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STEM Degrees: **STEM Participants:**

Major Goals: We address an important research area in stochastic multiscale modeling, namely, the propagation of uncertainty across heterogeneous domains characterized by partially correlated processes with vastly different correlation lengths. This class of problems arises very often when computing stochastic PDEs and particle models with stochastic/stochastic domain interaction but also with stochastic/deterministic coupling. The domains may be fully embedded, adjacent, or partially overlapping. The fundamental open question we address is the construction of proper transmission boundary conditions that preserve global statistical properties of the solution across different subdomains. Often, the codes that model different parts of the domains are black box and hence a domain decomposition technique is required. No rigorous theory or even effective empirical algorithms have yet been developed for this purpose, although interfaces defined in terms of functionals of random fields (e.g., multipoint cumulants) can overcome the computationally prohibitive problem of preserving sample-path continuity across domains.

Accomplishments: 1. Algorithms for propagating uncertainty across heterogeneous domains based on the Schwarz algorithm and on constrained optimization; see I below.
2. Stochastic domain decomposition via moment minimization – an improved general algorithm for both linear and nonlinear stochastic PDEs; see II below.
3. Bi-directional coupling between a PDE-domain and an adjacent Data-domain equipped with multi-fidelity sensors; see III below.
4. Thermal fluctuations in multiscale coupling of heterogeneous solvers at non-equilibrium via domain decomposition method for particle methods; see IV below.
5. Multi-fidelity Gaussian process regression for prediction of random fields (deep learning); see V below.
6. A resilient and efficient CFD framework: Statistical learning tools for multi-fidelity and heterogeneous information fusion; see VI below.

To the best of our knowledge, these are the first algorithms capable of propagating uncertainty seamlessly across heterogeneous domains both for PDEs but also for particle-based simulations using molecular dynamics (MD) and dissipative particle dynamics (DPD). They are based on ideas from diverse fields, i.e., domain decomposition, optimization, generalized polynomial representation, Gaussian process regression, deep learning and statistical physics. Each of the algorithms in 1-6 represents a major development with potential applications in multiscale modeling of materials, complex fluids, statistical physics, and information domains.

This work was presented in the annual SIAM conferences by the PhD students involved in the project. The papers completed were based on collaboration of Brown University with researchers from MIT and Princeton University.

Training Opportunities: Nothing to Report

Results Dissemination: There have been 7 publications acknowledging this award:

Bian, Xin, et al. "Analysis of hydrodynamic fluctuations in heterogeneous adjacent multidomains in shear flow." Physical Review E 93.3 (2016): 033312.

Bian, Xin, Mingge Deng and George Em Karniadakis. "Analytical and Computational Studies of Correlations of Hydrodynamic Fluctuations in Shear Flow", arXiv preprint arXiv:1703.03762 (2017), to appear in Communications in Computational Physics.

Cho, H., et al. "Algorithms for propagating uncertainty across heterogeneous domains", SIAM Journal on Scientific Computing 37 (2015): A3030-A3054.

Lee, Seungjoon, Ioannis G. Kevrekidis and George Em Karniadakis. "A resilient and efficient CFD framework: Statistical learning tools for multi-fidelity and heterogeneous information fusion", Journal of Computational Physics (2017): 516-533.

Parussini, L., et al. "Multi-fidelity Gaussian process regression for prediction of random fields", Journal of Computational Physics (2017): 36-50.

Zhang, Dongkun, Hessam Babaee and George Em Karniadakis. "Stochastic domian decomposition via moment minimization", submitted to SIAM Journal on Scientific Computing.

Zhang, Dongkun, Liu Yang and George Em Karniadakis. "Bi-directional coupling between a PDE-domain and an adjacent Data-domain equipped with multi-fidelity sensors." in preparation.

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Technology Transfer: Nothing to Report

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Objectives

We address an important research area in stochastic multiscale modeling, namely, the propagation of uncertainty across heterogeneous domains characterized by partially correlated processes with vastly different correlation lengths. This class of problems arises very often when computing stochastic PDEs and particle models with stochastic/stochastic domain interaction but also with stochastic/deterministic coupling. The domains may be fully embedded, adjacent, or partially overlapping. *The fundamental open question we address is the construction of proper transmission boundary conditions that preserve global statistical properties of the solution across different subdomains.* Often, the codes that model different parts of the domains are black box and hence a domain decomposition technique is required. No rigorous theory or even effective empirical algorithms have yet been developed for this purpose, although interfaces defined in terms of functionals of random fields (e.g., multipoint cumulants) can overcome the computationally prohibitive problem of preserving sample-path continuity across domains.

Research Team

During the period from 07/18/2014 to the end of the grant 07/17/2017, PI Karniadakis was supported for 1.23 months. The Co-PI, Dr. Daniele Venturi was supported for 0.9 months before he left Brown University. In addition, a postdoctoral researcher, Dr. Fangying Song, was supported for 3 months. The following PhD students were also supported: Heyrim Cho (4.5 months), Anna Lischke (4.5 months), Seungjoon Lee (1.25 months), Yu-hang Tang (1.5 months), Liu Yang (1.5 months), and Dongkun Zhang (24.5 months).

