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# MULTI-SCALE MODELING OF PARTICLE-LADEN BLAST WAVES MACHINE LEARNING OF CLOSURE LAWS WITH INTER-SCALE COUPLING AND UNCERTAINTY QUANTIFICATION

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Multi-scale methods were developed that learn closure terms using high-resolution meso-scale simulations of shocked particulate flows. Advances were made in data-driving learning of closure terms, (multidfidelity) surrogate modeling, stochastic macro-modeling of Eulerian-Lagrangian models, uncertainty quantification and verification and validation of the multi-scale framework.

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Final Report on

# MULTI-SCALE MODELING OF PARTICLE-LADEN BLAST WAVES

Machine Learning of Closure Laws with Inter-Scale Coupling and Uncertainty Quantification

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## Abstract

State-of-the-art process scale simulations of particle-laden blasts still rely on empirical models to close the governing equations. Such empirical models typically involve extrapolations from small sets of physical experiments conducted in restricted regions of parameter space. In this project, multi-scale methods were developed that learn closure terms using high-resolution meso-scale simulations of shocked particulate flows. Several advances were made in this project which have pushed the envelope on accuracy and fidelity of multi-scale blast wave simulations. They include: 1) New surrogate modeling methods were developed and tested in multi-dimensional parameter spaces by machine learning from ensembles of *in silico* meso scale experiments; 2) Multi-fidelity surrogate-modeling techniques were evaluated as inexpensive alternatives to high-fidelity surrogate models for obtaining closure laws for drag in shock-particle interactions. This enables construction of surrogates from otherwise prohibitive three-dimensional meso-scale simulations; it also opens the door to accessing higher-dimensional parameter spaces which have been hitherto plagued by the curse of dimensionality; 3) A new, general stochastic framework for Eulerian-Lagrangian macro-models was developed through methods of averaging. Uncertainty in closure models is quantified and propagated through the stochastic macro-model to a quantity of interest. Comparison with Monte-Carlo results shows that the stochastic macro-model is computationally efficient and accurate; 4) Eulerian-Lagrangian macro-models were developed that incorporate subgrid-scale dynamics of clouds of particles. The finite time deformation and sub-grid stresses of a cloud of particles are determined through a combination of averaging techniques and continuum mechanics theory. Closure was obtained through data-driven forcing and turbulence models. The method was shown to improve upon modeling accuracy when compared to the state-of-the-art models for blast problems with shocks and significant cloud deformations; 5) Higher-order (pseudo-turbulence) effects in the closure laws were examined for the first time and it was shown that such effects are considerably more important than is conventionally acknowledged. Without taking fluctuations and stochasticity into account closure models and macro-models will incorrectly predict the evolution of particle and flow fields. 6) Finally, the macro-models and closure models were extended to include not only momentum closure but heat transfer as well, including phase change and chemical reactivity of the particles in the flow. Thus, the foundation for a comprehensive framework for accurate prediction of particle-laden blast scenarios is laid, which are of crucial importance to the Air Force and other DoD agencies.

## 1. Objective

The objective of this project was to develop and test a data-driven, multi-scale computational method that enables predictive simulations of high-speed particle-laden flows, with uncertainty quantification of quantities of interest.

## 2. Approach

Starting from a previously developed set of tools for meso-scale and macro-scale simulations, and surrogate/response surface reconstruction (or meta-modeling), a machine-learned, multi-scale method was developed that quantifies uncertainty in the surrogate models constructed from meso-scale simulations. Stochastic macro-models are developed that quantify and propagate this uncertainty in and onto a quantity of interest. Figure 1 shows a summarizing schematic of the multi-scale method. Several computationally intensive meso-scale simulations are performed to obtain input data points for the response surface approximation. To ensure computational efficiency and an approximation within an acceptable uncertainty range, the meta-model has to rely on a sparse set of input data points. The macro-scale model takes information from the surrogate and uses a computationally efficient reduced model to obtain accurate results for a quantity of interest. The uncertainty in the surrogate is propagated through the macro-model to this quantity of interest.

