SAND2015-6869 TR

Dakota Software Training

Input Syntax: Configuring Dakota Components

http://dakota.sandia.gov

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Module Learning Goals

- Develop an accurate "mental model" of Dakota components
- Understand how to configure Dakota components using a Dakota input file
- Become familiar with the Dakota Reference Manual

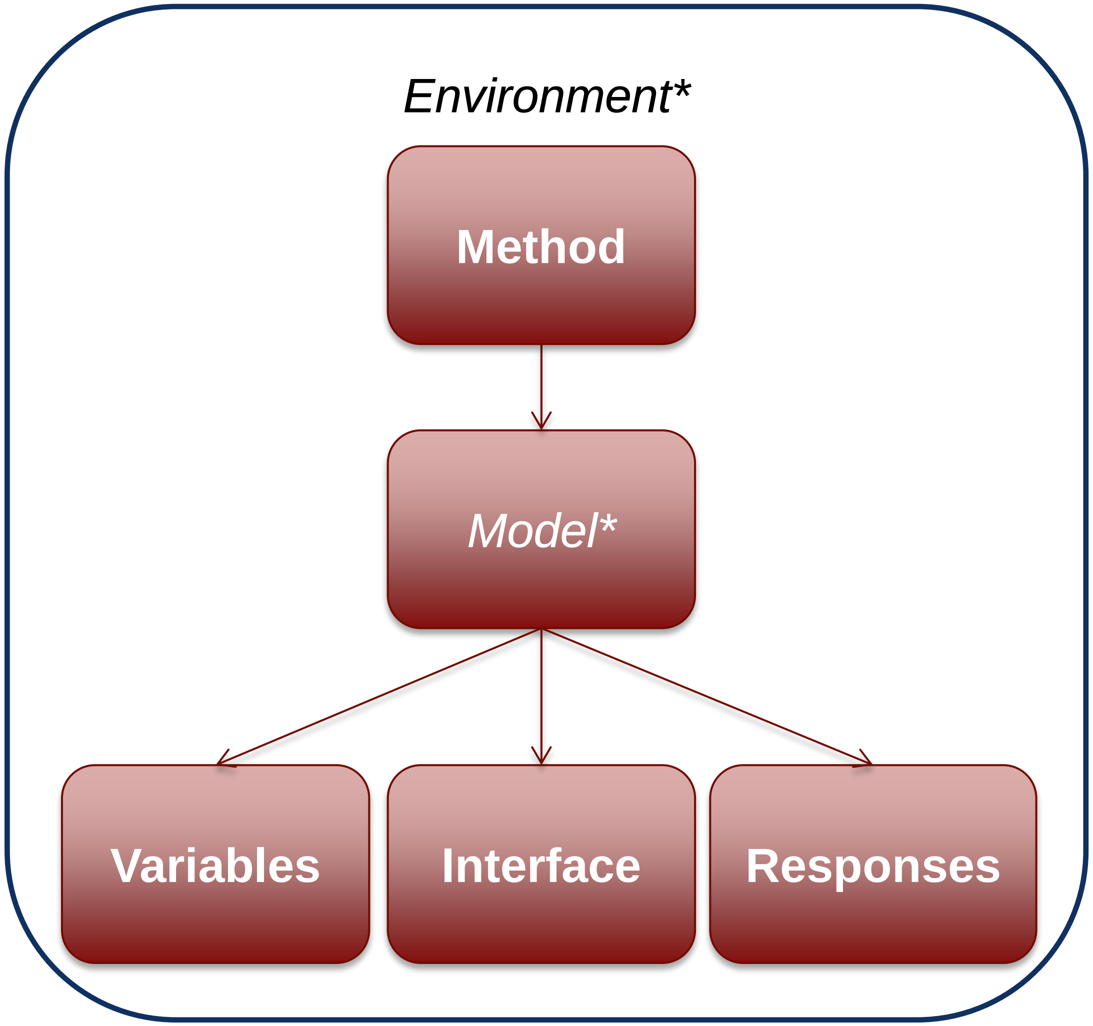
Dakota Input and Components

DAKOTA COMPONENTS

Dakota Blocks

Every Dakota study is composed of six types of blocks

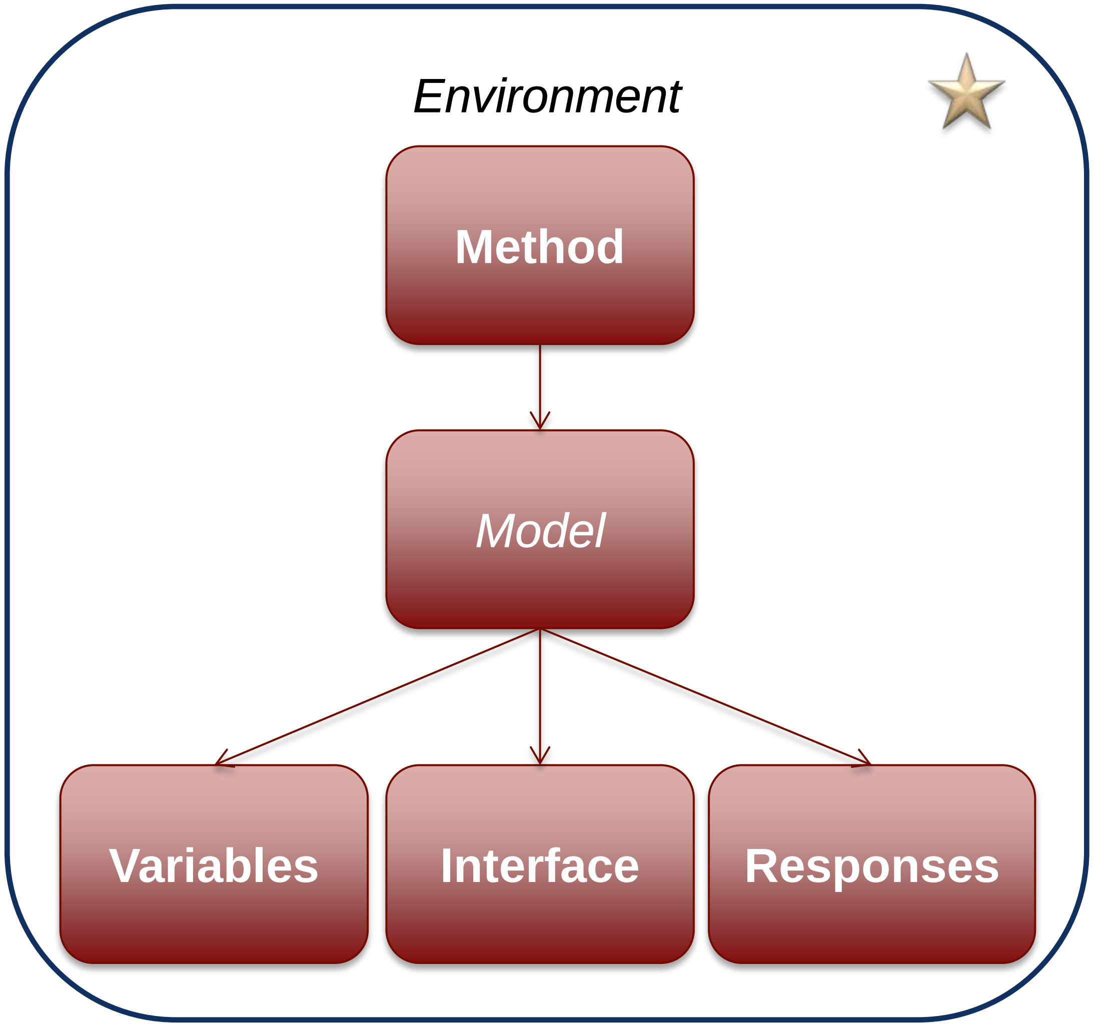
- *Environment**
- **Method**
- *Model**
- **Variables**
- **Interface**
- **Responses**