Major Highlights

1. Algorithms for propagating uncertainty across heterogeneous domains based on the Schwarz algorithm and on constrained optimization; see I below.
2. Stochastic domain decomposition via moment minimization – an improved general algorithm for both linear and nonlinear stochastic PDEs; see II below.
3. Bi-directional coupling between a PDE-domain and an adjacent Data-domain equipped with multi-fidelity sensors; see III below.
4. Thermal fluctuations in multiscale coupling of heterogeneous solvers at non-equilibrium via domain decomposition method for particle methods; see IV below.
5. Multi-fidelity Gaussian process regression for prediction of random fields (deep learning); see V below.
6. A resilient and efficient CFD framework: Statistical learning tools for multi-fidelity and heterogeneous information fusion; see VI below.

To the best of our knowledge, these are the first algorithms capable of propagating uncertainty seamlessly across heterogeneous domains both for PDEs but also for particle-based simulations using molecular dynamics (MD) and dissipative particle dynamics (DPD). They are based on ideas from diverse fields, i.e., domain decomposition, optimization, generalized polynomial representation, Gaussian process regression, deep learning and statistical physics. Each of the algorithms in 1-6 represents a major development with potential applications in multiscale modeling of materials, complex fluids, statistical physics, and information domains.

This work was presented in the annual SIAM conferences by the PhD students involved in the project. The papers completed were based on collaboration of Brown University with researchers from MIT and Princeton University.

I. Algorithms for propagating uncertainty across heterogeneous domains[1]

The key idea of the different methods we propose relies on combining local reduced-order representations of random fields with multilevel domain decom-position. Specifically, we propose two new algorithms: The first one (SDD-M) enforces the continuity of the conditional mean and variance of the solution across adjacent subdomains by using Schwarz iterations. The second algorithm (PDE-constrained interface method) is based on PDE-constrained multi objective optimization, and it allows us to set more general interface conditions. The effectiveness of these new algorithms is demonstrated in numerical examples involving elliptic problems with random diffusion coefficients, stochastically advected scalar fields, and nonlinear advection-reaction problems with random reaction rates.

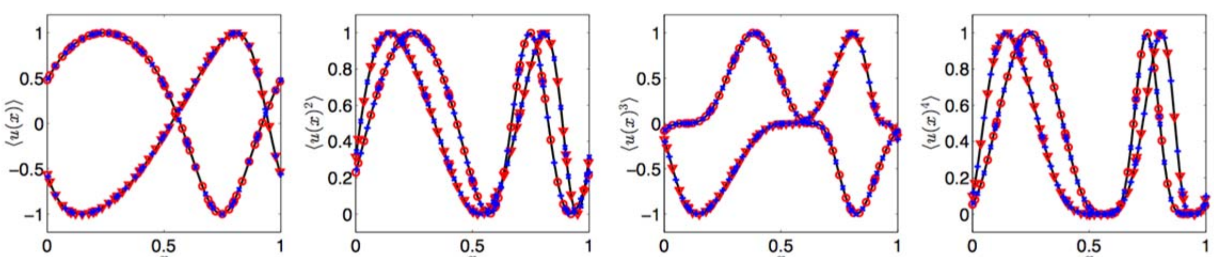

Figure 1: Stochastic advection-reaction problem. First four statistical moments of the solution with correlation length that varies from 0.02 to 0.08. The reference solution (black line) is compared with the SDD-M method (red line) and the PDE-constrained interface method (blue line) at two different times: t = 0.5 (red triangle, blue +) and t = 1.0 (red circle, blue x).

Here, we present the results of the advection-reaction equation by using two subdomains in Figure 1, where we plot the first four moments of the stochastic solution at different times obtained by using the SDD-M and PDE-constrained interface methods. The relative L_2 error of such moments is plotted in Figure 2(a) versus time. It is seen that the SDD-M method is more accurate than the PDE-constrained method. Both algorithms produce the same error slope in time. In addition, we consider a random reaction rate with a Gaussian covariance kernel having correlation length $l_c = 0.008$, and compute the solution by using the SDD algorithm on multiple subdomains. We emphasize that the local dimensionality of the random space

[1] Cho, H., et al. "Algorithms for propagating uncertainty across heterogeneous domains." *SIAM Journal on Scientific Computing* 37 (2015): A3030-A3054.

associated with this decomposition reduces from 119 to 23 and 6, respectively. In Figure 2(b), although the errors slightly increase as we divide the domain into smaller subdomains, the accuracy does not depend strongly on P as the error stays in the same order of magnitude.