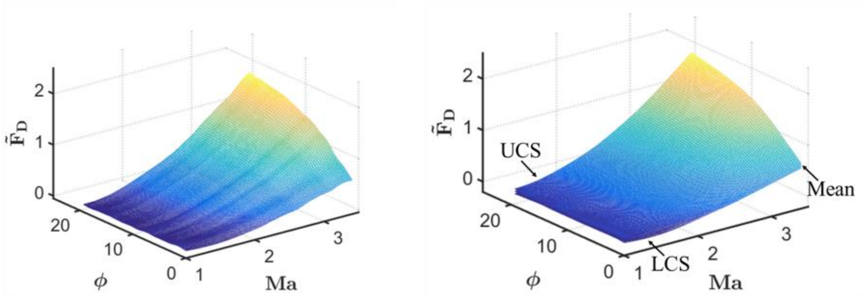
Our multi-scale modeling approach has been to: (1) develop computationally efficient Kriging based surrogate reconstruction surface models that quantify uncertainty through Bayesian inference, (2) develop multi-fidelity methods that reduce the computational cost of construction of surrogate models, (3) develop stochastic macro-models that propagate moments of uncertainty to a quantity of interest, (4) develop sub-scale cloud models to enhance the range of scales that can be simulated and to account for sub-grid pseudo-turbulent stresses, (5) develop multi-scale methods with inter-scale coupling of particle-fluid mass, momentum and energy forcing and pseudo-turbulent stresses using the techniques developed in (1)-(4), and conduct tests on the interaction between a shock and a cloud of particles to show that the method increases modeling accuracy, (6) extend both macro- and meso-models to account for heat and mass transfer, and chemical reaction in blast waves.

In the sections below a summary is given for each of the accomplishments in these six advances in the multi-scale approach. Although the multi-scale approach is applied to shock-particle cloud dynamics, the general framework and techniques are applicable for a wide range of shocked heterogeneous materials.

## 3. Kriging based meta-modeling with uncertainty quantification

Construction of machine-learned closure models from high-fidelity computations presents several challenges. First, the process of learning from expensive meso-scale computations should be considered a “small data” (as opposed to big data) problem; because resolved meso-scale simulations are computationally expensive, only a limited number of numerical experiments can be performed to obtain the training data for typical machine-learning algorithms. Second, each meso-scale simulation must yield an improved approximation of the surrogate; i.e. the machine-learning algorithm must converge monotonically with respect to the number of training points. In a comparison of several leading surrogate 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 (DKG) [2], it was found that for a sufficiently large number of training points, Stochastic Collocation methods generally converge faster than the other metamodeling techniques; however, for smaller training data sets, 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, DKG is favored.

Mesoscale computations of shock-particle interactions were performed to construct surrogate models for the drag force on a cluster of particles for different Mach numbers and particle volume fractions. The effect of inhomogeneity in both space and time on the accuracy of the surrogate model was assessed. To improve robustness and to obtain estimates for uncertainty in the meta-model, two Kriging-based methods were co-developed and/or tested with collaborators, viz. the Dynamic Kriging Method (DKG) and a Modified Bayesian Kriging Method (MBKG). The DKG method converges poorly for noisy data arising from numerical experiments, as shown by the oscillatory hypersurface constructed by DKG in Figure 2. The MBKG method converges monotonically even with noisy input data. In addition to the superior convergence, MBKG can also provide an invaluable estimate of the uncertainty in the surrogate model through Bayesian inference. Figure 2 shows an example of MBKG's ability to predict the upper and lower bound for a surrogate. For noisy, small data, such as the input data drawn from meso-scale simulations, MKBG was found to be the best choice.

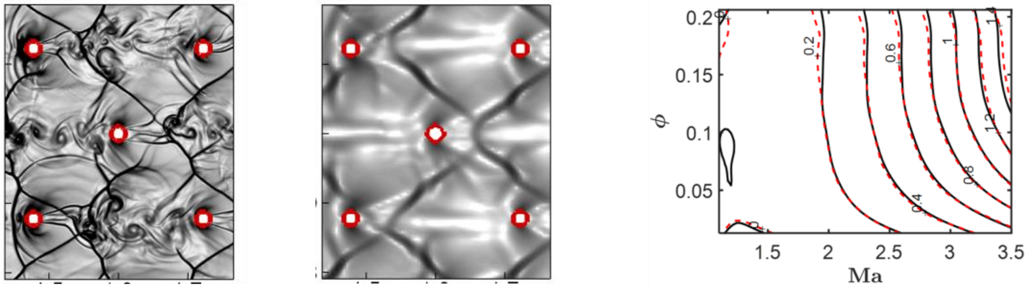


(a) (b)

