Data driven Computational Mechanics at EXascale

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A NOVEL LOAD-BALANCED TMCMC-BASED METHOD FOR SCALABLE SAMPLING

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Description

In this task we have proposed the research and development of an algorithm for the sampling of distributions based on the transitional-MCMC algorithm that allows for scalable parallelisation but also prevents, to the maximum extent possible, the problem of load imbalance among samples in the same sampling generation. The high computational cost of the sampling algorithms comes from the computation of the likelihood function that involves the evaluation of a computationally expensive computational model.

Problems with the proposed algorithm

The proposed algorithm was based on the idea of starting further generations of TMCMC before all the samples in the current generation had finished. At the early stages of the project, we realized that this approach will introduce a destructive bias towards samples with low probability. Moreover, there is no way to correct the bias without wasting extra computational resources. This makes the algorithm practically unusable since the computational resources that will be saved by running early samples on further generations will be used to correct the bias that has been introduced.

Alternative algorithm

We propose the following alternatives to mitigate the problems of the high computational cost of the computational models involved in the evaluation of the likelihood function.

First, we note that load imbalance in sampling will no longer be a bottleneck once we start using the surrogate model. This is based on the observation that the surrogates can be run in seconds, as simple forward propagation of NNs in a GPU. In addition, using a surrogate model with available derivatives with respect to its parameters, will benefit from the usage of gradient based sampling algorithms. So far, the Hamiltonian Markov chain algorithm has been implemented in Korali.

Second, we plan to implement in Korali the stochastic approximation expectation maximization (SAEM) algorithm. This algorithm has been proposed for the optimization of the observable variables in latent variable models (LVMs). The hierarchical Bayesian models that we will consider in this project can be viewed as LVMs. In addition, the uncertainty in the observable variables can be approximated by the Laplace approximation technique. The involved Hessian of the posterior is analytically tractable in the models and applications that we will consider. Since the SAEM algorithm optimizes and does not sample the posterior distribution, we believe that the computational savings will be significant compared to TMCMC. We have started with the implementation of the SAEM algorithm in Korali. The implementation has been tested on simple LVMs and we plan to test it and compare it with TMCMC on a hierarchical Bayesian problem in the next months.

Finally, we plan to explore ideas on parallelizing the SAEM algorithm by fusing ideas from evolution strategy (ES) algorithms and especially the covariance matrix adaptation ES algorithm (CMA-ES).

The alternative procedure will be included in Task 4.4 Integration of the new methods in the Korali framework (M12-M18) without any amendments in the effort or budget.