*Optional

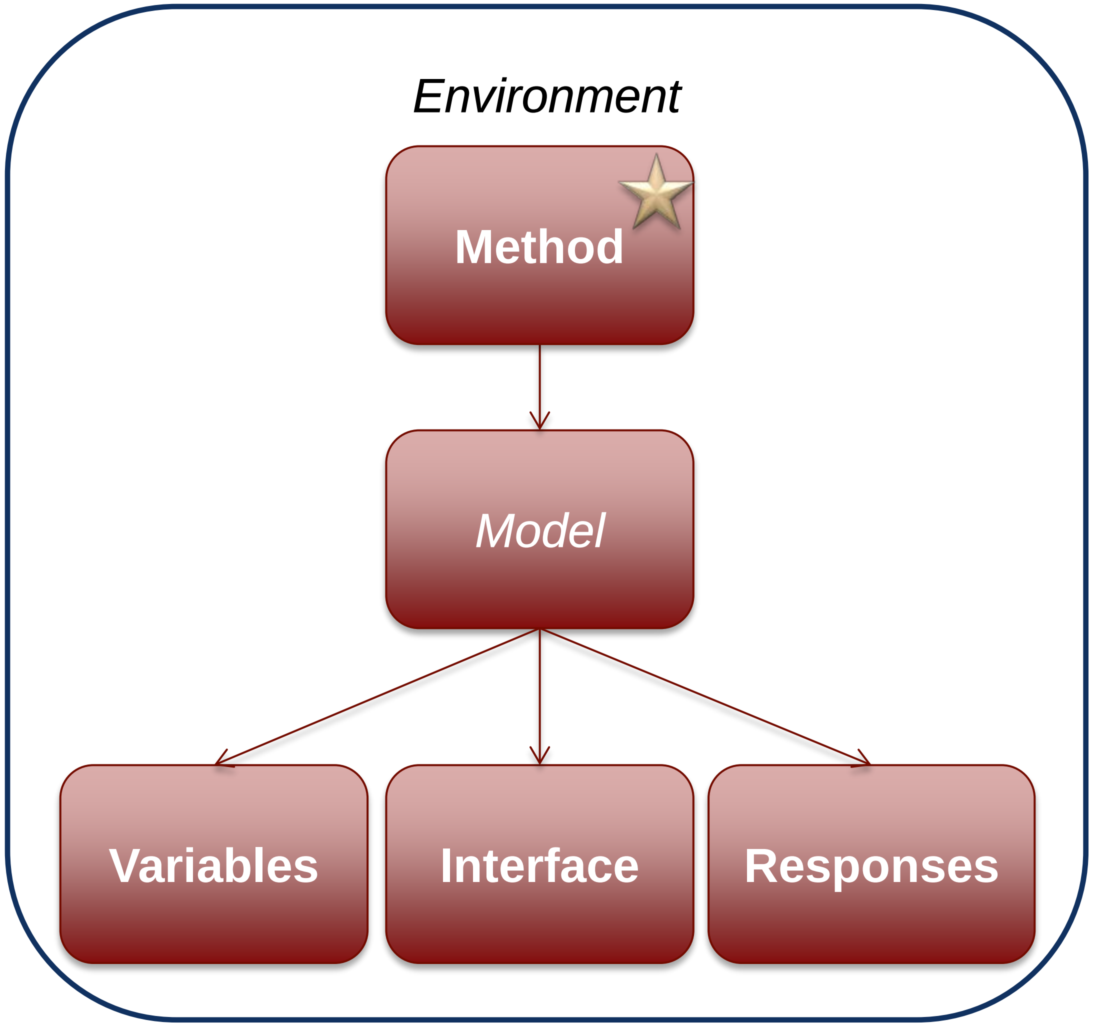
Environment: General Study Settings

- All other blocks are embedded in one environment block
- Example settings
  - Output precision
  - Name of output & error files
- At most one environment specification is permitted
- Environment specification is *optional*