Figure 2. Hypersurfaces of drag obtained from high-fidelity mesoscale computations of shock-particle interactions computed using (a) the DKG method and (b) the MBKG method. The DKG method has high-frequency oscillations resulting from over-fitting the drag. THE MBKG method has minimum variance and shows the mean and the Upper and Lower credible sets (UCS and LCS) for the drag, providing a measure of the fitting (epistemic) uncertainty.

## 4. Computationally feasible, multi-fidelity meso- and meta-modeling

The parameter space for the shock-particle interaction problems can be large; in addition to the Mach number and volume fraction for inviscid models, the Reynolds number and Nusselt number are also affecting the drag force for viscous problems. This will make the surrogate construction onerous, since orders of magnitude more high-resolution meso-scale simulations will need to be performed. If 3D simulations are used instead of the 2D simulations that were mostly used, the computational burden will become prohibitive. To reduce the computational burden and address the curse of dimensionality, multi-fidelity methods were developed [5] that construct surrogates from ensembles of low-fidelity (coarse grid) and high-fidelity mesoscale computations: preliminary surrogates constructed from low-fidelity



(a) (b) (c)

Figure 3. Results from a multifidelity surrogate modeling approach. (a) High-fidelity solution of shock-particle interactions, (b) Low-fidelity solution of the flow in the same cluster, (c) Contours on drag in the parameter space, showing that the high-fidelity (blask lines) and multi-fidelity (red dotted line) approaches overlap.

meso-scale simulations are corrected using only a few high-fidelity computations to obtain multifidelity surrogate models. Figure 3a shows that the high-fidelity computations capture finer scale structures, whereas the low-fidelity simulations (Figure 3b) only capture the general shock structure. Three different multifidelity methods, viz. Space Mapping, Radial Basis Functions and MBKG were developed and evaluated for correcting an initial low-fidelity surrogate. MBKG provided the most accurate and robust metamodels and simultaneously minimized the computational cost and error in the constructed surrogate. The MBKG multi-fidelity method was shown to decrease the computational cost by more than 20% for a modest increase (only 5%) in an approximation error as shown in Figure 3c. For 3-D computations of particle-shock interactions the computational savings from using multi-fidelity approaches will be significantly greater than for the 2D case studied.

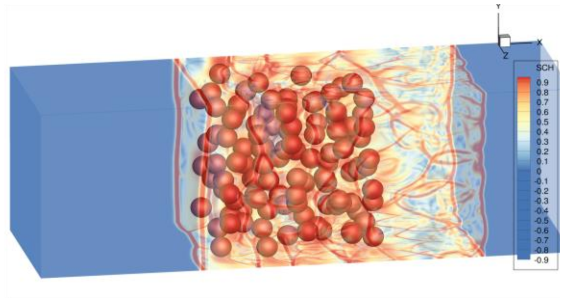


Figure 4. Representative 3D mesoscale simulation of shock-particle interaction used to obtain training data points.

To further reduce computational cost, various strategies were explored that specifically apply to particle-laden flows. The cost of the generation of training data was reduced by selecting optimal grid resolutions, particle arrangements in clusters and size of particle clusters, i.e. by selecting suitable representative volumes (RVEs). The use of multifidelity methods was investigated to correct a surrogate for the average drag force in a cluster of particles constructed from 2D simulations for 3D effects. Figure 4 shows a results of such a three-dimensional simulation [6] [7]. The multi-fidelity technique was shown to decrease the computational effort by an order of magnitude.

