AI-Solver: Uncertainty in Prediction and Error Estimation for AI in Engineering

Ahmed Al-Jarro[1], Loic Beheshti[1], Serban Georgescu[1], Koichi Shirahata[2], Yasumoto Tomita[2], and Kouta Nakashima[2]

[1]Fujitsu Laboratories of Europe Ltd., Hayes Park Central, Hayes End Road, Hayes UB4 8FE, Greater London, UK

[2]Fujitsu Laboratories Ltd., 4-1-1 Kamikodanaka, Nakahara-ku, Kawasaki, Kanagawa 211-8588, Japan

FUJITSU

Abstract

The AI-Solver is a deep learning platform that learns from simulation data to extract general behavior based on physical parameters. The AI-Solver can handle a wide variety of classes of problems including those commonly identified in FEA, CFD and CEM, to name a few, with speedups of up to 250000X and extremely low error rate of 2-3% [1, 2]. In this work, we build on this recent effort. We first integrate uncertainty quantification, via exploiting the approximation of Bayesian Deep Learning. Second, we develop bespoke error estimation mechanisms capable of processing this uncertainty to provide instant feedback on the confidence in predictions without relying on the availability of ground truth data. To our knowledge, the ability to estimate the discrepancy in predictions without labels is a first in the field of AI for Engineering.

AI-Solver : Uncertainty Quantification in Prediction

In the AI-Solver [1, 2], we quantify the uncertainty in prediction as a Bayesian Approximation (BA) at inference via applying Monte-Carlo Dropout (MC-Dropout) [3], as shown below.

