazdelao/ (F.A. DiazDelaO), http://engweb.swan.ac.uk/~adhikaris/ (S. Adhikari).
[1] Project officer at ASTUTE (http://www.astutewales.com/).
[2] Professor of Aerospace Engineering.

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metamodeling is given in Section 3. Section 4 discusses the theory behind the Gaussian process emulation. Section 5 explains the proposed coupling between domain decomposition and Gaussian process emulators. Section 6 presents some numerical results of the proposed method applied to the deformation of a membrane on a domain with different geometries. Section 7 offers some conclusions based on the results obtained in the paper.

2. Multi-fidelity finite element modeling

Let Ω be a bounded domain in $\mathbb{R}^2$ with Lipschitz continuous boundary $\partial\Omega$, that is, there exist a finite number of covering open sets $\mathcal{O}_\ell$ such that, for every $\ell, \partial\Omega \cap \mathcal{O}_\ell$ is the graph of a Lipschitz continuous function and $\Omega \cap \mathcal{O}_\ell$ lies on one side of this graph. Let $\mathcal{T}^h$ be a family of conforming meshes (triangles) which are shape-regular as the mesh size $h \to 0$. Consider the elliptic PDE with the following Dirichlet boundary condition

$$\begin{aligned} &-\nabla[\alpha(\mathbf{x})\nabla u(\mathbf{x})] + \beta(\mathbf{x})u(\mathbf{x}) = \phi(\mathbf{x}); \quad \mathbf{x} \in \Omega \\ &u(\mathbf{x}) = 0; \quad \mathbf{x} \in \partial\Omega \end{aligned} \tag{1}$$

The Hilbert space $L^2(\Omega)$ and Sobolev space $H^k(\Omega)$ are respectively endowed with inner products $(u, v) = \int_\Omega u(\mathbf{x})v(\mathbf{x})d\mathbf{x}$ and $(u, v)_k = \int_\Omega u(\mathbf{x})v(\mathbf{x})d\mathbf{x} + \int_\Omega \left(\frac{du}{d\mathbf{x}}\right)\left(\frac{dv}{d\mathbf{x}}\right)d\mathbf{x} + \cdots + \int_\Omega \left(\frac{d^k u}{d\mathbf{x}^k}\right)\left(\frac{d^k v}{d\mathbf{x}^k}\right)d\mathbf{x}$. The aim is to obtain the function $u : \Omega \to \mathbb{R}$ which satisfies the conditions of problem (1) for a given $\phi : \Omega \to \mathbb{R}$.

Applying the standard finite element method [23,24], the PDE in problem (1) can be expressed in the matrix form as

$$\mathcal{K}u = f \tag{2}$$

where $\mathcal{K} \in \mathbb{R}^{N\times N}$ is the stiffness matrix, $u \in \mathbb{R}^N$ is the displacement vector and $f \in \mathbb{R}^N$ is the forcing vector. Note that N is the number of degrees of freedom in the underlying finite element mesh.

Suppose L_f and H_f are two finite element models to solve problem (1). Let $n_e^{(L_f)}$ and $n_e^{(H_f)}$ denote the number of elements in the finite element meshes of L_f and H_f induced by Eq. (2) and let $N^{(L_f)}$ and $N^{(H_f)}$ be the number of degrees of freedom. Let $h^{(L_f)}$ and $h^{(H_f)}$ be the respective element size. Also, let $u^*(\mathbf{x})$ and $U^*(\mathbf{x})$ be a solution to L_f and H_f respectively, and let $u^{(r)}$ be the exact solution to (1). That way, $\|u^{(r)}(\mathbf{x}) - u^*(\mathbf{x})\|$ and $\|u^{(r)}(\mathbf{x}) - U^*(\mathbf{x})\|$ are the differences between the exact solution and the solution to the models L_f and H_f, with $\|\cdot\|$ being the Euclidean norm. We call L_f a low-fidelity model and H_f a high-fidelity model if the following inequalities hold:

1. $\|u^{(r)}(\mathbf{x}) - u^*(\mathbf{x})\| > \|u^{(r)}(\mathbf{x}) - U^*(\mathbf{x})\|$ (Accuracy)
2. $h^{(L_f)} > h^{(H_f)}$ (Resolution)
3. $N^{(L_f)} < N^{(H_f)}$ (number of degrees of freedom)
4. $n_e^{(L_f)} < n_e^{(H_f)}$ (number of elements)

It is important to note that the concepts of low and high fidelity based on the above definition are relative. A single refinement of a given low-fidelity mesh would imply a different increase in the fidelity of the model depending on the particular characteristics of the problem at hand. A more accurate description of L_f and H_f would therefore be “lower” and “higher” fidelity models respectively. Keeping this note in mind, the current low and high fidelity terminology is kept in the remainder of the paper. Also, note that in the above definition it is implicitly assumed that both models L_f and H_f have same polynomial order p. A general hp finite element model is beyond the scope of this paper (see for example [25]). Fig. 1 shows two finite element models on a D-shaped domain, each with a different fidelity level.