## 5. Development of stochastic macro-models with uncertainty propagation

From the macro-scale perspective, we investigated the impact of uncertainty in surrogates on a macro-scale quantity of interest. At the macro- or process scale the number of particles is too large to model

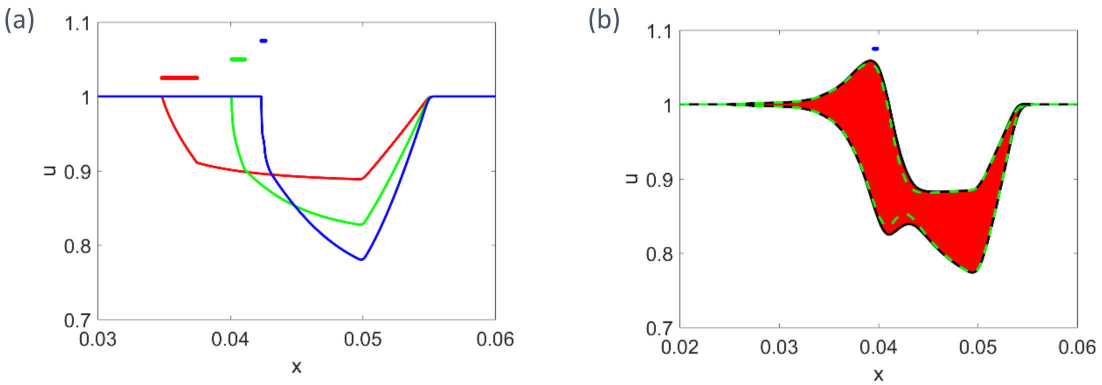


Figure 5. Three Monte-Carlo realizations of the interaction between a transported property and a group of inertial particles (left figure) show that the uncertainty in the random forcing leads to a significant variation in the realizations. The that propagates from the random forcing into the solutions and as quantified by the second moment shown by the green dotted line the right figure is captured well by averaged model equations (second moment identified by red area).

with first-principles meso-scale models. Macro-scale models and simulation techniques are necessary to simulate such problems. An Eulerian-Lagrangian (EL) approach combined with point-particle modeling is commonly used to make computations more efficient. In these EL models, the carrier flow is solved in the Eulerian frame, while the volumeless particles (Particle-Source-In-Cell, or PSIC) are traced along their Lagrangian path. The interactions between the particles and the carrier fluid are modeled though momentum exchange via singular point source terms [8, 9]. These point particle approaches require a model for the drag force exerted on the particles. Whereas empirical models are commonly used, we employ the more versatile surrogate modeling techniques described above.

Meta-models used here, but also broadly used reduced empirical models, have associated uncertainties arising from measurement, numerical errors and sparsity of the data points in the surrogate models. To understand how this modeling uncertainty affects the solution on the macro-scale, one must understand how uncertainty propagates through the non-linear Eulerian-Lagrangian model. This understanding begins by using a probabilistic perspective and by modeling the drag force as a random variable. The quantities of interest (QoIs), such as the flow dynamics and particle dispersion and mixing, are greatly

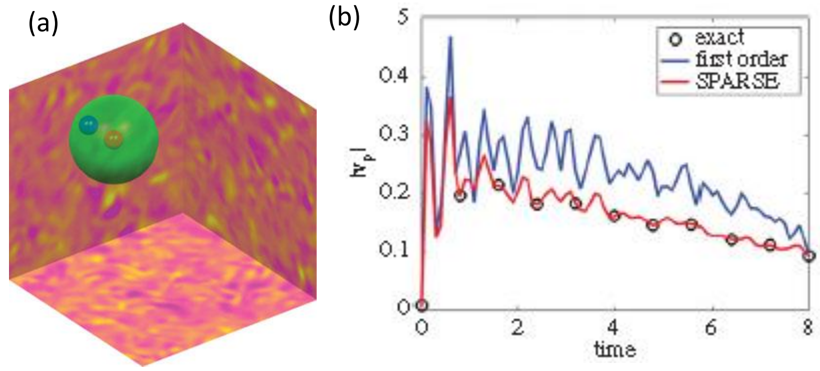


Figure 6. By accounting for sub-particle cloud scale stresses, the Subgrid Particle Averaged Reynolds Stress Equivalent (SPARSE) model, the mean cloud position (green cloud) in an isotorpic turbulence is more accuractly predicted by SPARSE (red dot) than with the first-order cloud-in-cel model, CIC1 (blue dot). The mean velocity predicted also shows improved accuracy by SPARSE as compared to CIC1.

influenced by the epistemic uncertainty in the drag forces. As a consequence, the QoIs have to be modeled as random variables also. This yields a classic stochastic formulation that requires techniques from the field of uncertainty quantification (UQ).