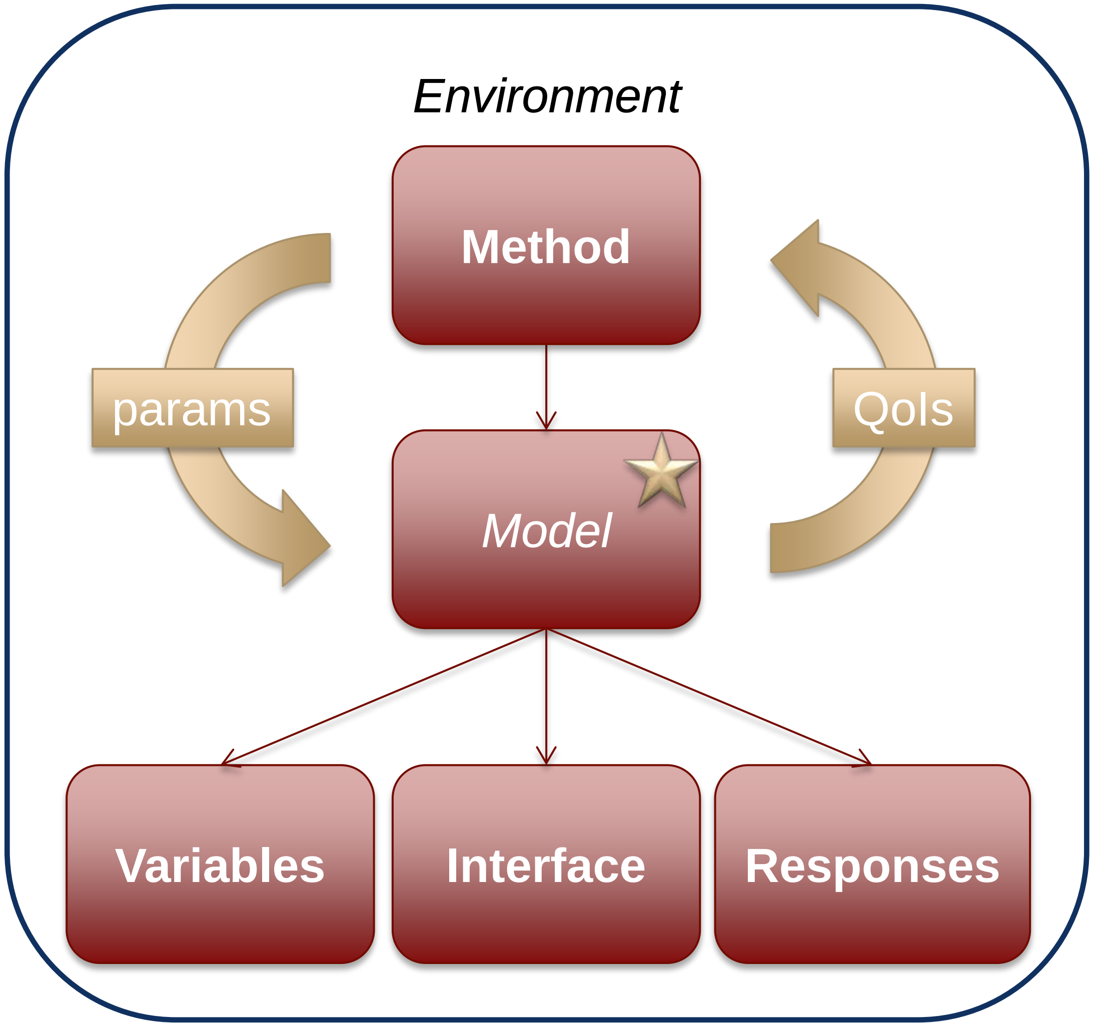
Method: What Dakota Does

- Specifies an algorithm, e.g., sampling, along with its options
- Invokes the model for a variables-to-responses map
- At least one method block is **required**
  - Multiple may be specified in complex studies



