

# Optimization - Dakota

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# Dakota

- Open source
- Interfacing with simulation models
- Multiple analysis capabilities

# Parameter Studies

- Exploring the effects of parametric changes on the model
  - Smoothness
  - Multi-modality
  - Robustness
  - Nonlinearity
- Can cover the whole parameter space, or be centered around a point of interest
- Typically an introductory analysis

# Design of Experiments

- Design of computer experiments are different than design of physical experiments
  - High dimensionality (many factors), no need for replicates
- Some computational models might have a long run time
- Response surface approximation
  - Surrogate models

# Uncertainty Quantification

- Analyzing uncertainty propagation
- Brute force
  - Sampling inputs from a statistical distribution
  - Analyzing the distribution of model outputs

# Optimization

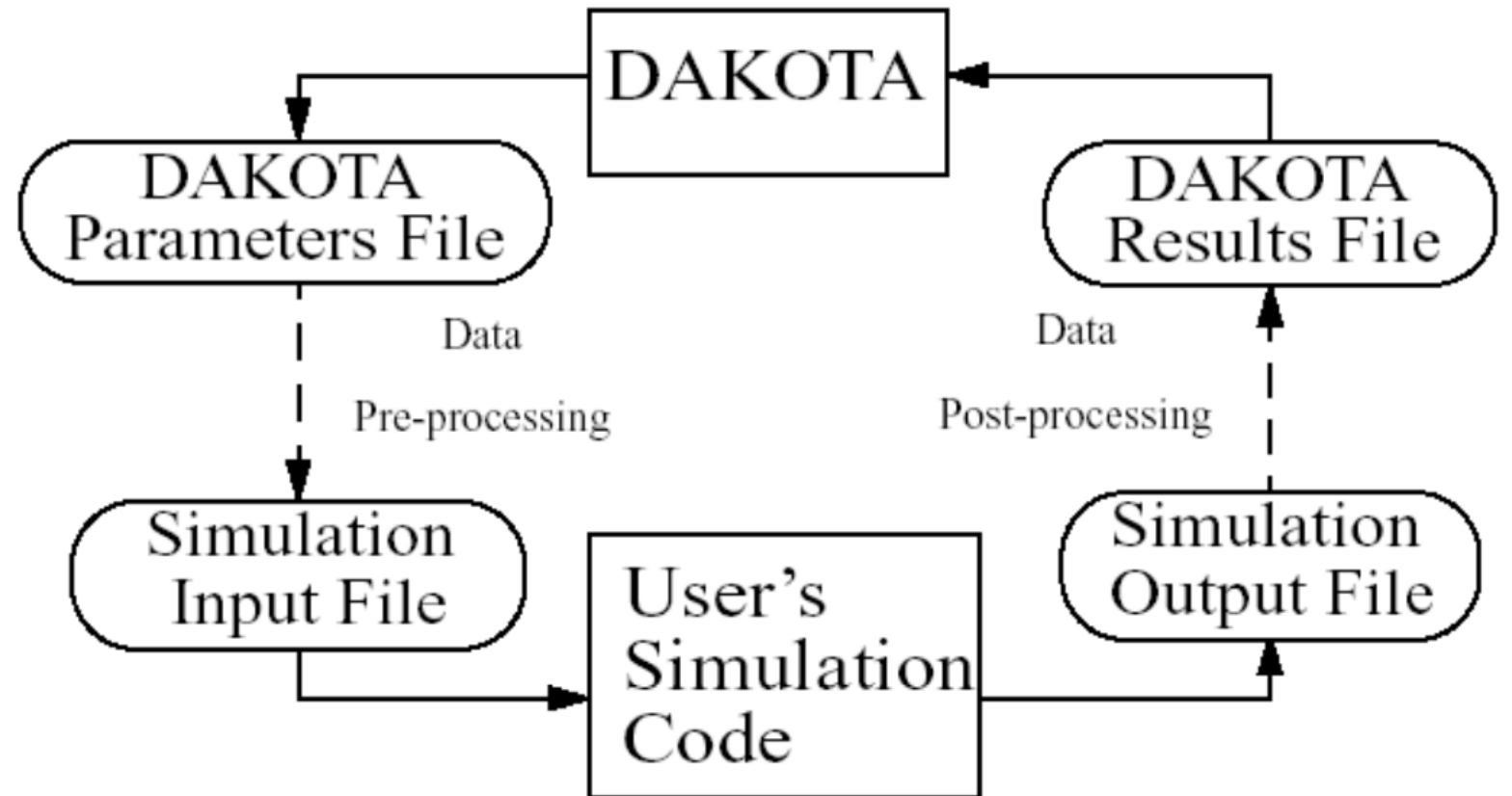
- Optimization of some objective function based on model outputs
- Large collection of third-party algorithms
- Multiple types
  - Gradient based local methods
  - Derivative-free local methods
  - Derivative free global methods

# Model Calibration

- Optimization methods specialized for least squares optimization

# The Dakota/Model Interface

- Black box
- No direct interface to the simulation code
- Requires wrapper functions





# Example Input File

```
environment,  
    tabular_data  
        tabular_data_file = 'rosen_opt.dat'  
  
method,  
    optpp_newton  
        max_iterations = 50  
        convergence_tolerance = 1e-4  
  
model,  
    single  
  
variables,  
    continuous_design = 2  
    cdv_initial_point -1.2  1.0  
    cdv_lower_bounds  -2.0 -2.0  
    cdv_upper_bounds  2.0  2.0  
    cdv_descriptor    'x1' 'x2'  
  
interface,  
    fork  
    analysis_drivers = 'python.exe rosenbrock_bb_di.py'  
    parameters_file = 'params.in'  
    results_file = 'results.out'  
  
responses,  
    num_objective_functions = 1  
    analytic_gradients  
    analytic_hessians
```

# Conclusion

- Useful for evaluating already implemented, complex models
- Multiple kinds of analyses
- Interface adds additional overhead
  - Both on the user- and computer side