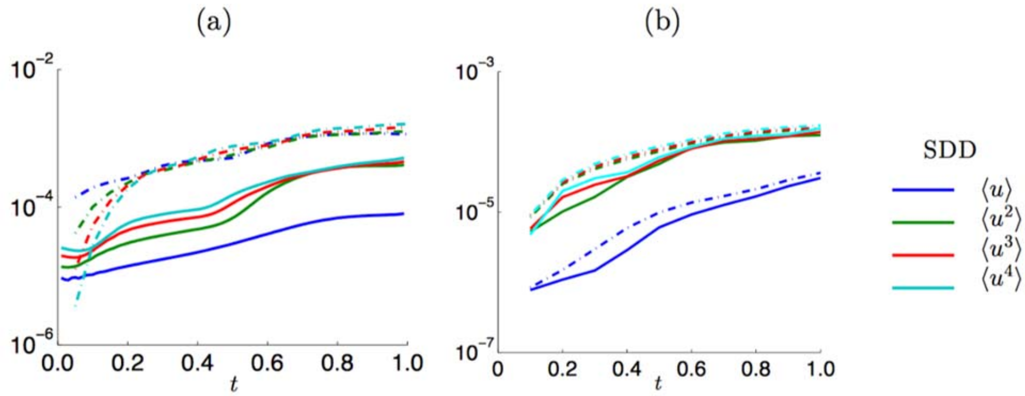

Figure 2: Stochastic advection-reaction problem. Relative L_2 errors in the first four statistical moments of the solution versus time. We show results computed by using the moment interface SDD-M (−) and the PDE-constrained (− · −) methods where D is decomposed into two subdomains (a) and by using SDD-M with multiple number of subdomains P = 5 (−) and P = 20 (− · −) (b).

II. Stochastic domain decomposition via moment minimization[2]

Propagating uncertainty accurately across different domains in multi-scale physical systems with vastly different correlation lengths is of fundamental importance in stochastic simulations. We propose a new method to address this issue, namely the stochastic domain decomposition via moment minimization (SDD-MM). Specifically, we develop a new moment minimizing interface condition to match the stochastic solutions at the interface of the non-overlapping domains. Unlike other stochastic domain decomposition methods, the proposed method serves as a general framework that works with heterogeneous local stochastic solvers, and does not rely on accessing global random trajectories, which are typically not available in realistic multi-scale simulations. We analyze the computational complexity of the method and we quantify the contributing errors. The convergence property of SDD-MM is tested in several examples that include the stochastic reaction equation, Fisher's equation, as well as a two-dimensional Allen-Cahn equation. We observe good performance of the method for nonlinear problems as well as problems with different correlation lengths.

[2] Zhang, Dongkun, Hessam Babaee and George Em Karniadakis. "Stochastic domian decomposition via moment minimization." *submitted to SIAM Journal on Scientific Computing*.

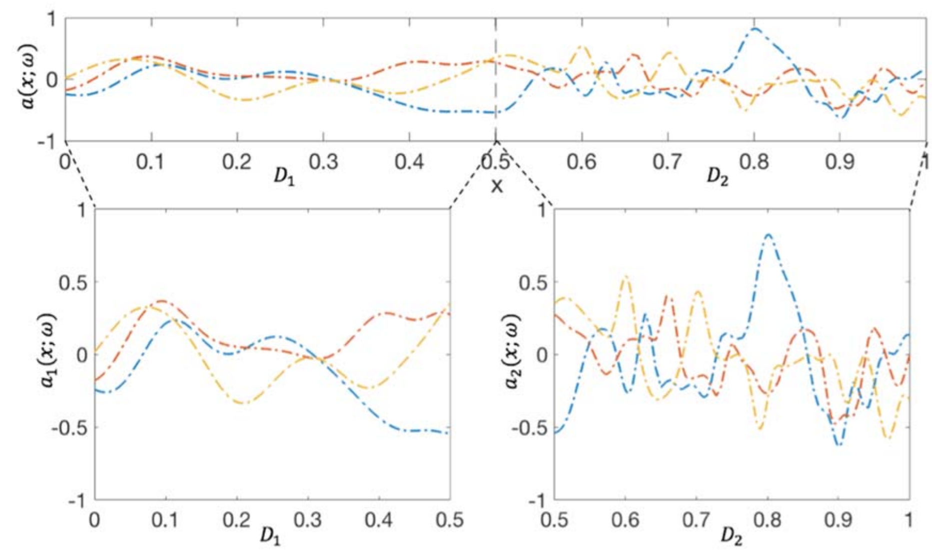

Figure 3: Decomposing domain $[0,1]$ into two non-overlapping subdomains D_1 and D_2, where $a(x;\omega)$ is a global random process with varying correlation lengths; $a_1(x;\omega)$ and $a_2(x;\omega)$ are the embedded local random processes.

1. Local randomness parametrization

Figure 3 illustrates the non-overlapping domain decomposition of a one-dimensional domain $[0,1]$. Suppose the random input takes form of a random process, $a(x;\omega)$, which is naturally embedded into local subdomains by directly truncating at the subdomain interface. K-L expansion can be performed independently inside each subdomain, thus $a_1(x;\omega)$ and $a_2(x;\omega)$ can be locally represented as random variables $\boldsymbol{\xi_1}$ and $\boldsymbol{\xi_2}$. However, to generate continuous sample trajectories of $a(x;\omega)$, $\boldsymbol{\xi_1}$ and $\boldsymbol{\xi_2}$ cannot be sampled independently. The cross-correlation between ξ_1 and ξ_2 shall be explicitly computed from the global covariance kernel of $a(x;\omega)$:

$$Cov[\boldsymbol{\xi_1},\boldsymbol{\xi_2}] = \sqrt{\Lambda_1^{-1}}\Phi_1^{-1}K_{12}(\Phi_2^{-1})^T\sqrt{\Lambda_2^{-1}},$$

where Λ_i is the diagonal eigenvalue matrix of domain D_i, and Φ_i is the matrix of eigenvectors. K_{12} is the cross-covariance matrix of $a(x;\omega)$ between D_1 and D_2.

