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Sandia National Laboratories

Overview of the latest features and capabilities in the Dakota software

DAKOTA

Explore and predict with confidence

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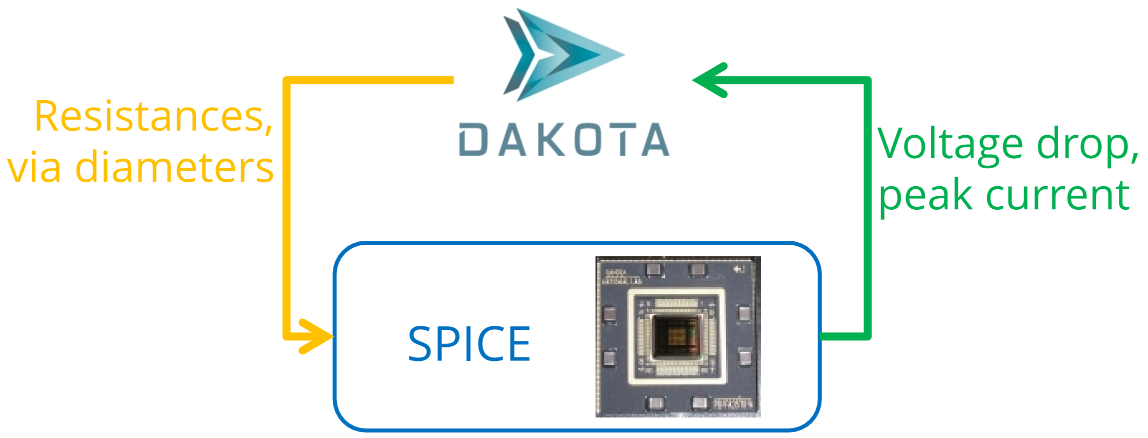
What is Dakota?

Open-source software for black-box, ensemble analysis of computational simulations

- Suite of iterative mathematical and statistical methods and a convenient means of interfacing with (just about) any simulation software
- Provides scientists, engineers, and decision makers greater insight into the predictions of their models via:
  - Global Sensitivity Analysis
  - Uncertainty Quantification
  - Optimization
  - Calibration
- Production and Research focus
- Works on desktops and HPCs and the major operating systems (*nix, OS X, Windows)
- Command line interface, GUI, and API



Capabilities

Common interface to established and cutting edge algorithms

Sensitivity Analysis
- Designs: MC/LHS, DACE, sparse grid, one-at-a-time
- Analysis: correlations, scatter, Morris effects, Sobol indices

Uncertainty Quantification
- MC/LHS/Adaptive Sampling
- MF/ML sampling and surrogates
- Reliability
- Stochastic expansions
- Epistemic methods

Optimization
- Gradient-based local
- Derivative-free local
- Global/heuristics
- Surrogate-based

Calibration
- Tailored gradient-based
- Use any optimizer
- Bayesian inference

- Mixed aleatory/epistemic UQ
- Optimization under uncertainty

- Parallel execution
- HDF5 Output
- Direct Python interface

Develop simulation driver once; use in different kinds of studies

Multifidelity and Multilevel UQ Methods

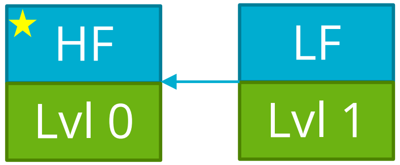
Exploit hierarchies of models to compute lower variance estimates of moments at lower cost

- Dakota 6.10 (May ‘19) included Control Variate Monte Carlo (CVMC), Multilevel (ML)MC, and MLCV MC.

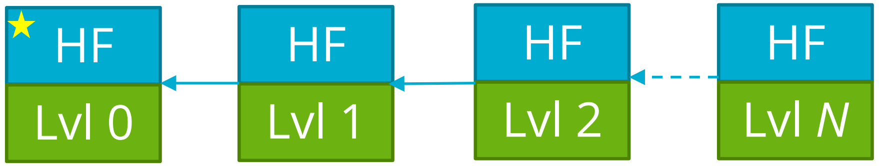
Multifidelity Hierarchy
Predictions of lower fidelity models are biased, regardless of model resolution

