PSAAP III
INTEGRATED SIMULATIONS USING EXASCALE MULTIPHYSICS ENSEMBLES

Multi-fidelity Hamiltonian Monte Carlo Method for Stochastic Inference of Ignition Parameters

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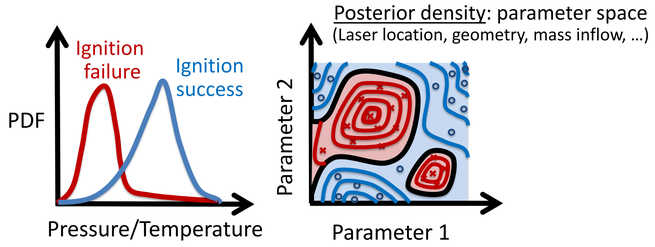
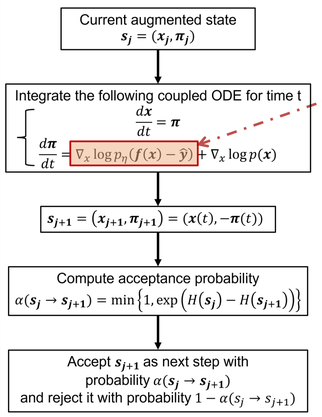
I. Motivation

- Finding the values of parameters which are responsible for the ignition success/failure is critical for robust performance, optimization, and prediction.
- The goal of this work is to infer the probability distribution of these parameters given the ignition success/failure condition by casting this inference problem in a Bayesian setting.



Current state-of-the-art:

- Markov Chain Monte Carlo (MCMC) method is a promising sampling technique to infer such probability distribution. However, it is intractable in high dimensional parameter space.
- Hamiltonian Monte Carlo (HMC) method makes such high-dimensional sampling possible by exploiting the geometry of the target probability distribution.



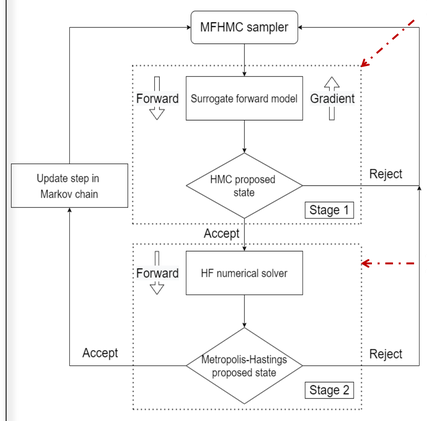
Challenges:

$\nabla_x \mathbf{f}(\mathbf{x})$ is required.

1. Impossible to compute for Black-box solvers (such as HTR)
2. Expensive gradient computation (1 gradient evaluation = 2 forward solves)
3. Low statistical efficiency

II. Multi-fidelity Hamiltonian Monte Carlo (MFHMC)

Key idea: Split the HMC algorithm in two stages:



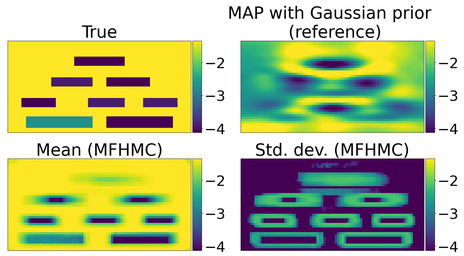
1. Use a DNN-based surrogate in the first (HMC) stage (by leveraging automatic differentiation capability for efficient gradient computation)
2. Use HF numerical solver in the second stage of Metropolis-Hastings step for accurate posterior sampling

Results on benchmark problems:

Darcy's flow (*experimentally* obtained data)

$$-\nabla \cdot (\boldsymbol{x}\, \nabla \boldsymbol{y}) = \boldsymbol{f_i} \quad \text{in } \Omega$$
$$\boldsymbol{y} = \mathbf{g} \quad \text{on } \partial\Omega$$

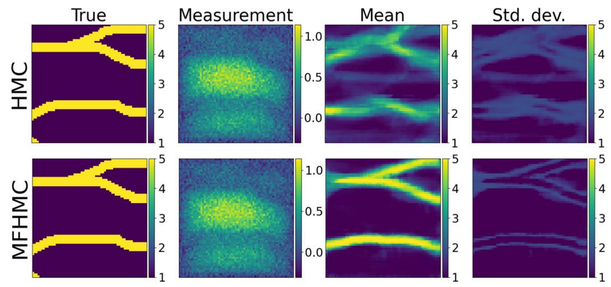
For a fixed stats. error:



Fixed stats. error	HMC	MFHMC
# of HF evaluations ↓	O(1000)	**O(100)**
Statistical efficiency ↑	O(1e-5)	**O(1e-4)**

Darcy's flow (*synthetic data*)

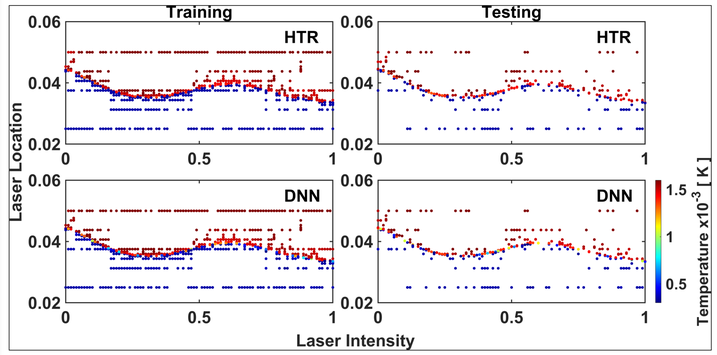
For a fixed no. of HF evaluations:



QoI	HMC	MFHMC
Error in mean (in %) ↓	51.4	**31.4**
Time (in Sec.) ↓	11777.5	**3401.5**

III. Ongoing Work

- A multi-layer perceptron neural network is used as a forward surrogate model to train different operating conditions. Mainly, two laser parameters, laser intensity and location, are used to train the model with 1292 sample points.



References:

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- Andrew Gelman, John B. B. Carlin, Hal S. S. Stern, and Donald B. B. Rubin (2014) "Bayesian Data Analysis", Third Edition (Texts in Statistical Science). page 675.
- D. Patel, J. Lee, M. Forghani, M. Farthing, T. Hesser, P. Kitanidis, E. Darve "Multi-Fidelity Hamiltonian Monte Carlo Method with Deep Learning-based Surrogate", *Second symposium on science-guided AI, AAAI Fall Symposium Series (FSS)*, 2021.

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