2. Moment minimizing interface condition

Consider the second-order statistical moment of the difference of local solutions at the subdomain interface x_b, that is:

$$\mathcal{J}_1 = \mathbb{E}\left[\left(\sum_{i=0}^{M_1} u_{1,i}(x_b,t)\Phi_i(\boldsymbol{\xi_1},\boldsymbol{\xi_2}) - \sum_{j=0}^{M_2} u_{2,j}(x_b,t)\Phi_j(\boldsymbol{\xi_1},\boldsymbol{\xi_2})\right)^2\right],$$

where M_1 and M_2 are the numbers of terms of the gPC expansion of $u(x;\omega)$ in each subdomain. Given $u_{2,j}$, by minimizing $\mathcal{J}_1$, we end up with a Dirichlet type boundary condition for $u_{1,i}$ in domain D_1. Similarly, if we consider minimizing the second moment of the difference of flux across the interface x_b, i.e.

$$\mathcal{J}_2 = \mathbb{E}\left[\left(\sum_{i=0}^{M_1} u'_{1,i}(x_b,t)\Phi_i(\boldsymbol{\xi_1},\boldsymbol{\xi_2}) - \sum_{j=0}^{M_2} u'_{2,j}(x_b,t)\Phi_j(\boldsymbol{\xi_1},\boldsymbol{\xi_2})\right)^2\right],$$

we end up with a Neumann type boundary condition for $u_{2,j}$, given $u_{1,i}$. We therefore build our Schwarz type iterative method upon these two minimizing problems.

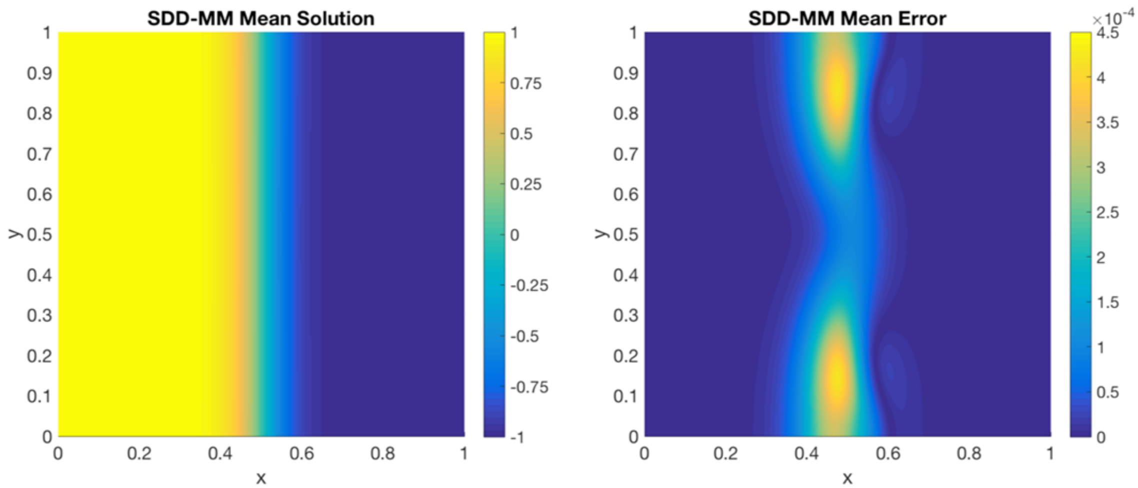

Figure 4: Mean field solution of the 2D stochastic Allen-Cahn equation, obtained from the domain decomposition method, and its error.