Multilevel Hierarchy
Model predictions converge as resolution is improved

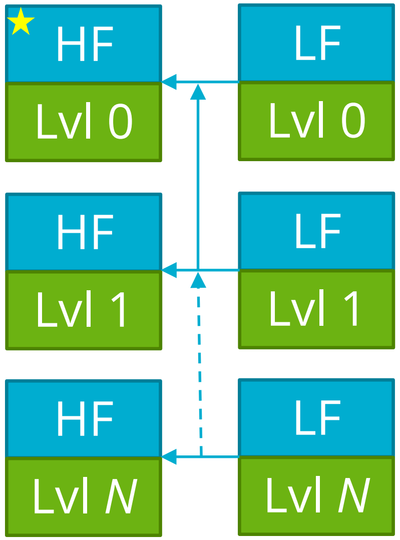
- Model costs, variance, and correlations are estimated by a pilot study, and a constrained optimization problem is solved to select a sample schedule that minimizes the cost for a desired estimator variance



CVMC
High and Low Fidelity
(LF prediction is biased)



MLMC
Multiple model resolutions
(Prediction converges as resolution is improved)

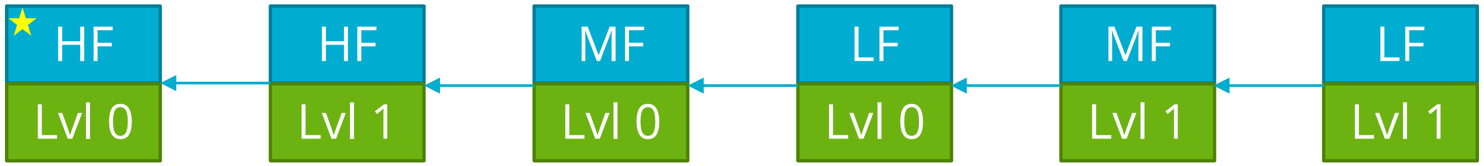


MLCV MC
(2D hierarchy)

Multifidelity and Multilevel UQ Methods

Reduce Restrictions on Model Hierarchies

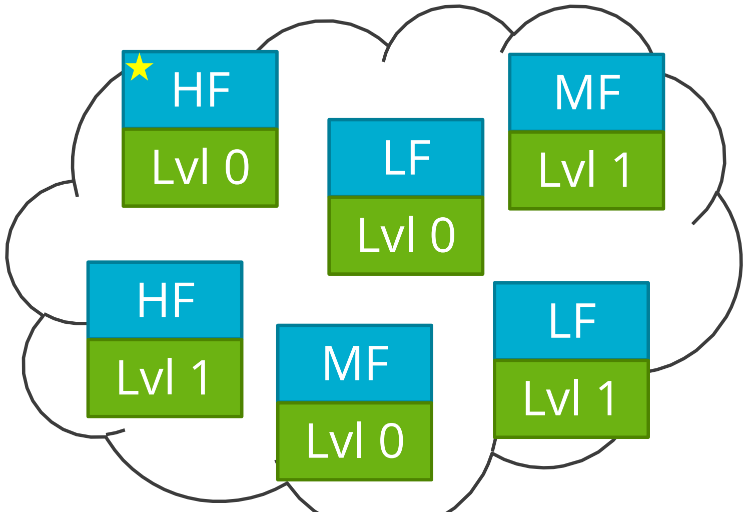
Multifidelity Monte Carlo - 6.15 (Nov ‘21)



1D hierarchy of models of unlimited depth; convergence requirement lifted

Approximate Control Variate – 6.15 (Nov ‘21)

- “Cloud” of models; no hierarchy assumed
- Recursion limit on variance reduction $(1-\rho^2)$ is lifted



