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Strategies for efficient machine learning of surrogate drag models from three-dimensional mesoscale computations of shocked particulate flows

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ABSTRACT

Macroscale simulations of shocked particulate flows rely on closure laws to model momentum transfer between the fluid and dispersed particles phase. Developing closure models from experimental data is expensive. Robust and accurate closures laws can be obtained through surrogate modeling using high-resolution mesoscale simulations. However, development of surrogate models for drag from 3D high-fidelity simulations of shock interaction with clusters of particles can be computationally prohibitive. This paper explores various strategies to efficiently construct surrogate models for drag on particles in the shocked flow. The cost of generating training data is reduced by selecting optimal grid resolutions, particle arrangements in clusters, and size of particle clusters, i.e., by selecting suitable representative volumes (RVEs). Different surrogate modeling strategies such as multi-fidelity and parameter-by-parameter construction approaches are examined. The surrogate models obtained from the different methods are compared to determine the most cost-effective machine learning based surrogate modeling method in the context of shock-particle interactions.

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1. Introduction

Shocked particle-laden flows are found in many engineering processes such as combustion in solid rocket motors (Carlson and Hoglund, 1964), pneumatic conveyance of particles in industries (Crowe, 1982), thermal spraying techniques (Dongmo et al., 2008), explosive dispersal of particles (Boiko et al., 1997), etc. Such processes involve large numbers of solid particles transported in a shocked flow field, with length scales ranging from particle scale (μm) to process scale (m). Particle resolved simulations of such engineering processes are cost prohibitive and impractical. The computational burden of resolving each particle in the flow field can be circumvented by modeling the particle phase either as a cloud of dimensionless points (Davis et al., 2017; Jacobs and Don, 2009) or as a continuous two-phase medium (Saito et al., 2003; Shotorban et al., 2013). In such methods, the exchange of momentum and energy between the particulate and fluid phases are not computed directly, but are obtained from empirical laws (Boiko et al., 1997; Parmar et al., 2010) or surrogate models (Lu et al., 2012; Sen et al., 2018a,b;2017) of drag and Nusselt number as functions of the local flow parameters such as Mach number (M_s), Reynolds number (Re), particle volume fraction (ϕ), etc. This paper compares techniques for constructing accurate and computationally affordable surrogate models for drag from ensembles of three-dimensional mesoscale computations.

Typically, models for drag in shocked particle-laden flows are obtained from correlations developed via physical experiments. Such experiments (Boiko et al., 1997; Ling et al., 2012) are expensive and confined to restricted regions in parameter spaces. Recently, there has been considerable efforts in learning drag laws from ensembles of resolved mesoscale computations (Lu et al., 2012; Sen et al., 2018a,b; 2017; 2015). In this approach, several particle-resolved computations are performed to train a surrogate model for the drag coefficient ($\overline{\langle C_D \rangle}$) in particle clouds as functions of M_s and ϕ. While the surrogate-based approach spans a more extensive parameter space than physical experiments, performing large number of such simulations to generate the training data can be computationally intensive and often prohibitively expensive. This is particularly true when 3D mesoscale computations are used to generate the training data.

The first step to mitigate the computational cost for generating training data is to select a robust surrogate modeling technique, i.e., one which offers high rates of convergence for relatively sparse training data sets. Artificial neural networks

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(Ghaboussi et al., 1998; Hambli, 2011; Lu et al., 2012), Radial Basis Functions (Sen et al., 2015), Polynomial Stochastic Collocation Methods (Ma and Zabaras, 2009), Kriging-Based Methods (Zhao et al., 2010) are popular methods for this purpose. Previous work (Sen et al., 2017; 2015) carefully examined these methods and showed that the Modified Bayesian Kriging (MBKG) method (Gaul et al., 2015) is particularly suited for sparse inputs and converges monotonically with fewer, possibly noisy training data. Previously, the MBKG method has been used for developing surrogate models for drag and Nusselt number in shock-particle interaction problems (Das et al., 2018; Sen et al., 2018a,b; 2017). However, these applications have so far been limited to training data obtained from 2D mesoscale simulations. But in 2D simulations particles are represented by cylinders, rather than spheres and the incoming shock wave encounters higher blockage in 2D clusters of particle. Therefore, the drag is over-predicted in 2D simulations. Such modeling limitations in the 2D simulation of shock-particle interactions introduce inherent epistemic uncertainties in the surrogate model for the drag. The uncertainty propagates to the macroscale resulting in lower fidelity of the macro-response. This motivates the use of 3D computations for obtaining the training data.