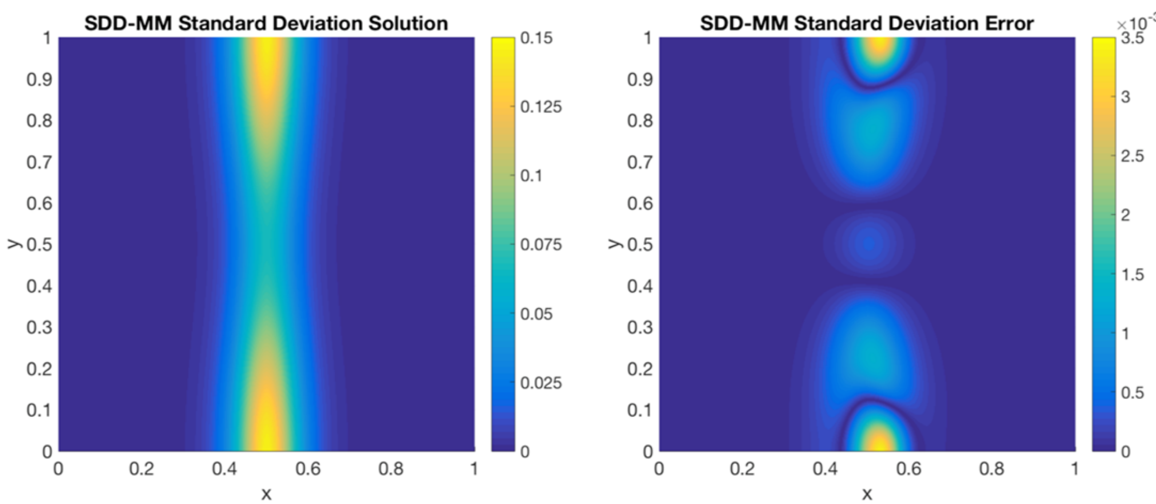

Figure 5: The standard deviation of the 2D stochastic Allen-Cahn equation solution, and its error.

Figure 4 and Figure 5 demonstrate the performance of SDD-MM method for solving a two-dimensional stochastic Allen-Cahn equation. The relative L_2 error for the mean field is 0.03% and the relative L_2 error for the standard deviation is 5.23%.

III. Bi-directional coupling between a PDE-domain and an adjacent Data-domain equipped with multi-fidelity sensors[3]

The increasing collection of data in essentially all facets of our lives has heralded concomitant growth in statistical and machine learning (ML) techniques to analyze the data. Researchers are looking for data-driven algorithms that will solve a partial differential equation (PDE) as an inverse problem. However, few focuses on combining the information provided by the traditional PDE solver and the big data. In this work, we are devoted to propagating information between those two paradigms, and specifically, we address on coupling the solution of a PDE governed domain with the big data domain. Our method builds upon the Schwarz alternating method and the recent work on numerical Gaussian process regression (GPR). We further extend our method to deal with data with variate fidelities, using an auto-regressive multi-fidelity model.

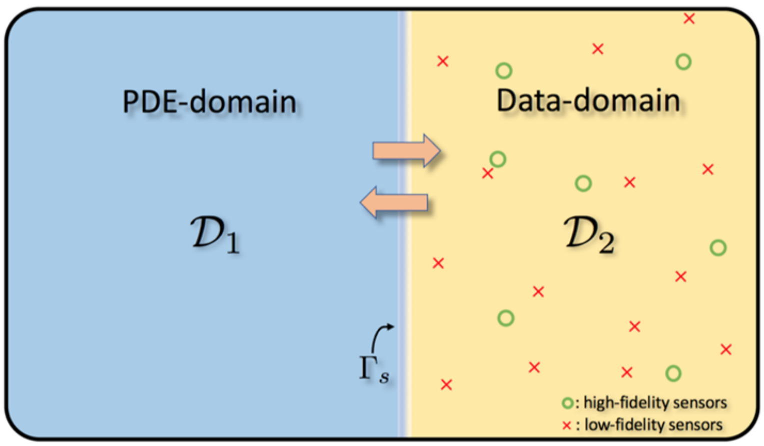

Figure 6: The physical domain D is decomposed into non-overlapping subdomains D_1 and D_2 , where D_1 is the PDE-domain and D_2 is the Data-domain equipped with high-fidelity sensors (green circles) and low-fidelity sensors (red crosses). Information from the PDE-domain and the Data-domain propagates in both directions across the interface Γ_s.

Suppose D is the physical domain and is divided into two non-overlapping Data-domain D_1 and PDE-domain D_2 as depicted in Figure 6. The quantity of interest (QoI), $u(x)$, is governed by a partial differential equation in D_1:

$$\begin{cases} L_x\, u(x) = f(x), & x \in D_1, \\ B_x\, u(x) = g(x), & x \in \partial D_1 \backslash \Gamma_s. \end{cases}$$

We place multi-fidelity sensors of $u(x)$ or $f(x)$ at sparse locations in D_2, and collect the sensors data. Our goal is to design a domain decomposition algorithm that will make use of both the PDE in D_1 and the sparse multi-fidelity sensors data in D_2 to solve for the QoI, $u(x)$, in the entire domain D.

[3] Zhang, Dongkun, Liu Yang and George Em Karniadakis. "Bi-directional coupling between a PDE-domain and an adjacent Data-domain equipped with multi-fidelity sensors." *in preparation*.

We took the two-dimensional Helmholtz equation as our demonstration example. The global physical domain $D: [0, 1.5] \times [0, 1]$ is divided into two non-overlapping subdomains: the PDE-domain $D_1: [0, 1] \times [0, 1]$ and the Data-domain $D_2: [1, 1.5] \times [0, 1]$. The positions of the samples were illustrated in Figure 7. As we could see in Figure 8(a), our coupling method displays very good accuracy. Figure 8(b) shows that as the number of low fidelity data increases, the error of numerical solution shows a decreasing trend. Therefore, the low fidelity data could help improve the precision of the numerical solution.