Multifidelity and Multilevel UQ Methods

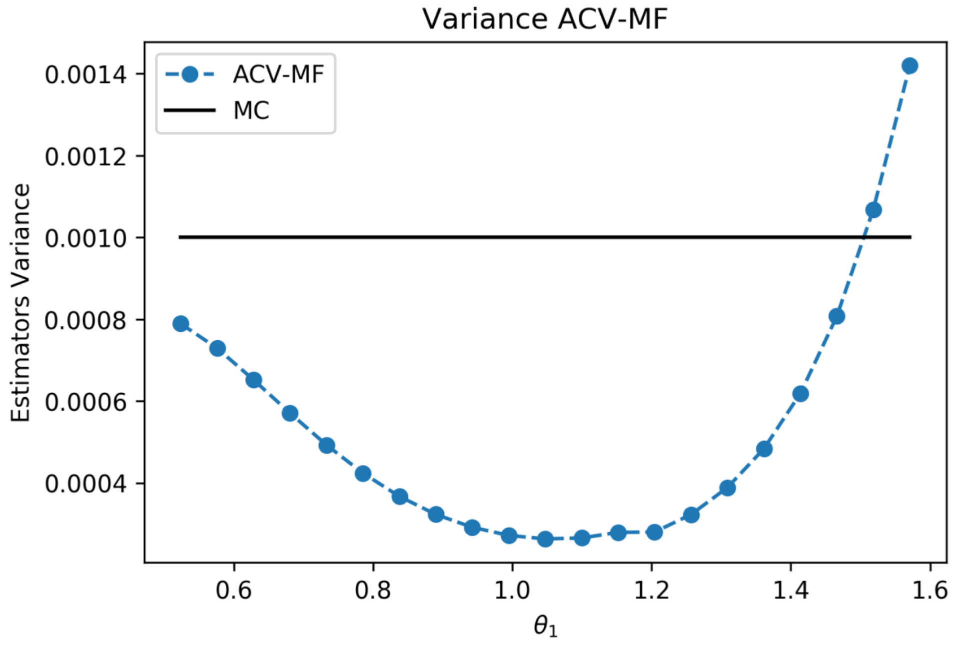
Other Recent Algorithmic and Usability Improvements

Pilot Projection - 6.16 (May ‘22)

Which estimator (CVMC, MLMC, ACV, etc) provides the greatest variance reduction at the least cost?

Model Tuning – 6.16 (May ‘22)

Tune solution level to achieve the best variance reduction and cost

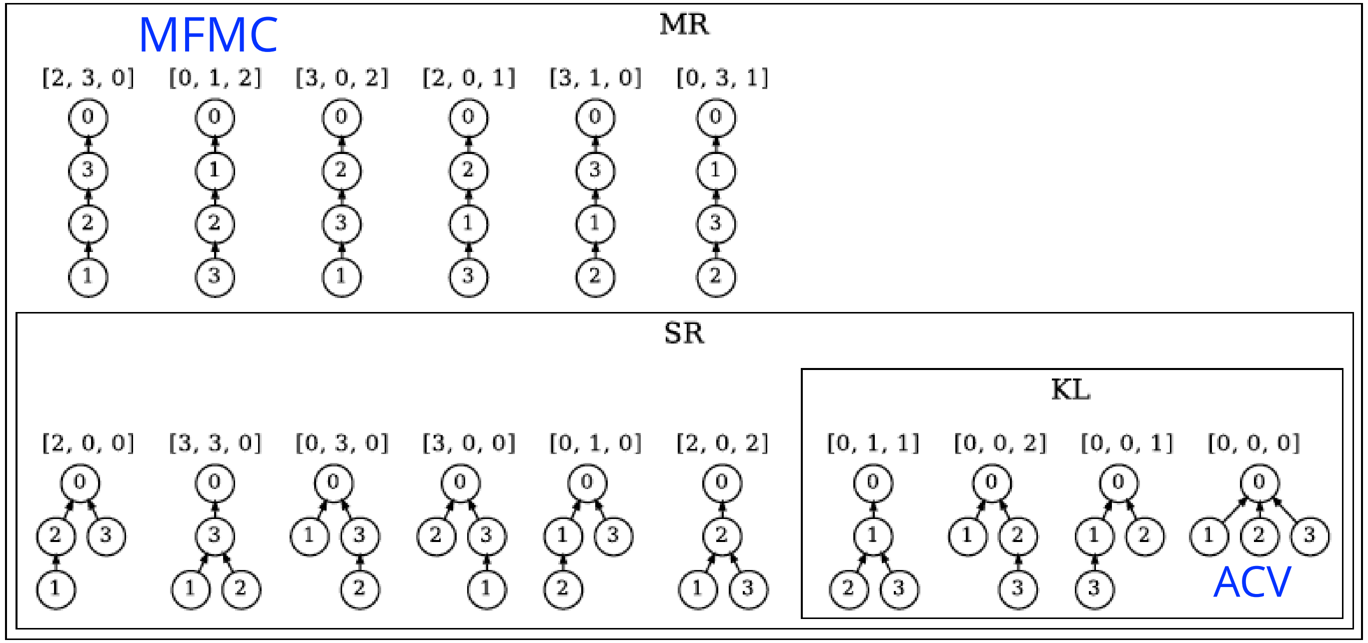


Multifidelity and Multilevel UQ Methods

Other Recent Algorithmic and Usability Improvements

Generalized ACV: graph enumeration - 6.18 (May ‘23)

Explores all possible model dependencies, as defined by directed acyclic graphs defining control variate pairs