We have addressed the uncertainty by deriving an Eulerian-Lagrangian model through averaging that propagates moments of this random variable into the solution. Simulations with the averaged moment equations are compared to Monte-Carlo simulations[10]. As compared to the state-of-the-art, the contributions of this development include a first investigation into the effects of uncertainty in the random force model on solutions of Eulerian-Lagrangian point-particle simulations from a probabilistic point of view. In particle-laden shocked flows a number of singularities occur in the systems that have to be regularized. We have developed such regularization techniques. We have quantified uncertainty and validated the stochastic model for a system whose carrier phase is governed by a linear equation, followed by uncertainty quantification in shock-particle-laden flows. Figure 5a shows three different Monte-Carlo realizations for a problem where a transported medium interacts with a cloud of particles. For a stochastics forcing with a variance of 10%, both the particle and the fluid phase show a non-linear propagation of the uncertainty to their solution, respectively. Figure 5b shows that the uncertainty is non-uniformly distributed and is largest in regions where the solution has the highest gradients.

## 6. Extending the scale range: macro-and multi-scale models with sub-cloud stresses

To extend the scale range and to be able to account for sub-grid level fluctuations in both the turbulent carrier phase and the dynamic particle phase, we have developed models for clouds of particles using a combination of averaging methods and methods that account for deformation of the clouds of particles. We developed an augmented cloud model called "SPARSE" (Subgrid Particle-Averaged Reynolds Stress-Equivalent)[11], which accounts for the subgrid pseudo-turbulence or Reynolds-equivalent stresses in the macro-particle momentum equation. It is based on a combination of a truncated Taylor expansion of a drag correction function and Reynolds averaging of the resulting momentum equations for the individual particles. The pseudo-turbulent stresses were computed via Particle-Source-In-Cell(PSIC) model [8] simulations, i.e., the averaged momentum equation was closed a posteriori. For one-way coupled, incompressible and isothermal flows, the importance of accounting for these SGS inter-phase fluctuations in traditional Cloud-In-Cell (CIC) approaches was demonstrated by showing that SPARSE predicts the average cloud position more accurately than a CIC model that does not account for

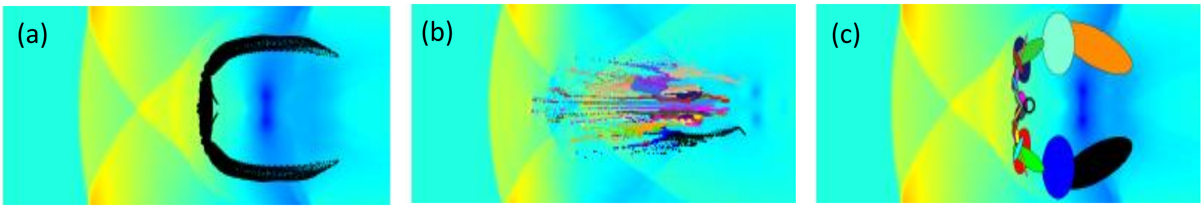


Figure 7. A comparison of macro-scale model for the interaction between a shock and a cloud of particles: (a) the point particle-source-in-cell (PSIC) model with 40,000 particles, (b) the commonly used first-order Cloud-In-Cell model, (c) the SPARSE model with 24 clouds. The SPARSE model compares well with the PSIC, but only uses a fraction of the degrees of freedom and is hence more computationally efficient. The commonly used CIC model does not perform well 24 clouds.

these stresses. Figure 6, for example, shows that a cloud's spatially averaged, unsteady location and velocity in an isotropic turbulent field is significantly better predicted by SPARSE as compared to the CIC approach.

In two-way coupled formulations, the flow does not just affect the particles (one-way coupling), but the particles also force the flow (two-way coupling). This particle-fluid forcing is modeled through a source term in the carrier-phase momentum equation. We have formulated a two-way coupled version of the SPARSE model [19]. Rather than weighting the influence of individual point particles to the Eulerian grid as occurs in PSIC, we weight the influence of macro-particles representing subgroups of particles to the grid. We account for the deformation of these subclouds by representing them as bivariate Gaussian distributions rather than using a local weighing that only accounts for their mean motion. The variance and rotation of the Gaussian are linked to the principle strain and using a decomposition of the deformation tensor in terms of rotation and stretching.