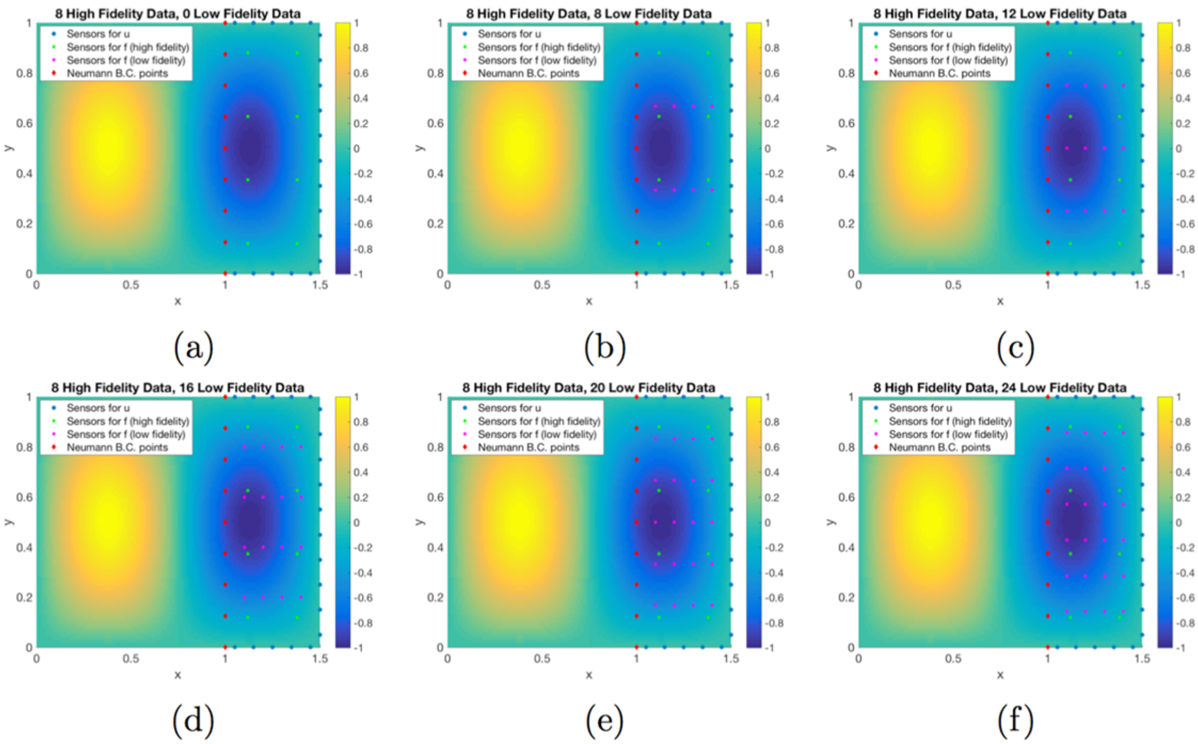

Figure 7: Locations and numbers of the high fidelity data and low fidelity data.

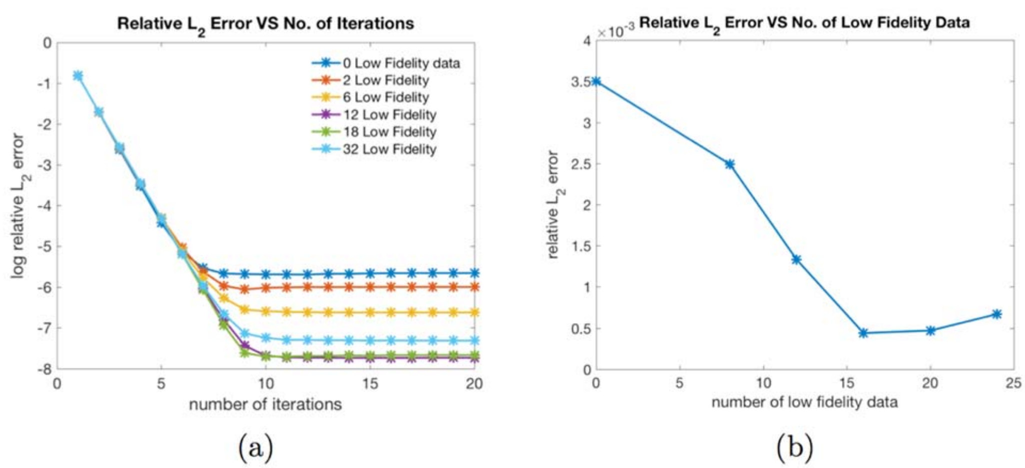

Figure 8: (a) The relative L_2 error of solution decays as iteration goes on and finally converges. (b) As the number of low-fidelity sensors increases, the error of numerical solution shows a decreasing trend.

IV. Thermal fluctuations in multiscale coupling of heterogeneous solvers at non-equilibrium via domain decomposition method

We analyze stochastic hydrodynamic fluctuations of both standalone particle simulations[4] and hybrid simulations[5] under shear flow. In the former case of pure particle simulations, we study spatial Fourier transform of various correlation functions of thermal fluctuations under a periodic shear flow (Lees-Edwards boundary condition). Therefore, there is no limitation on the choice of wave-vectors and we are able to quantify the behavior of both transversal and longitudinal current autocorrelation functions. In the latter case of hybrid simulations, we focus on the wall-bounded shear flow. The spatial Fourier transform is possible only in two periodic directions and therefore we focus on the transversal autocorrelation functions.