3. A brief overview of domain decomposition and metamodeling

3.1. The domain decomposition method

Let Ω be partitioned in S subdomains $\{\Omega_j : 1 \leqslant j \leqslant S\}$, such that $\overline{\Omega} = \bigcup_j \overline{\Omega}_j$. Suppose these domains are non-overlapping, that is $\Omega_j \bigcap \Omega_k = \emptyset$, $\forall j \neq k$. The interface is denoted by Γ, where

$$\Gamma = \bigcup_{i,j} (\partial\Omega_i \cap \partial\Omega_j) \setminus \partial\Omega \tag{3}$$

In Fig. 2, the D-shaped domain Ω from Fig. 1 is partitioned into subdomains Ω_1 and Ω_2. The interface Γ separates both subdomains. Fig. 3 shows the finite element mesh of the partitioned low-fidelity model L_f and the partitioned high-fidelity model H_f. In order to obtain the solution to these finite element models, it can be shown [1] that if Ω is the disjoint union of the subdomains $\Omega_1, \ldots, \Omega_S$, then the discretised PDEs governing the system's response can be recast as the following partitioned linear system

$$\begin{pmatrix} \mathcal{K}_1 & 0 & \cdots & 0 & \mathcal{B}_1^{\mathrm{T}} \\ 0 & \mathcal{K}_2 & \cdots & 0 & \mathcal{B}_2^{\mathrm{T}} \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & \mathcal{K}_n & \mathcal{B}_S^{\mathrm{T}} \\ \mathcal{B}_1 & \mathcal{B}_2 & \cdots & \mathcal{B}_S & C \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \\ \vdots \\ u_n \\ u_c \end{pmatrix} = \begin{pmatrix} f_1 \\ f_2 \\ \vdots \\ f_S \\ f_c \end{pmatrix} \tag{4}$$

The solution of the partitioned linear system (4) is obtained by solving the interface problem

$$\begin{aligned} &(C - \mathcal{B}_1\mathcal{K}_1^{-1}\mathcal{B}_1^{\mathrm{T}} - \cdots - \mathcal{B}_S\mathcal{K}_S^{-1}\mathcal{B}_S^{\mathrm{T}})u_c \\ &\quad = f_c - \mathcal{B}_1\mathcal{K}_1^{-1}f_1 - \cdots - \mathcal{B}_S\mathcal{K}_S^{-1}f_S \end{aligned} \tag{5}$$

and then solving in parallel

$$\begin{aligned} &u_1 = \mathcal{K}_1^{-1}(f_1 - \mathcal{B}_1^{\mathrm{T}}u_c) \\ &\vdots \\ &u_S = \mathcal{K}_S^{-1}(f_S - \mathcal{B}_S^{\mathrm{T}}u_c) \end{aligned} \tag{6}$$

Fig. 4 shows the domain decomposition solution of problem (1) for H_f and for the values $\alpha(\mathbf{x}) = 1$, $\beta(\mathbf{x}) = 0$, and $\phi = 1$. The model represents the deformation of a membrane in the domain Ω.

The main problem with solving a finite element model using domain decomposition is that the Schur complement matrix

$$\Sigma = C - \mathcal{B}_1\mathcal{K}_1^{-1}\mathcal{B}_1^{\mathrm{T}} - \cdots - \mathcal{B}_S\mathcal{K}_S^{-1}\mathcal{B}_S^{\mathrm{T}} \tag{7}$$

is numerically expensive to obtain. Hence, solving the linear system (5) is likely to become a bottleneck of the domain decomposition strategy for a high-fidelity model H_f. A metamodeling approach is therefore proposed, whereby the solution to the interface problem (5) is approximated using only a few evaluations of a lower-fidelity model L_f.

3.2. Metamodeling approach

Let $u^*(\mathbf{x}) : \Omega \subset \mathbb{R}^2 \to \mathbb{R}$ be a finite element solution to problem (1). If $\mathbf{x} = (x,y)$ and $u^*(\mathbf{x}) = z$, then u^* is a function that maps $(x,y) \mapsto z$. Adopting this notation, a level set of the domain Ω with respect to the x-axis is defined as

$$\mathcal{L}^x(c) = \{z | u^*(c, y) = z; c \in \mathbb{R}\} \tag{8}$$

and analogously for a level set with respect to the y-axis

$$\mathcal{L}^y(d) = \{z | u^*(x, d) = z; d \in \mathbb{R}\} \tag{9}$$

For $n_x, n_y \in \mathbb{Z}^+$, let Λ denote

$$\Lambda = \{\mathcal{L}^x(c_i), \mathcal{L}^y(d_j) | 1 \leqslant i \leqslant n_x, 1 \leqslant j \leqslant n_y\} \tag{10}$$