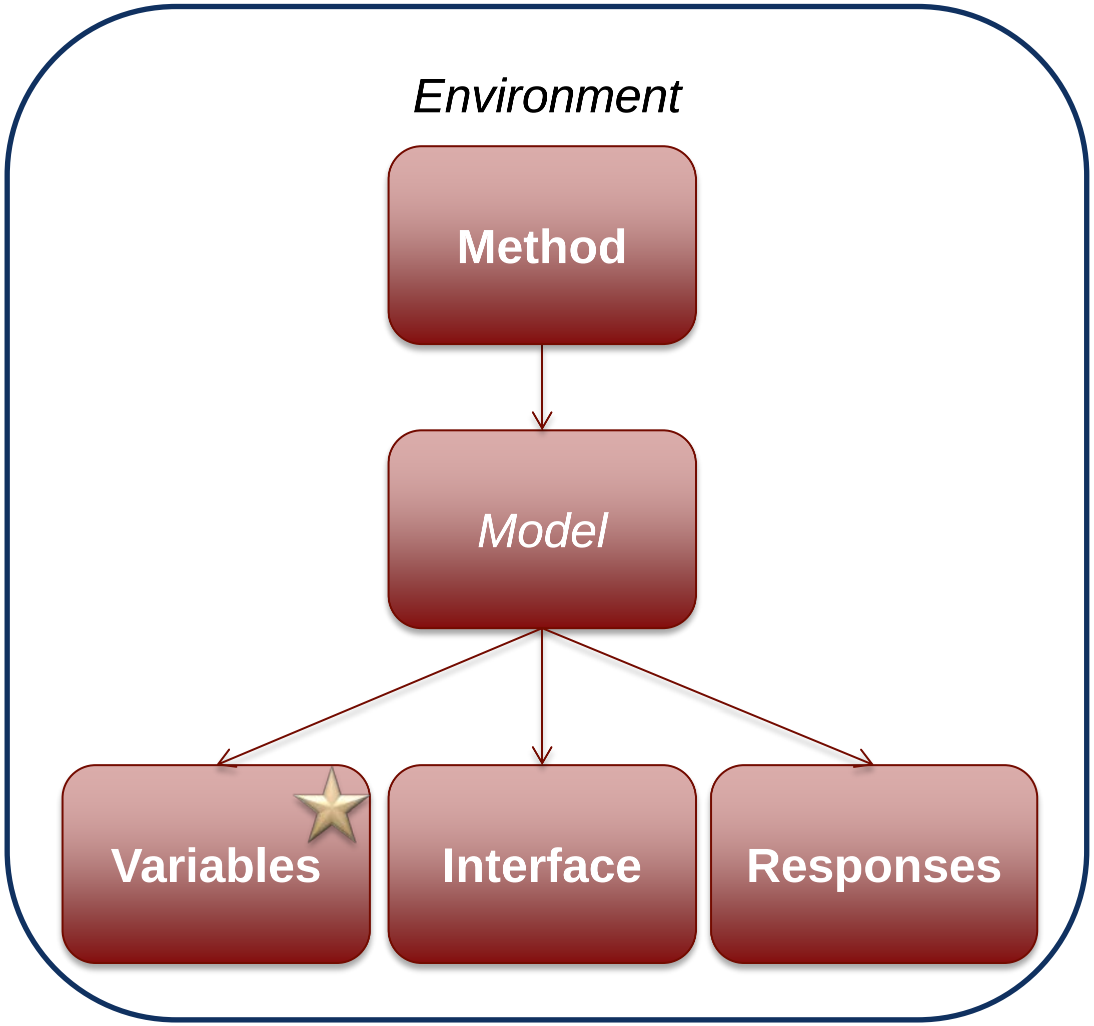
Model: Maps Variables to Responses

- A model block fulfills requests from a method to compute responses from variables
- Mapping can be through a simulation interface
  - Complex studies may use surrogate model, nested model/method
- Model is *optional* in simple studies
  - Multiple may be specified in complex studies