Bomarito et al., 2022

Batch Parallel Efficient Global Optimization (EGO)

Efficiently use parallel computing resources to perform global optimization

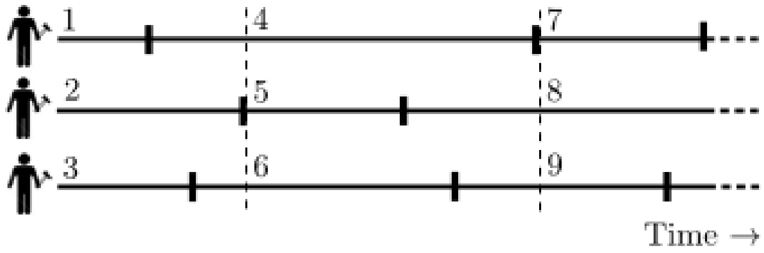
EGO uses the mean and variance prediction of a Gaussian process to balance exploration and exploitation

Original EGO Algorithm

1. Train a GP on an initial set of samples.
2. Identify candidate: $\underset{u}{\operatorname{argmax}}\, EI\left(\hat{G}(u)\right)$, where $EI\left(\hat{G}(u)\right) \equiv \mathbb{E}\left[\max\left(\hat{G}(u^*) - \hat{G}(u), 0\right)\right]$
3. Evaluate candidate using the truth model; incorporate into the GP's training set
4. If not converged, go to 2.

Improvement 1 - 6.12 (May '20)

Batch Sequential EGO. Instead of a single point, batches are added. The additional points are based on *hallucination.*



Improvement 2 - 6.14 (May '21)

Batch Parallel EGO. Evaluations and updates to the GP occur asynchronously.

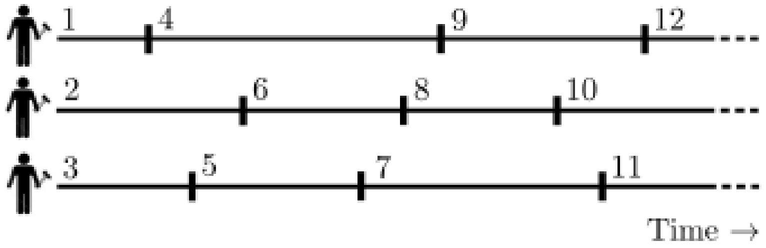
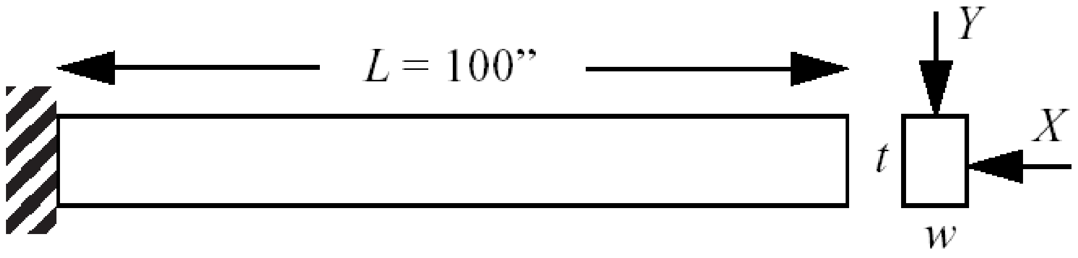


Figure courtesy Kandasamy et al. 2017

1. Tran, Anh, et al. https://doi.org/10.1007/s00158-021-03102-y
2. Tran, Anh, et al. https://doi.org/10.1016/j.cma.2018.12.033

Standardized Regression Coefficients – GSA Improvements




```
sampling
  samples 360
  std_regression_coeffs
```