Case 1: DPD simulations and analytical solutions

We study correlations of hydrodynamic fluctuations in shear flow analytically and also by dissipative particle dynamics (DPD) simulations under periodic shear flow. The hydrodynamic equations are linearized around the macroscopic velocity field and then solved by a perturbation method in Fourier-transformed space. The autocorrelation functions (ACFs) from the analytical method are compared with results obtained from DPD simulations under the same shear-flow conditions. Up to a moderate shear rate, various ACFs from the two approaches agree with each other well. At large shear rates, discrepancies between the two methods are observed, hence revealing strong additional coupling between different fluctuating variables, which is not considered in the analytical approach. In addition, the results at low and moderate shear rates can serve as benchmarks for developing multiscale algorithms for coupling of heterogeneous solvers, such as a hybrid simulation of molecular dynamics and fluctuating hydrodynamics solver, where thermal fluctuations are indispensable.

Case 2: Hybrid simulations

We analyze hydrodynamic fluctuations of hybrid simulations under shear flow. The hybrid simulation is based on the Navier-Stokes (N-S) equations on one domain and Dissipative Particle Dynamics (DPD) on the other domain. The two domains overlap and there is an artificial boundary for each domain within the overlapping region. To impose the artificial boundary of the N-S solver, a simple spatial-temporal averaging is performed on the DPD simulation. In the artificial boundary of the particle simulation, four popular strategies of constraint dynamics are implemented, namely, the Maxwell buffer[6], the relaxation dynamics[7], the least constraint

[4] Bian, Xin, Mingge Deng and George Em Karniadakis. "Analytical and Computational Studies of Correlations of Hydrodynamic Fluctuations in Shear Flow." *arXiv preprint arXiv:1703.03762* (2017).
[5] Bian, Xin, et al. "Analysis of hydrodynamic fluctuations in heterogeneous adjacent multidomains in shear flow." *Physical Review E* 93.3 (2016): 033312.
[6] Hadjiconstantinou, Nicolas G., and Anthony T. Patera. "Heterogeneous atomistic-continuum representations for dense fluid systems." International Journal of Modern Physics C 8.04 (1997): 967-976.
[7] O'Connell, Sean T., and Peter A. Thompson. "Molecular dynamics–continuum hybrid computations: a tool for studying complex fluid flows."*Physical Review E* 52.6 (1995): R5792.

dynamics[8] [9], and the flux imposition[10] to achieve a target mean value given by the N-S solver. Going beyond the mean flow field of the hybrid simulations, we investigate the hydrodynamic fluctuations in the DPD domain. To this end, we calculate the transversal autocorrelation functions of the fluctuating variables in k-space, to evaluate the generation, transport and dissipation of fluctuations in the presence of a hybrid interface. We quantify the unavoidable errors in the fluctuations, due to both the truncation of the domain and the constraint dynamics performed in the artificial boundary. Furthermore, we compare the four methods of constraint dynamics and demonstrate how to reduce the errors in fluctuations. The analysis and findings of this work are directly applicable to other hybrid simulations of fluid flow with thermal fluctuations. Some representative results are in Figure 9.

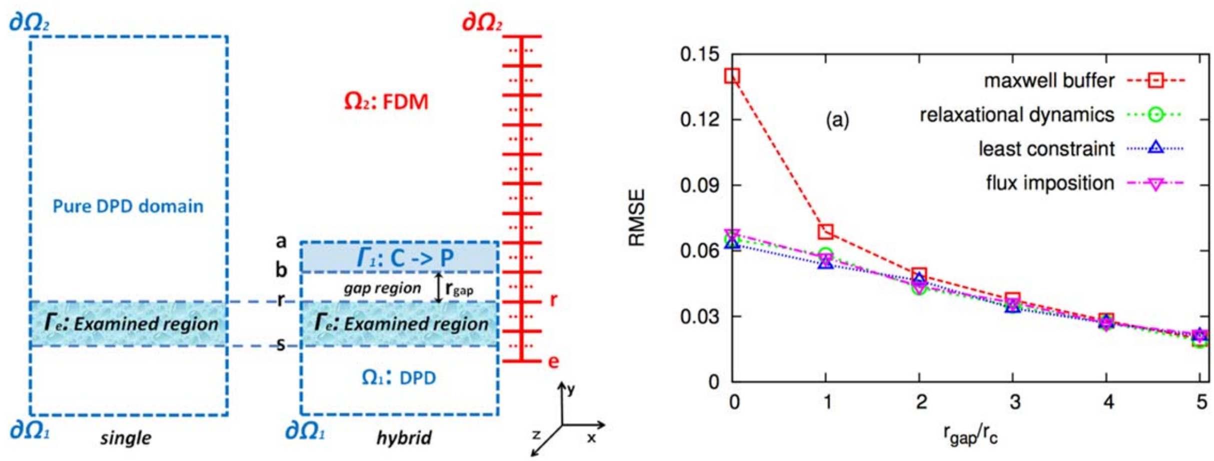

Figure 9: Left figure: the transversal current autocorrelation function of thermal fluctuations are examined in the same geographical region Γ_e. between standalone DPD simulations and hybrid simulations of DPD and finite difference method. A gap region with height r_{gap} is introduced to regulate the errors introduced by the constraint dynamics in the artificial boundary Γ_1 for the particle simulations. Right figure: root mean square errors (RMSE) are quantified on the hybrid simulations against the reference DPD simulations. In particular, errors of four coupling protocols are evaluated as functions of r_{gap}.