SPARSE improves upon the results of CIC as it captures the cloud's average position and spatial spread more accurately, as shown in Figure 7 for a shock-particle cloud interaction. The CIC results are not prediciting the motion of the particle cloud well. The SPARSE predictions of the cloud's average position and spread converge to those from PSIC simulations when the number of macro-particles in the horizontal and vertical directions is appropriately increased. Using fewer than 200 macro-particles, SPARSE predicts the time-averaged horizontal and vertical cloud spread in our benchmark problem to within less than 4% and 1%, respectively, of the reference PSIC result obtained with 40000 point particles. This makes SPARSE a game changer in particle-laden flow simulations as it enables the accurate computation of process-scale flows that would be infeasible with PSIC.

## 7. Multi-scale method with inter-scale coupling for forcing and pseudo-turbulent stresses

The meso-, meta-, and macro-models were combined to achieve the project's objective; i.e. a multi-scale framework for simulation of particle-laden blast waves [12]. To test the performance of the multi-scale method, we performed a full resolution simulation of a shock interaction with a rectangular cloud of particles and used that as a ground truth reference for comparison with existing multi-scale methods. Initially only surrogates for the interphase coupling were considered to couple the scales. Figure 8 shows that the multi-scale results are in good agreement with the full resolution results but require only a fraction of the cost. Because the test case showed that the effects of pseudo-turbulence are significant on particle dispersion and cloud acceleration, surrogates were also developed for the closure terms in the SPARSE model [13]. Multi-scale simulations based on SPARSE showed significantly improved agreement with the reference case. These results show, for the first time, direct head-to-head comparison between a fully resolved DNS simulation of shocked flows through a particle cloud and a data-driven, i.e. meso-scale informed macro-scale particle-in-cell simulation under identical conditions. The good agreement in the particle dispersion patterns as well as resulting downstream wake flow patterns demonstrates the successful completion of the multi-scale effort in this project. We show, for the first time, that data-driven models can be used to produce improved simulation of shocked particle cloud dynamics; such closure models can not be used to supplant limited empirical closure models that have been traditionally used in macro-scale models of particle-laden shocked flows.

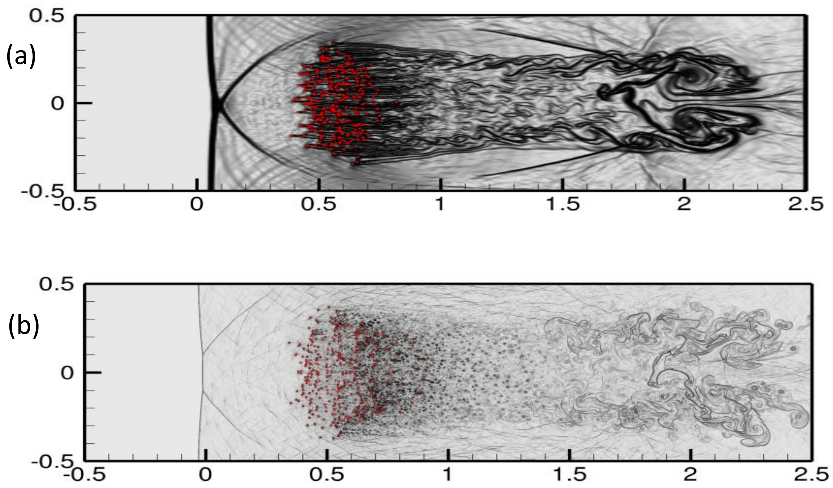


Figure 8. Comparison of: (a) macro-scale simulation informed by a meso-scale data-driven surrogate model and (b) a high-fidelity simulation with full resolution of each particle. The multi-scale simulation compares well with the high-fidelity simulation but only requires a fraction of the computational cost.