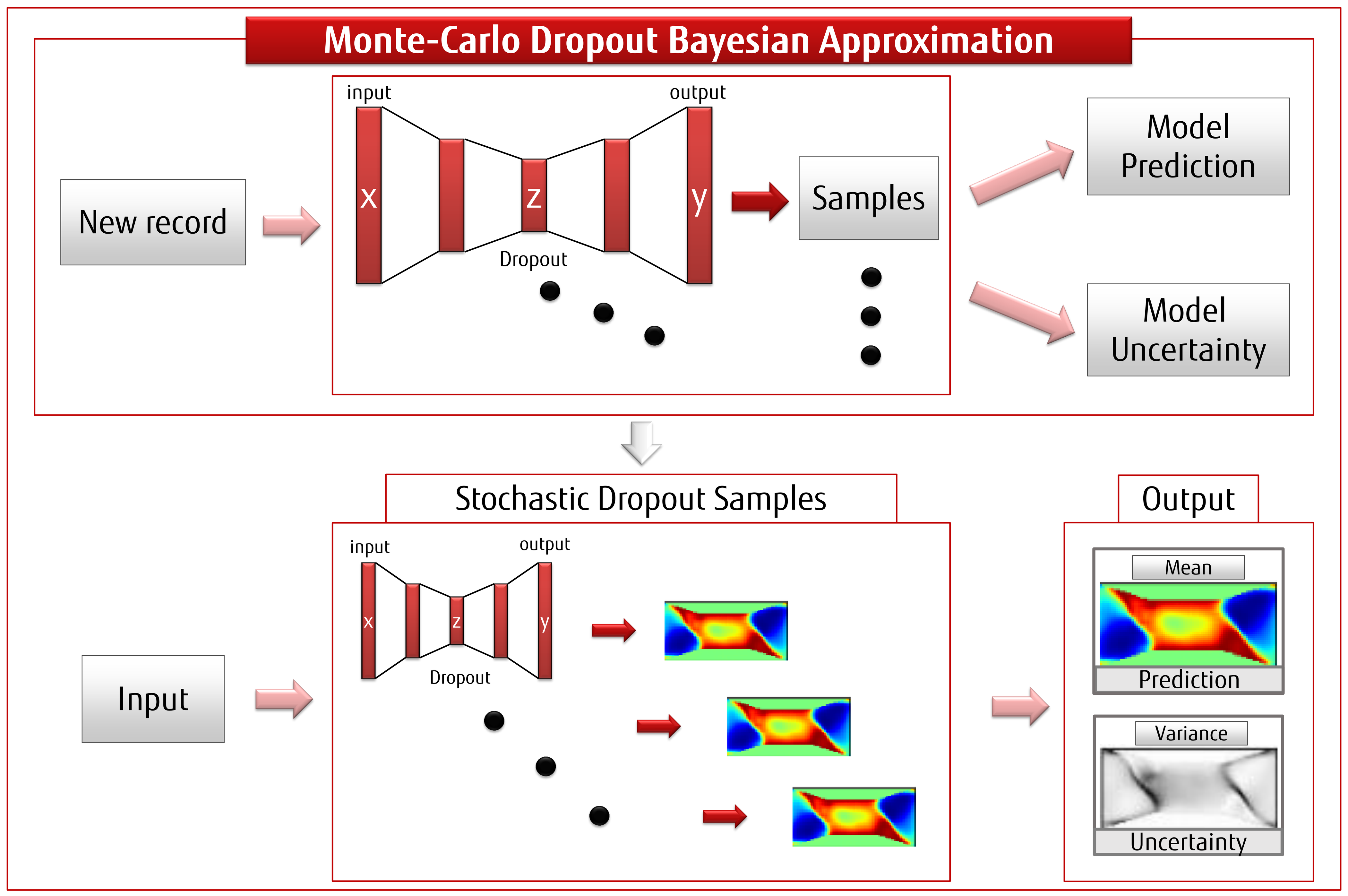

Figure 1: MC-Dropout Bayesian approximation integrated into the AI-Solver

Conclusion

The potential errors associated with deep learning predictions are important to tackle. In this work, we provide a novel system and mechanism to detect such imperfections and failures. We demonstrate this work to provide effective tools related to uncertainty quantification and error estimation where a statistically derived model and metric is applied to translate this uncertainty into reliable error estimation. A metric that is easy to understand and interpret by engineers as well as non-expert end-users. This ability to estimate the discrepancy of predictions in deep learning without labels is a first in the field of AI for Engineering.

Method and Results

- The problem setup considers the magnetisation of solids that are of different layouts and subjected to the influence of external sources, often used in the design of hard drive heads or other memory devices.
- The top panel shows the ground truth simulations (S). The second and third panels show the prediction (P) and uncertainty (U) produced by the AI-Solver that integrates MC-Dropout at inference. The bottom panel plots the absolute difference between the sets of ground truth, S, and predicted results, P, across all principal field components, i.e. diff = |P - S| for x, y and z fields, where the average diff_x,y,z ≈ 0.0436.

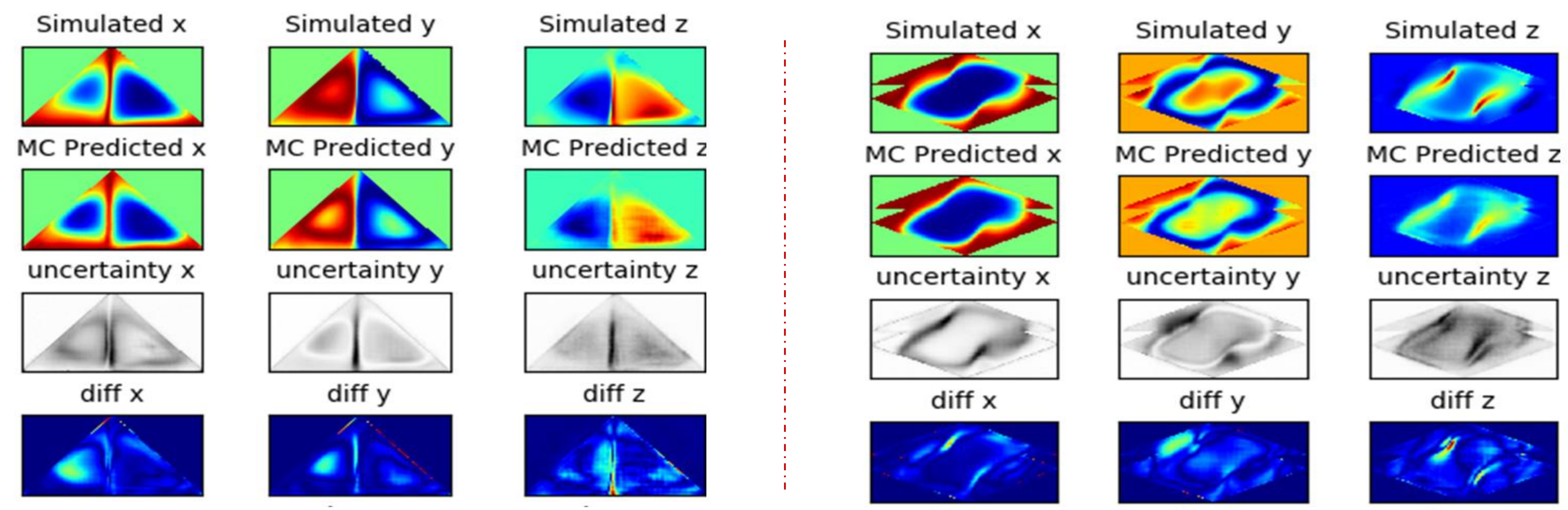

Figure 2: Prediction (P) and uncertainty (U) in the AI-Solver via MC-Dropout at inference

Uncertainty to Error Estimation

- **Uncertainty, U, from BA via MC-Dropout at inference is strongly correlated with inference error, i.e. diff.**
- **However, it does not produce a direct metric of final error, e.g. diff. This can lead to misinterpretation of U, particularly for the non-expert end-user.**
- **Here, we present a custom model that statistically evaluates a reliable metric of error, E, and margins of confidence, std, given an uncertainty value, U.**
- **Our custom model requires few data points and is developed as an alternative to Gaussian Processes (GP), where GP are judged incompatible with this particular nature of the observed data distribution.**
- **As an example of the application of our proposed method, Figure 3 plots the estimated errors, E, and corresponding margins as a function of uncertainty.**
- **Red points are used to derive our model, and green points correspond to new records (test data). Crosses and circles represent actual error, diff, and estimated error, E, respectively, with excellent fitting.**