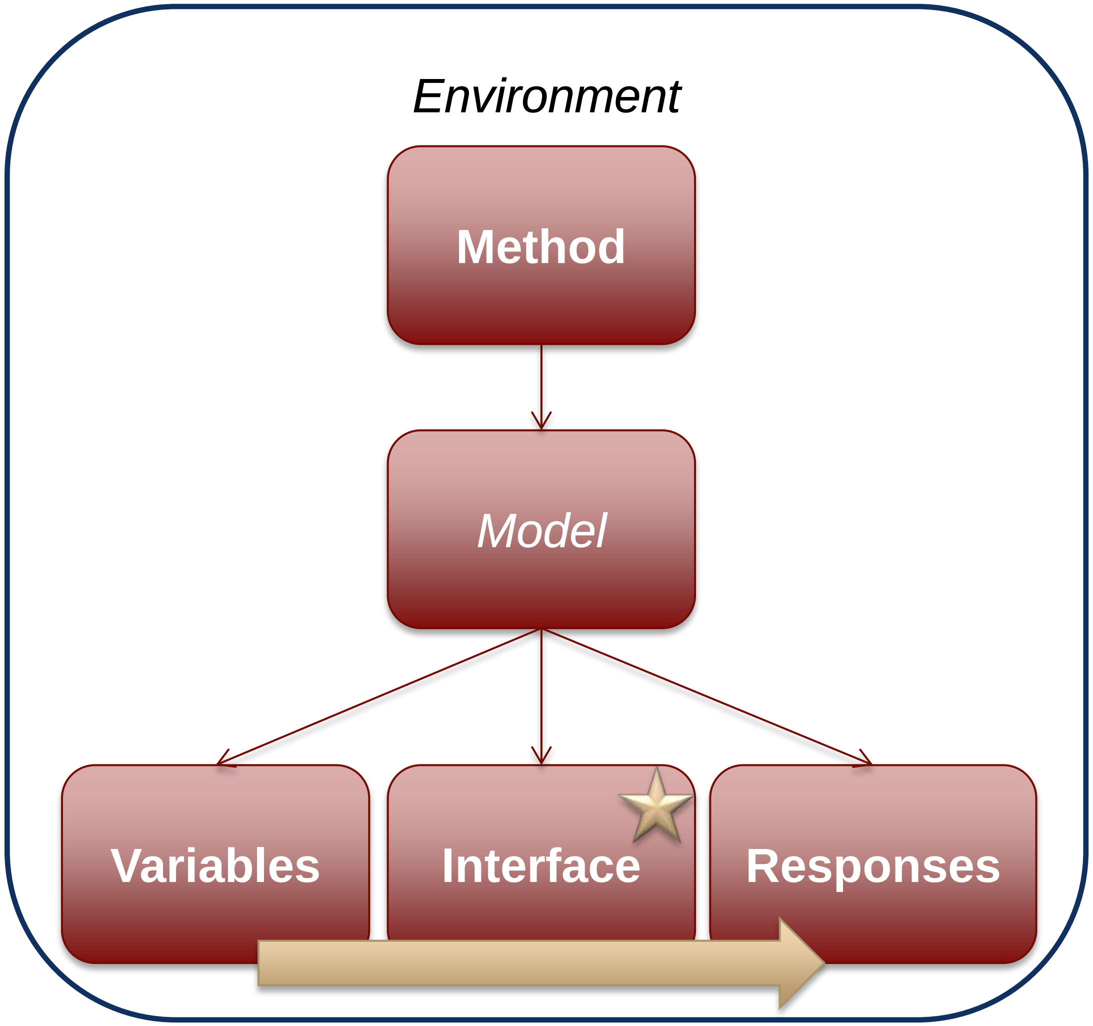
Variables: What Dakota… Varies

- Specify the number, type, other properties of the parameters
- Types are categorized along three dimensions
  - Design, uncertain, or state
  - Continuous or discrete
  - Real, integer, or string
- *Design* variables are used in optimization and calibration
- *Uncertain* variables are used in UQ and sensitivity studies
- *State* variables are typically fixed parameters and not varied by the method
- At least one variables block is **required**



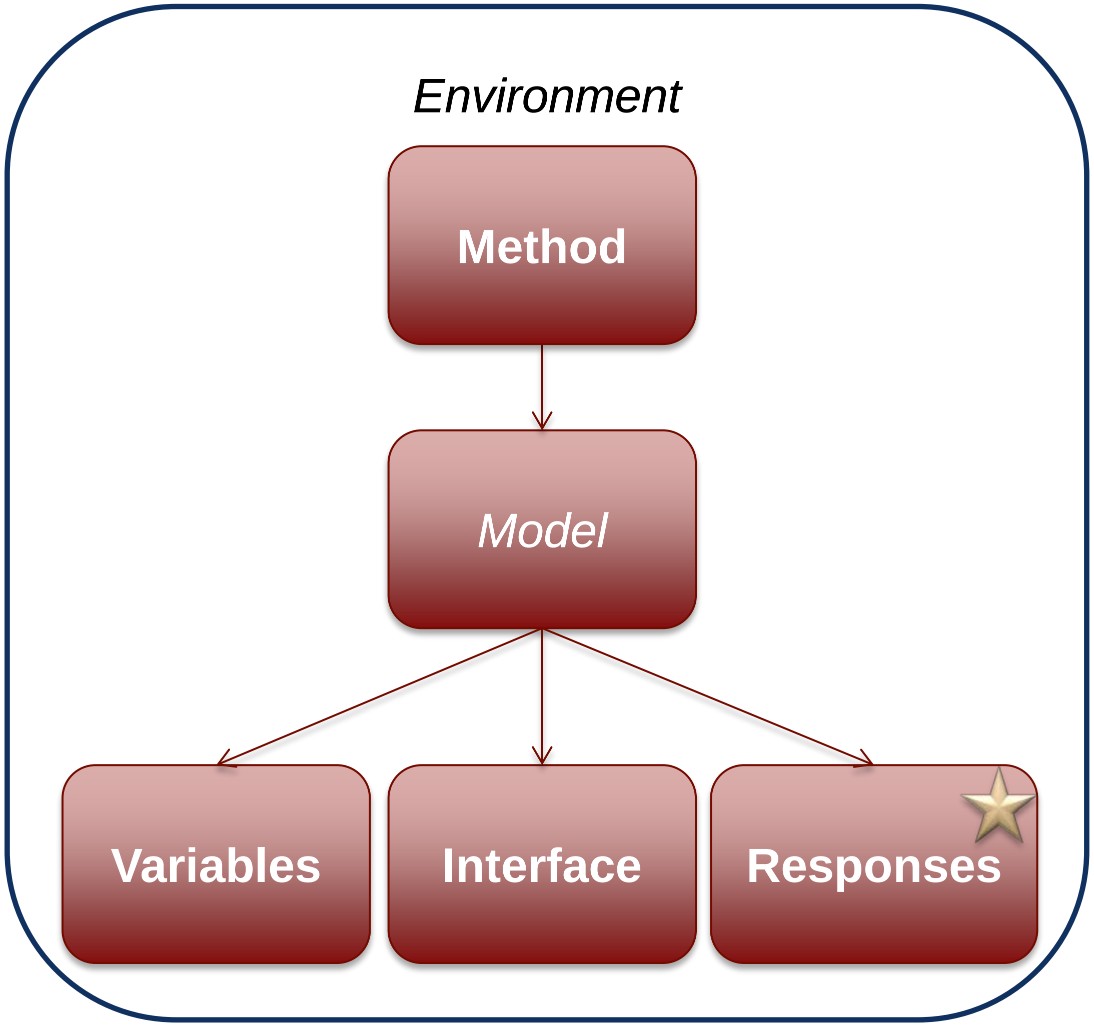
Interface: Communicate with a Simulation

