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Accelerated scale bridging with sparsely approximated Gaussian learning

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ABSTRACT

Multiscale modeling is a systematic approach to describe the behavior of complex systems by coupling models from different scales. The approach has been demonstrated to be very effective in areas of science as diverse as materials science, climate modeling and chemistry. However, routine use of multiscale simulations is often hindered by the very high cost of individual at-scale models. Approaches aiming to alleviate that cost by means of Gaussian process regression based surrogate models have been proposed. Yet, many of these surrogate models are expensive to construct, especially when the number of data needed is large. In this article, we employ a hierarchical sparse Cholesky decomposition to develop a sparse Gaussian process regression method and apply the method to approximate the equation of state of a material in a multiscale model of dynamic deformation. We demonstrate that the method provides a substantial reduction both in computational cost and solution error as compared with previous methods.

1. Introduction

Multiscale modeling has now become a *de facto* standard approach for the construction of high-fidelity models of complex phenomena and systems encountered in many areas of science and engineering [1–6]. The process of building a multiscale model starts with identification of relevant phenomena occurring at individual scales, both spatial and temporal. Thereafter, appropriate at-scale models characterizing these phenomena are selected and combined together into a single multiscale model. Computation is fundamental to multiscale modeling as at-scale models are usually cast in the form of computer models. In recent years, computational aspects of multiscale modeling have become the focal point of numerous research efforts (cf. [7] for an in-depth review of recent developments). These efforts have led to a conclusion that practicality of multiscale modeling hinges on the ability to significantly reduce the often staggering computational cost of at-scale models. Many different approaches have been proposed in order to reduce this cost, with the vast majority falling under the name of surrogate models. A surrogate model is a cheaper-to-evaluate approximation of a model, constructed from direct observations of the model. Surrogate models have been employed with great success in design optimization [8,9], where a model is repeatedly evaluated in the search for an optimal design. In physical sciences, the use of surrogate models can be traced back to the pioneering work of Pope [10], who employed surrogate modeling to enable simulations of combustion chemistry. Other examples of the applications of surrogate models in physical sciences include crystal plasticity [11,12],

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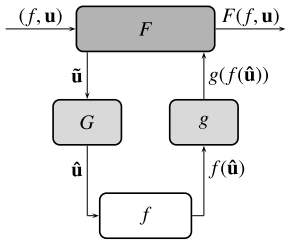

Fig. 1. A two-scale model consisting of macroscale model F and microscale model f. Two mappings transform data between scales: the input filter G which transforms data into an appropriate form for the microscale model and the output filter g which extracts relevant data from the microscale model to inform the macroscale model.

elastodynamics [13,14], atomistic modeling [15,16], quantum chemistry [17,18], and fluid dynamics [19]. A comprehensive survey of surrogate modeling techniques, including polynomial regression, kriging, multivariate adaptive regression splines, polynomial stochastic collocation, adaptive stochastic collocation, and radial basis functions can be found in [20,21].

Gaussian process regression has been advocated as a particularly flexible technique for surrogate model development [22, 23,16]. However, due to a significant cost of construction, Gaussian process regression is rarely employed to build a single surrogate model. Instead, the domain is often partitioned into a set of subdomains and separate surrogate models are built over each of the subdomains. While such an approach inevitably reduces the overall cost of constructing a surrogate model, this reduction in cost may be accompanied by considerable disadvantages, such as, for example, the loss of smoothness of the surrogate model. In this article, we introduce a methodology to reduce the cost of constructing surrogate models based on Gaussian process regression and apply it in the context of multiscale modeling. The methodology relies on the recently developed hierarchical Cholesky decomposition in order to reduce the computational cost for inverting the dense covariance matrix [25]. The computational complexity can be shown to be near-linear with respect to the size of the data set, which is a significant savings compared to the original cubic cost. However, it should be pointed out that the method does not completely resolve the curse of dimensionality issue of Gaussian process regression. Since it requires the construction of a data set over the uniform grid, the number of data points needed grows exponentially with respect to the dimension of the problem. Therefore, the method is particularly suited to low dimensional Gaussian process regression with a large number of data.

The manuscript is organized as follows. We describe the multiscale modeling context of our work in Section 2. The details of our approach are provided in Section 3, along with an application of the technique to constructing a surrogate model of an energetic material in Section 4.

2. A computational framework for scale-bridging in multi-scale simulations

The overarching context of the developments presented in this article is the scale-bridging framework for multiscale modeling of Leiter et al. [16]. Here, we only give a brief description of the framework, the reader is referred to [16] for a full exposition. The most elemental multiscale model consists of two at-scale models, the macroscale model F and the microscale model f (cf. Fig. 1). The macroscale model is a mapping $F : I \times D \mapsto R$, where I is a collection of microscale models, domain $D \subset \mathbb{R}^H$, and range $R \subset \mathbb{R}^\Xi$. Similarly, the microscale model is a mapping $f : \hat{D} \mapsto \hat{R}$ where $\hat{D} \subset \mathbb{R}^\eta$ and $\hat{R} \subset \mathbb{R}^\xi$ denote the domain and range of f, respectively. In addition, the framework includes two mappings to transform data between at-scale models. The mapping $G : \tilde{D} \mapsto \hat{D}$, where $\tilde{D} \subset \mathbb{R}^{\tilde{\eta}}$ is the set of intermediate values derived from values in D by F. Henceforth, we refer to G as the "input filter" since it generates the input to f in the set $\hat{D}$. Likewise, the mapping $g : \hat{R} \mapsto \tilde{R}$, where $\tilde{R} \subset \mathbb{R}^{\tilde{\xi}}$, is referred to as the "output filter" as it extracts relevant data from the microscale model output to be passed to the macroscale model. More complex multiscale models can, of course, be formed through assemblies of multiple two-scale model building blocks.

The centerpiece of the scale-bridging framework is a module coordinating data exchanges between at-scale models, the Evaluation Module (cf. Fig. 2 (a)). The act of sending of $\tilde{\mathbf{u}} \in \tilde{D}$ from F to the Evaluation Module is denoted as an evaluation request. The Evaluation Module carries out five distinct tasks: 1) it collects requests for evaluation of f from F; 2) it applies the input filter to the evaluation requests to prepare input data for microscale models; 3) it schedules evaluation requests on available resources; 4) it monitors progress of evaluations to detect completion and handle failures; and 5) it applies the output filter to extract relevant data from completed f evaluations to return to F. However, in many practical applications, microscale models may be extremely costly to evaluate and methods to lower the evaluation cost are necessary in order to render the approach feasible. A popular approach, pioneered by Pope [10] in combustion modeling, relies on adaptive surrogate modeling, where evaluation requests are utilized to on-the-fly build an approximation to the microscale model. Such an approach is particularly advantageous as the modular structure of the scale-bridging framework allows to incorporate surrogate models with ease. Therefore, the framework can be simply augmented by the Surrogate Module operating along side of the macroscale model and the Evaluation Module (cf. Fig. 2 (b)). The role of the Surrogate Module is to automatically construct a surrogate model from completed microscale model evaluation data and subsequently