V. Multi-fidelity Gaussian process regression for prediction of random fields[11]

We propose a new multi-fidelity Gaussian process regression (GPR) approach for prediction of random fields based on observations of surrogate models or hierarchies of surrogate models. Our method builds upon recent work on recursive Bayesian techniques, in particular recursive co-kriging, and extends it to vector-valued fields and various types of covariances, including separable and non-separable ones. The framework we propose is general and can be used to

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[8] Nie, X. B., S. Y. Chen, and M. O. Robbins. "A continuum and molecular dynamics hybrid method for micro-and nano-fluid flow." *Journal of Fluid Mechanics* 500 (2004): 55-64.

[9] Werder, Thomas, Jens H. Walther, and Petros Koumoutsakos. "Hybrid atomistic–continuum method for the simulation of dense fluid flows." *Journal of Computational Physics* 205.1 (2005): 373-390.

[10] Flekkøy, E. G., G. Wagner, and J. Feder. "Hybrid model for combined particle and continuum dynamics." *EPL (Europhysics Letters)* 52.3 (2000): 271.

[11] Parussini, L., et al. "Multi-fidelity Gaussian process regression for prediction of random fields." *Journal of Computational Physics* (2017): 36-50.

perform uncertainty propagation and quantification in model-based simulations, multi-fidelity data fusion, and surrogate-based optimization. We demonstrate the effectiveness of the proposed recursive GPR techniques through various examples. Specifically, we study the stochastic Burgers equation and the stochastic Oberbeck–Boussinesq equations describing natural convection within a square enclosure. In both cases we find that the standard deviation of the Gaussian predictors as well as the absolute errors relative to benchmark stochastic solutions are very small, suggesting that the proposed multi-fidelity GPR approaches can yield highly accurate results.

VI. A resilient and efficient CFD framework: Statistical learning tools for multi-fidelity and heterogeneous information fusion[12]

Exascale-level simulations require fault-resilient algorithms that are robust against repeated and expected software and/or hardware failures during computations, which may render the simulation results unsatisfactory. If each processor can share some global information about the simulation from a coarse, limited accuracy but relatively costless auxiliary simulator we can effectively fill-in the missing spatial data at the required times by a statistical learning technique – multi-level Gaussian process regression, on the fly; this has been demonstrated in previous work [1]. Based on the previous work, we also employ another (nonlinear) statistical learning technique, Diffusion Maps, that detects computational redundancy in time and hence accelerate the simulation by projective time integration, giving the overall computation a "patch dynamics" flavor. Furthermore, we are now able to perform information fusion with multi-fidelity and heterogeneous data (including stochastic data). Finally, we set the foundations of a new framework in CFD, called patch simulation, that combines information fusion techniques from, in principle, multiple fidelity and resolution simulations (and even experiments) with a new adaptive time step refinement technique. We present two benchmark problems (the heat equation and the Navier–Stokes equations) to demonstrate the new capability that statistical learning tools can bring to traditional scientific computing algorithms. For each problem, we rely on heterogeneous and multi-fidelity data, either from a coarse simulation of the same equation or from a stochastic, particle-based, more "microscopic" simulation. We consider, as such "auxiliary" models, a Monte Carlo random walk for the heat equation and a dissipative particle dynamics (DPD) model for the Navier-Stokes equations. More broadly, in this paper we demonstrate the symbiotic and synergistic combination of statistical learning, domain decomposition, and scientific computing in exascale simulations.

[12] Lee, Seungjoon, Ioannis G. Kevrekidis and George Em Karniadakis. "A resilient and efficient CFD framework: Statistical learning tools for multi-fidelity and heterogeneous information fusion." *Journal of Computational Physics* (2017): 516-533.

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Cho, H., et al. "Algorithms for propagating uncertainty across heterogeneous domains", *SIAM Journal on Scientific Computing* 37 (2015): A3030-A3054.

Lee, Seungjoon, Ioannis G. Kevrekidis and George Em Karniadakis. "A resilient and efficient CFD framework: Statistical learning tools for multi-fidelity and heterogeneous information fusion", *Journal of Computational Physics* (2017): 516-533.

Parussini, L., et al. "Multi-fidelity Gaussian process regression for prediction of random fields", *Journal of Computational Physics* (2017): 36-50.

Zhang, Dongkun, Hessam Babaee and George Em Karniadakis. "Stochastic domian decomposition via moment minimization", *submitted to SIAM Journal on Scientific Computing*.

Zhang, Dongkun, Liu Yang and George Em Karniadakis. "Bi-directional coupling between a PDE-domain and an adjacent Data-domain equipped with multi-fidelity sensors." *in preparation*.