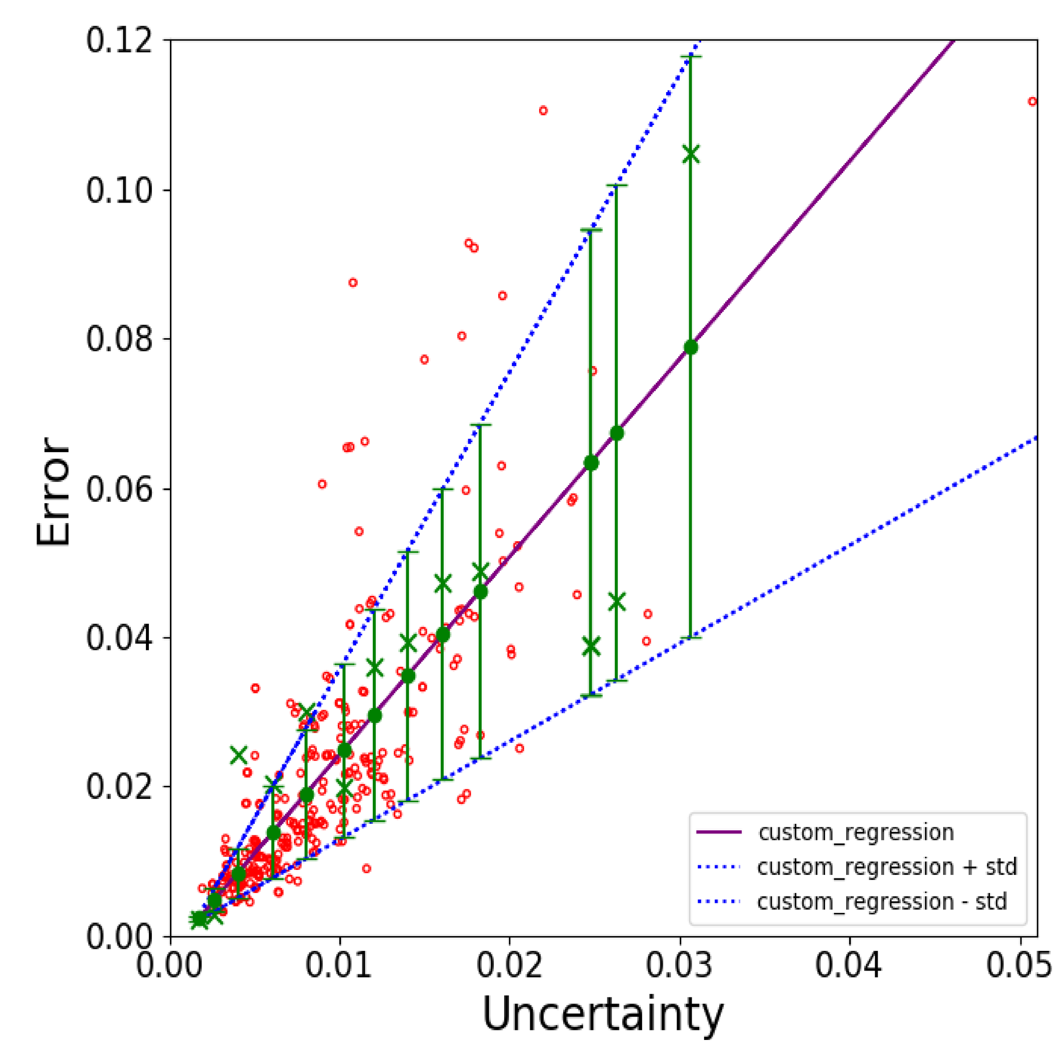

Figure 3: Uncertainty to error estimation

References: [1] A. Al-Jarro, L. Beheshti, S. Georgescu, Y. Tomita, and K. Nakashima, "DeepSim-HiPAC: Deep Learning-based Platform Converts Physics-based Simulators into Real-time AI Simulators", NVIDIA GPU Technology Conference, San Jose, Cal, USA, March 18-21, 2019. [2] A. Al-Jarro, S. Georgescu, Y. Tomita, and K. Nakashima, "DeepSim-HiPAC: Deep Learning High Performance Approximate Calculation for Interactive Design and Prototyping", SC 2018, Dallas, TX, USA, November 11-16, 2018. [3] Y. Gal and Z. Ghahramani. "Dropout as a Bayesian Approximation: Representing Model Uncertainty in Deep Learning", In International Conference on Machine Learning, pages 1050–1059, 2016.