Stress constraint

$$g_s = \frac{\frac{600}{wt^2}Y + \frac{600}{w^2 t}X}{R} - 1$$

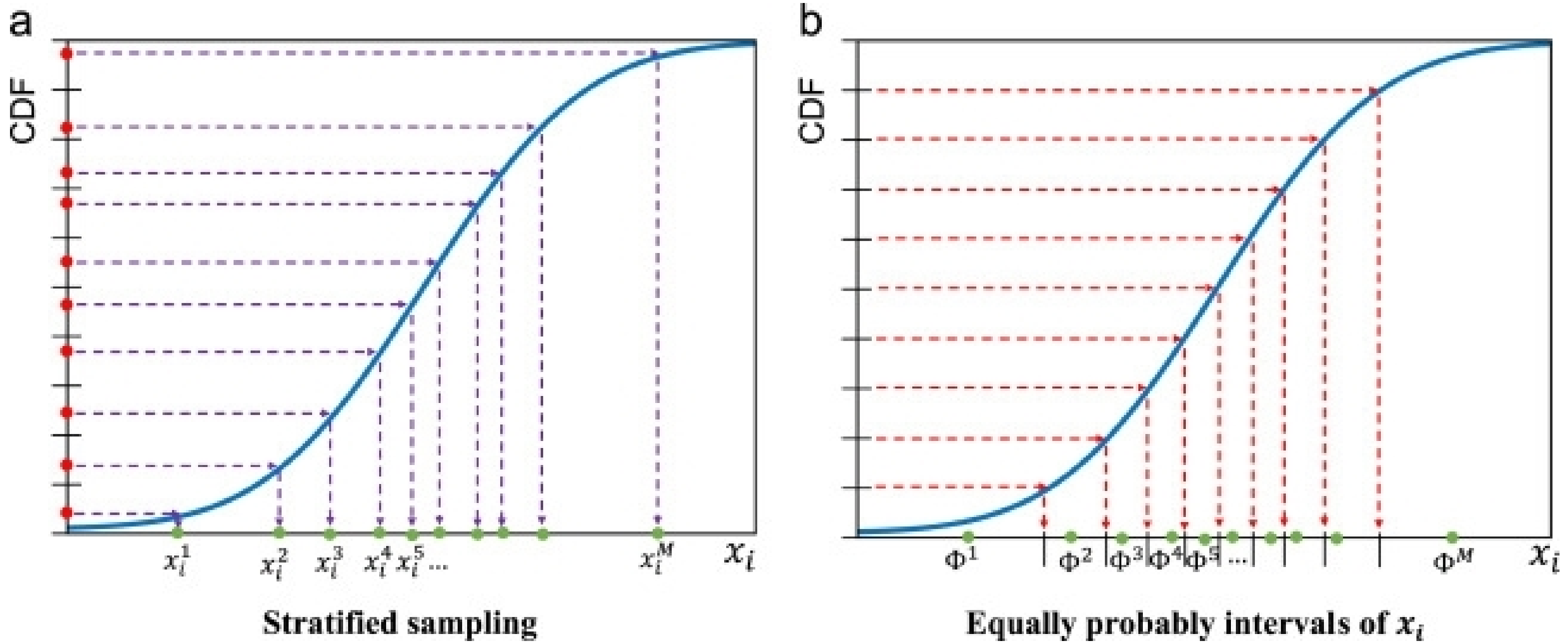
Displacement Constraint

$$g_d = \frac{\frac{4L^3}{Ewt}\sqrt{\left(\frac{Y}{t^2}\right)^2 + \left(\frac{X}{w^2}\right)^2}}{D_0} - 1$$

Variable	Distribution
w, t – width, thickness	*U*(2, 6) in
R – yield stress	*N*(30000, 1000) psi
E – elastic modulus	*N*(26e6, 1.45e6) psi
X – horizontal load	*N*(500, 100) lb
Y – vertical load	*N*(1000, 300) lb

Sampling-based first order Sobol indices – GSA Improvements

- For a function $y = f(\boldsymbol{x})$, the first order Sobol index is $S_i = \frac{V_{x_i}\left(E_{x_{\sim i}}(y|x_i)\right)}{V(y)}$
- As sensitivity measures, Sobol indices have some nice properties:
  - Attribute fractions of response variance to variables and combinations of variables
  - Do not assume linearity or monotonicity
- Existing “pick and freeze” approach requires hundreds of samples per dimension



Li and Mahadevan https://doi.org/10.1016/j.ress.2016.04.012

User Resources Migration to GitHub

https://github.com/snl-dakota

Unified documentation - https://snl-dakota.github.io

- Previously, Dakota's various manuals (GUI, Users, Reference, etc) were separate and even in different formats (CMS based, HTML, PDF)
- The new unified documentation provides "one stop shopping" for most of our materials

Discussions - https://github.com/orgs/snl-dakota/discussions

- Replaced the dakota-users listserv, which was deactivated February 15, 2023
- Offers numerous advantages: Markdown and latex support, threading, topics, etc

Examples Library - https://github.com/snl-dakota/dakota-examples

- Runnable examples with explanations for a wide variety of Dakota operations
- Authored by Dakota developers and routinely tested

Code Repositories - https://github.com/orgs/snl-dakota/repositories

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https://dakota.sandia.gov