## 8. Extension to include heat and mass transfer and chemistry

Shock-induced heating of particles is often followed by phase change, evaporation and combustion of the particles. Therefore, macro-scale models of shock-particle interaction would also require closure terms for mass and heat transfer between the dispersed phase and the gaseous phase caused by evaporation and energy deposition in the system caused by combustion of the particles. In ongoing work, we are developing closures for heat transfer [14] and are extending the multi-scale framework to account for shock-induced evaporation and combustion. Figure 9a shows show that the vapor fraction extends well into the wake of a droplet after interaction with a shock. Surrogate models of the shock-induced evaporation rate of the droplets are developed using mesoscale simulation data. On the macro-scale point particle-models have been implemented that account for evaporation through empiricism [15] For the chemical reaction modeling, the filter-mass density function (FMDF) model[16] has been adopted into our macro-scale solvers. In FDMF the filtered density function of each species is traced through stochastic differential equations. The velocity field is provided by the carrier-phase solver. We have implemented

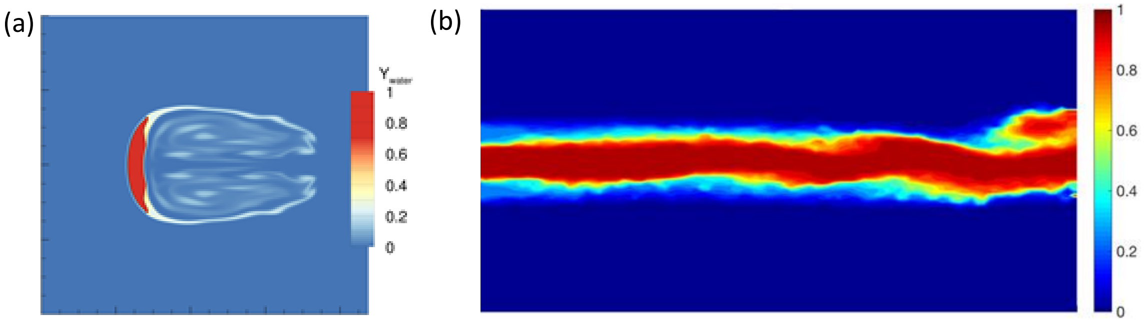


Figure 9. (a) Vapor fraction contours from a meso-scale simulation of an evaporating droplet in the accelerated flow behind a moving shock (b) fuel fraction contours from a macro-scale simulation with the filtered-mass density function model of a turbulent flame.

the FDMF into WENO and spectral element methods and hybridizations thereof [17]. Figure 9b shows a Sandia turbulent flame simulation, which compares well with an experimental database.

## 9. Summary

In this project, we made significant, carefully constructed and well thought out advances in the state-of-the-art of modeling and simulations of particle-laden blast waves. A machine-learning based, data-driven multi-scale modeling approach was created that can now connect subgrid meso-scale dynamics of particle clusters hit by shocks with the overall system scale simulation of particle clouds. This is a major advance and has created computer codes and techniques that set the foundations for much more accurate simulations of blast waves. We also put in place the fundamental components for efficiency of machine learning, investigated deeply many as yet unresolved questions connected with accuracy, robustness and efficiency of data-driven models and took foundational steps leading towards the simulation of reactive turbulent flows in particle clouds. All of this places us at the leading-edge of simulation capabilities for modeling reactive blast waves. There remains, of course, a lot to be done. Fully three-dimensional, turbulent, reactive blast wave simulations still remain out of reach. We are now well positioned to carve the path towards such simulations. We have the tools, techniques, ideas and vision required to track towards that goal. Our collaborative efforts, despite rather modest yet consistent support received from the AFOSR over the past decade has enabled us to carefully and judiciously construct these models and techniques. We hope to continue to work on these problems of great importance to DoD.

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## **Personnel Supported During Duration of Grant**

| | |
|---|---|
| Dr. Arnab Chauhduri | Postdoc, San Diego State University |
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| Dr. Vasilis Fountoulakis | Postdoc, San Diego State University |

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| Hareshram Natarjan | Ph.D. student, San Diego State University |
| Gustaaf B. Jacobs | Professor, San Diego State University |
| Dr. Oishik Sen | Postdoc, University of Iowa |
| Pratik Das | Ph.D. student, University of Iowa |
| Udaykumar, H.S. | Professor, University of Iowa |

**Publications resulting from this award**

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**AFRL Point of Contact**

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**Transitions**

none

**New Discoveries:**

**none**