Multivariate Adaptive Surrogate Modelling

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1. Overview

1.1 Goal

Given a black-box, multivariate simulator, create a ***global*** surrogate model that captures the complex behavior of the system over the complete design space as accurately and efficiently as possible.

1.2 Motivation

Accurate, physics based simulation codes are not always available or too costly to use for design exploration, parameter sweeping, *what-if* analysis,... Depending on complexity, a single sample evaluation may take many hours on modern hardware. Surrogate models are therefore a cost effective alternative.

1.3 Our Solution

We study and develop fully automated sequential metamodeling techniques for efficient design space exploration, which minimize the overall number of computational expensive simulations.

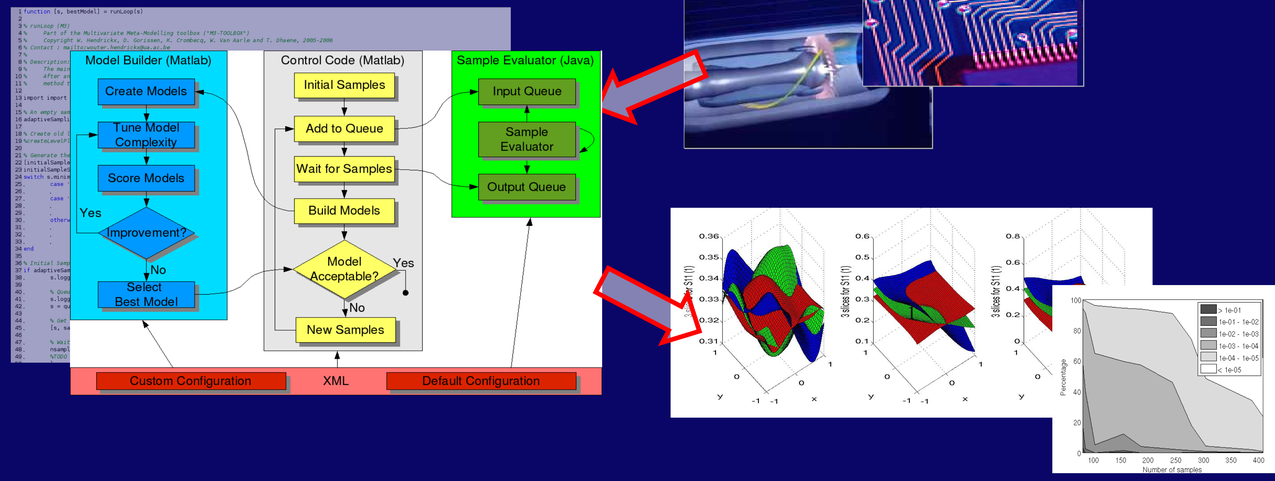

Figure 1: From physical model to metamodel.

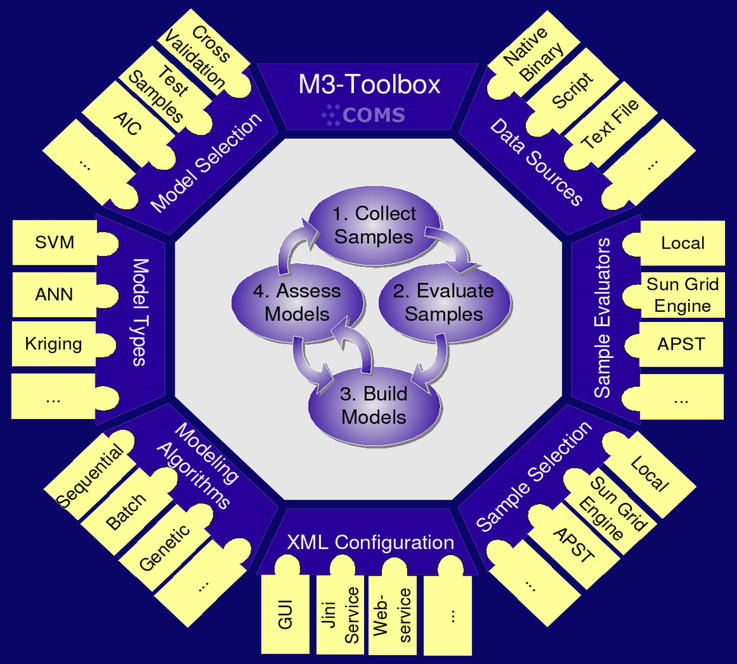

Figure 2: Modularity within the M3-Toolbox

2. M3-Toolbox

The *Multivariate MetaModeling toolbox* (M3) is a MATLAB toolkit for adaptive surrogate modeling. Given a datasource (simulation code, dataset, ...), the toolbox will iteratively generate a global surrogate model using as little datapoints as possible. Its algorithms are fully adaptive, requiring no user interaction and will run until a pre-defined accuracy level is reached.

There is no such thing as a "one-size-fits-all" solution. Each aspect of the toolbox has therefore been implemented with modularity and extensibility in mind and can be easily configured using XML (*see* figure 2).

Design Goals
- Construct standalone, global metamodels
- Minimize prior knowledge about the simulator
- Minimize the number of simulator evaluations
- Pre-defined accuracy
- Fully adaptive, minimizing user interaction
- Fully pluggable and extensible
- Easy configuration, use, and integration

3. Current Research Topics

- Surrogate model driven design optimization
- Simulator Preprocessing
  - Feature Selection (parameter screening)
  - Constraints
  - Knowledge integration (Fuzzy Techniques)
- Intelligent sample queueing
- Ensemble Modeling, Heterogeneous Evolutionary Modeling, Probabilistic Modelling

References

[1] **Gorissen D., Hendrickx W., Crombecq K., Dhaene T. (2006)**, *6th IEEE/ACM International Symposium on Cluster Computing and the Grid*, Singapore (Singapore), pp. 185-192.

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