- Specific values of variables are mapped through an interface to obtain responses at those values
- Settings include
  - Path/name to driver
  - Names of files used in I/O
  - Concurrency settings
- At least one interface specification is **required**



Responses: Your Simulation Results

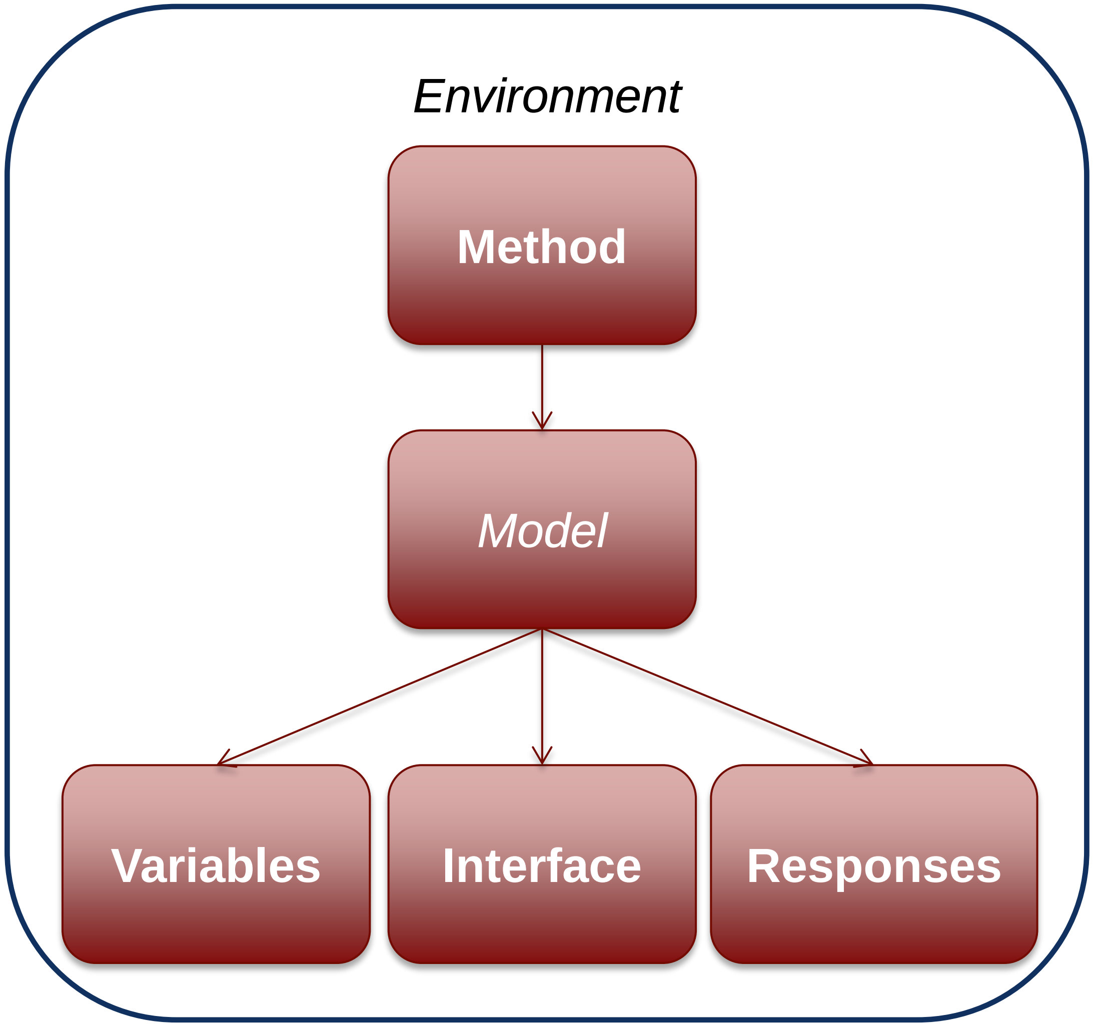
- Data Dakota expects back after setting parameters and running the interface
- Categorized based on usage
  - Objective functions→ optimization
  - Calibration terms → calibration
  - Response functions → SA & UQ
- At least one responses block is **required**