Development of the surrogate models from high-fidelity 3D numerical simulation is computationally expensive. As shown in Sen et al. (2017), for a 2D parameter space (i.e., when $\overline{\langle C_D \rangle}$ is a function of M_S and ϕ only), an ensemble of 50–100 mesoscale simulations are required to construct the surrogate model for $\overline{\langle C_D \rangle}$; typical 2D simulations require days of computing on multiprocessor systems for such an ensemble—for 3D, weeks or even months of calculations would be required. Therefore, generating even a sparse training data set from 3D computations is expensive. The cost is increased further if higher-dimensional parameter-spaces are necessary. For example, at the later stage of shock-particle interaction, i.e., after the shock has passed over the particles, the quasi-steady drag is a function of M_s, ϕ, and Re. Therefore, the curse-of-dimension and the mesh size requirements in 3D simulations make it nearly prohibitive to generate training data sets from high-fidelity mesoscale simulations. With current computing hardware capabilities, it is marginally feasible to “brute force” computations of 3D shock-particle simulations of ensembles large enough to extract surrogate models. However, a judicious choice of computational set-up, ensemble sizes and surrogate construction methods may provide strategies that will make utilization of 3D simulations more commonplace.

This paper addresses the issue of reducing the computational cost for developing training data-sets from 3D mesoscale computations. Two different strategies are adopted in pursuit of lowering the computational cost. First, the cost of generation of training data from the high-fidelity mesoscale simulations is reduced by selecting the optimal mesh resolution and the most compact cluster configurations (i.e., representative volumes, RVEs) required for mesh and geometry independent results. To reduce the computational cost of each simulation, first, grid convergence studies are performed to benchmark the minimum grid-resolution required to generate high-fidelity training data. The effect of cluster geometry on the average drag is then studied to decide the arrangement of particles in a cluster and the cluster size required for the simulations. It is important to study the effect of particle arrangements, i.e., whether to use structured (Mehta et al., 2016; Regele et al., 2014) or randomly Mehta et al., 2018) arranged clusters of particles; because spatial symmetry in a structured (e.g. simple cubic, face-centered cubic(FCC) (Mehta et al., 2016), body-centered cubic(BCC)) particle cluster can be exploited to reduce the computational cost by choosing a smaller length for the cluster in the transverse directions of the shock propagation. However, the selection of a structured arrangement introduces bias in the training data for surrogate modeling; Mehta et al. (2018) showed that particles in a simple cubic and FCC arrangement experience higher peak drag than particles in a random arrangement. In this work, the study on the effects of particle arrangement is further extended by comparing results obtained from numerical simulations of shock interactions with simple cubic, FCC, BCC and randomly arranged clusters of particles.

The size of the particle clusters is another parameter that needs to be chosen carefully while setting up the numerical experiments to obtain training data. The size of a particle cluster in a simulation may affect the averaged drag force on the particles. In a smaller cluster, the particles at the boundary of the cluster will influence the $\overline{\langle C_D \rangle}$. Such boundary effects can be mitigated by increasing the size of particle clusters in the simulations. But increasing the cluster size increases the computational cost as well. To determine the minimum size of particle cluster required to obtain results independent of the cluster size, simulations of shock interaction with particles are performed using clusters of varying sizes.

The total computational cost of surrogate model development is further reduced by using multi-fidelity surrogate modeling techniques (Sen et al., 2018a,b). In the multi-fidelity techniques, a preliminary low-fidelity surrogate model is obtained from computationally inexpensive simulations. Later, high-fidelity simulations are used to rectify the error in the low-fidelity surrogate model. A previous work used surrogate models obtained from 2D coarse grid simulations of shock-particle interaction as the initial low-fidelity model and showed that the MBKG method creates a multi-fidelity model with low error (Sen et al., 2018a,b) from 2D simulation data. In the current work, the MBKG method is used to develop multi-fidelity surrogate models from 3D mesoscale simulations. Two different strategies are explored to obtain multi-fidelity surrogate models from 3D simulations of shocked particulate flows. First, an initial low-fidelity model for multi-fidelity surrogate model is obtained from: ((1) 3D coarse mesh simulations, i.e. low-resolution models; and (2) 2D simulations, i.e. low-dimensional models. Then, both these initial surrogate models are corrected with a small number of 3D high-fidelity simulation data using the MBKG method. The two multi-fidelity surrogate models are compared to determine the cost-effectiveness of the methods.

Despite using an initial low-cost surrogate model, the multi-fidelity methods can still be expensive because of the computational cost associated with even the relatively few high-fidelity 3D simulations. The number of simulations required along each parameter direction, to develop the preliminary surrogate models are $\sim$O(10). Therefore, in a 2-parameter space(M_s, ϕ) the total simulations required for the development of the multi-fidelity surrogate models are $\sim$O(100). However, if M_s and ϕ are considered orthogonal bases of the functional space then the surrogate model $\overline{\langle C_D \rangle} = f(M_s, \phi)$, can be constructed from $\sim$20 simulations. Therefore, the orthogonality assumption in the parameter space provides another route to develop economical surrogate models; however, the error in the surrogate model entailed by the orthogonality assumption needs to be assessed. In this work, surrogate models obtained from the three machine-learning based metamodeling strategies discussed above are evaluated based on the error and associated computational cost.

The rest of the paper is organized as follows: In Section 2, the numerical methods used to obtain the simulation based surrogate model are described. The numerical method used for the mesoscale simulations is validated against benchmark results in Section 3.1. The grid convergence study is performed to find out the optimal grid resolution required for the high and low fidelity simulations in Section 3.1. The effect of the particle arrangement on the average drag in a cluster is studied in Section 3.2. The effect of cluster size on the average drag is studied in Section 3.3.

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