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Evaluation of convergence behavior of metamodeling techniques for bridging scales in multi-scale multimaterial simulation

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ABSTRACT

The effectiveness of several metamodeling techniques, viz. the Polynomial Stochastic Collocation method, Adaptive Stochastic Collocation method, a Radial Basis Function Neural Network, a Kriging Method and a Dynamic Kriging Method is evaluated. This is done with the express purpose of using metamodels to bridge scales between micro- and macro-scale models in a multi-scale multimaterial simulation. The rate of convergence of the error when used to reconstruct hypersurfaces of known functions is studied. For sufficiently large number of training points, Stochastic Collocation methods generally converge faster than the other metamodeling techniques, while the DKG method converges faster when the number of input points is less than 100 in a two-dimensional parameter space. Because the input points correspond to computationally expensive micro/meso-scale computations, the DKG is favored for bridging scales in a multi-scale solver.

1. Introduction

1.1. Motivation and applications

A wide variety of problems in multimaterial dynamics including the passage of a shockwave through a gas laden with particles [1], problems involving crack propagation in heterogeneous materials such as bones [2–5] or concrete structures [6,7] involve the intricate coupling of physics at two or more distinct length and time scales. Further examples of such problems include modeling of heterogeneous explosives [8–11], flow of mixtures including sediment transport in river beds [12], flow through fluidized beds [13] and flow of blood, i.e. plasma carrying cells and macromolecules [14]. In such systems, the physics of the micro/meso-scale needs to be represented in macro-scale simulations. This can be achieved by averaging over the heterogeneous micro/meso-scale. In such volume-averaged macro models [15], or homogenized models [16–18], micro/meso physics appear in the form of closure terms in the macro-scale equations.

Process-scale computations typically demand macro-scale governing equations and simulation techniques. For example, in the problem of a shock wave interacting with a dusty gas, the number of dust particles is extremely large. To follow

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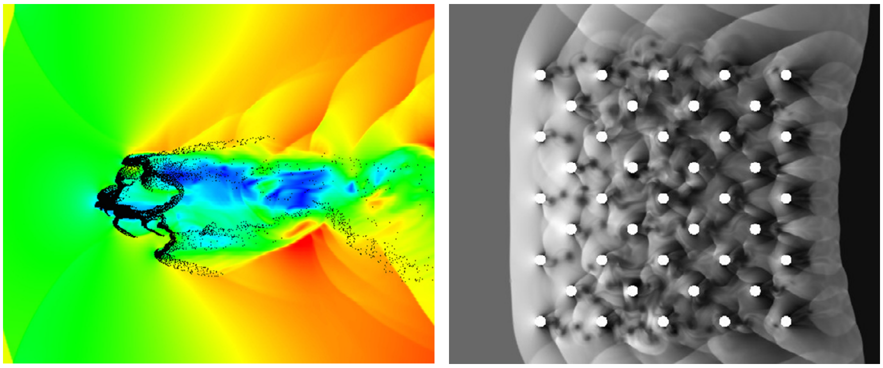

(a) (b)

Fig. 1. Two-dimensional examples of the (a) macro-scale interaction of a large number of modeled particles with a right running normal shock and (b) full resolution meso-scale computation of a small number of particles interacting with a right running normal shock.

the evolution of the gas–solid mixture, a common practice is to define a computational particle as an agglomerate of a number of dust particles and to adopt a mixed Eulerian–Lagrangian viewpoint [17], as in Fig. 1(a). Particle paths are traced in a Lagrangian reference frame while solving the fluid equations in a fixed Eulerian frame. In this approach, the computational particles are modeled as singular point sources, which couple with the carrier fluid through momentum exchange modeled via source terms in the fluid equations [17,19,20]. The source terms close the unresolved momentum exchange between the fluid and solid (particle) phases, providing the forces on the particles. For small particle Reynolds numbers and incompressible flow, the drag on a spherical particle can be determined analytically using Stokes drag law [21]. A range of empirical drag laws exist, which incorporate the effect of inertia [22], compressibility [23,24], slip coefficients [25], various shape factors [26] and/or viscosity ratio for droplets [27] for more complex flows. In general, closure models are obtained in the form of correlations developed in a physical experiment.

Empirical closure models such as drag correlations are only applicable in limited parameter spaces. To overcome this limitation, high resolution micro-scale methods that resolve the dynamics at the particle scale, as can be seen in Fig. 1(b) [28], can be used as surrogates for physical experiments to obtain closure models connecting the meso-scale physics to the macro-scale. In [29] for example, an artificial neural network (ANN) is used to construct a closure model for particle-laden shocked flow based on computational experiments. The neural network then supplies closure terms (drag force) to the macro-scale simulation. Further examples of closure terms constructed from computational experiments using an ANN can be seen in [2–7,30].

1.2. Bridging scales in a multi-scale multimaterial model

There are three components to the multi-scale modeling approach described above: a macro-scale solver which computes the interaction of a large number of particles with a carrier flow, a meso-scale solver, which resolves the fine-scale particle–fluid dynamics of a smaller number of particles and a closure model which calculates the drag and other relevant parameters from the meso-scale solver for use in the macro-scale solver. Generation of a closure model derived from an ensemble of full-resolution meso-scale computations requires quantifying the output from the meso-scale dynamics (for example, drag forces) under a number of different input parameters such as shock strength, particle loading, particle size distribution, etc.

1.3. Metamodels as surrogates to bridge scales

A metamodel, or a 'model of a model' [31], builds a hypersurface from a limited amount of input/output data and approximates the output over a much wider parameter space. An excellent overview of metamodeling techniques is given in [32–34]. Several studies have compared metamodels for reconstructing hypersurfaces from computational experiments. A review of the challenges and concerns in metamodeling techniques can be found in [35] and [36]. In addition, Jin et al. [37] compared the hypersurfaces approximated by a Polynomial Response Surface Method (RSM), a Kriging method, a Radial Basis Function Neural Network (RBFANN), and Multivariate Adaptive Regression splines (MARS) for 14 different test functions. Fang et al. [38] compared the RBFANN method and the RSM method, with the express purpose of reconstructing hypersurfaces in multi-objective crashworthiness optimization. However, these studies have been limited to comparing the quality of approximation only for a given number of input points, and not over a range of input points.

The choice of a "good" metamodeling technique depends on the application and the purpose of the metamodel. Because metamodels are constructed from expensive numerical computations in multi-scale modeling and because the multi-scale method should converge with increasing degrees of freedom, convergence of the metamodels with respect to the number of input points for a wide variety of hypersurfaces warrants careful investigation. This study shows that some metamodeling