

mumpce_py: A Python Implementation of the Method of Uncertainty Minimization Using Polynomial Chaos Expansions

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1. Summary

The Method of Uncertainty Minimization using Polynomial Chaos Expansions (MUM-PCE) [1-6] was developed as a software tool to constrain physical models against experimental measurements. These models contain parameters that cannot be easily determined from first principles and so must be measured, and some which cannot even be easily measured. In such cases, the models are validated and tuned against a set of global experiments which may depend on the underlying physical parameters in a complex way. The measurement uncertainty will affect the uncertainty in the parameter values.

MUM-PCE was written to provide a streamlined workflow for computational uncertainty analysis. The software provides the following functionality:

- Compiles a database of experimental measurements
- Compares calculations using a physical model with the measurements (validation)
- Constrains the physical model against the measurements (optimization)
- Determines the model uncertainty based on the measurement uncertainty (uncertainty analysis)
- Identifies measurements inconsistent with the constrained model (outlier detection)
- Identifies experimental measurements that do not strongly constrain the model (experimental design)

The software cannot be used out of the box. Users must create an interface to their own software, and that interface will be specific to the user's application. Two examples of how to write an interface are provided. One is a toy model that is intended to be as complete as possible while also simple. The other is an interface to the reaction kinetics program Cantera (<http://cantera.org>), which represents a research-level use case with multiple heterogeneous experiments and a highly complex interface to a detailed model.

2. Software Specifications

NIST Operating Unit(s)	Chemical Sciences Division, Material Measurement Laboratory
Category	Optimization and uncertainty analysis
Targeted Users	Users of any modeling code wishing to estimate uncertainty
Operating System(s)	Cross-platform, where Python, NumPy, and SciPy are installed
Programming Language	Python 3.6
Inputs/Outputs	This software is not usable out-of-the-box. The user must write additional code to interface their model with this software.
Documentation	https://pages.nist.gov/mumpce_py
Accessibility	N/A small-scale research tool
Disclaimer	https://www.nist.gov/director/licensing

3. Methods for Validation

The software is verified using the `toy_model` submodule. More details can be found in the documentation at <https://pages.nist.gov/toy.html>. This model is chosen to have an analytic solution.

4. References

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About the author: David Sheen is a Physicist at NIST. His work is on uncertainty analysis in complex systems including high-temperature chemical kinetics and metabolomics. The National Institute of Standards and Technology is an agency of the U.S. Department of Commerce.