Dakota Blocks In Summary

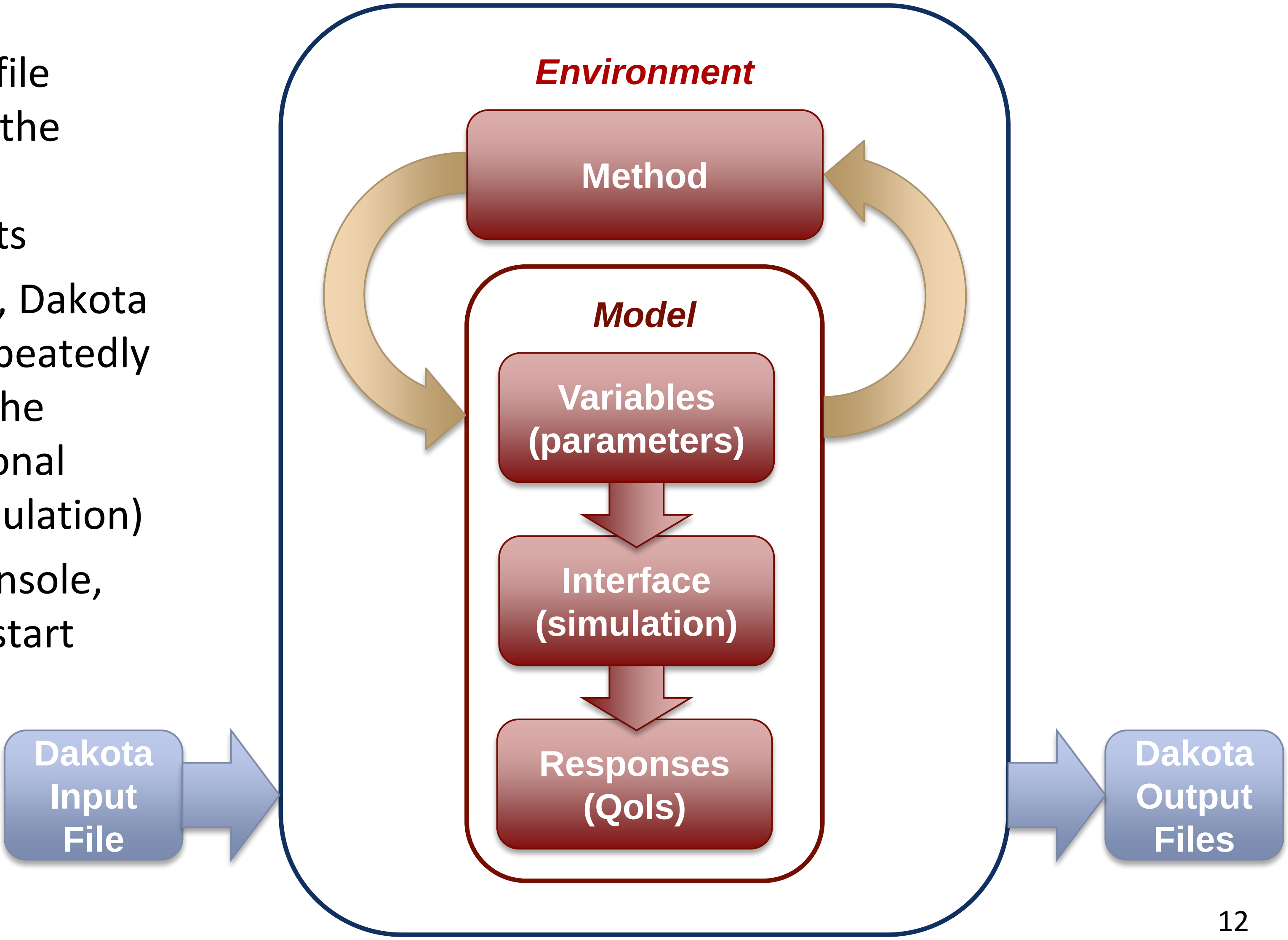
"In each iteration of its algorithm, a **method** block requests a **variables**-to-**responses** mapping from its **model**, which the model fulfills through an **interface***"

*Or surrogate or nested method



Overall Information Flow

- Text input file configures the Dakota components
- At runtime, Dakota method repeatedly evaluates the computational model (simulation)
- Output: console, tabular, restart

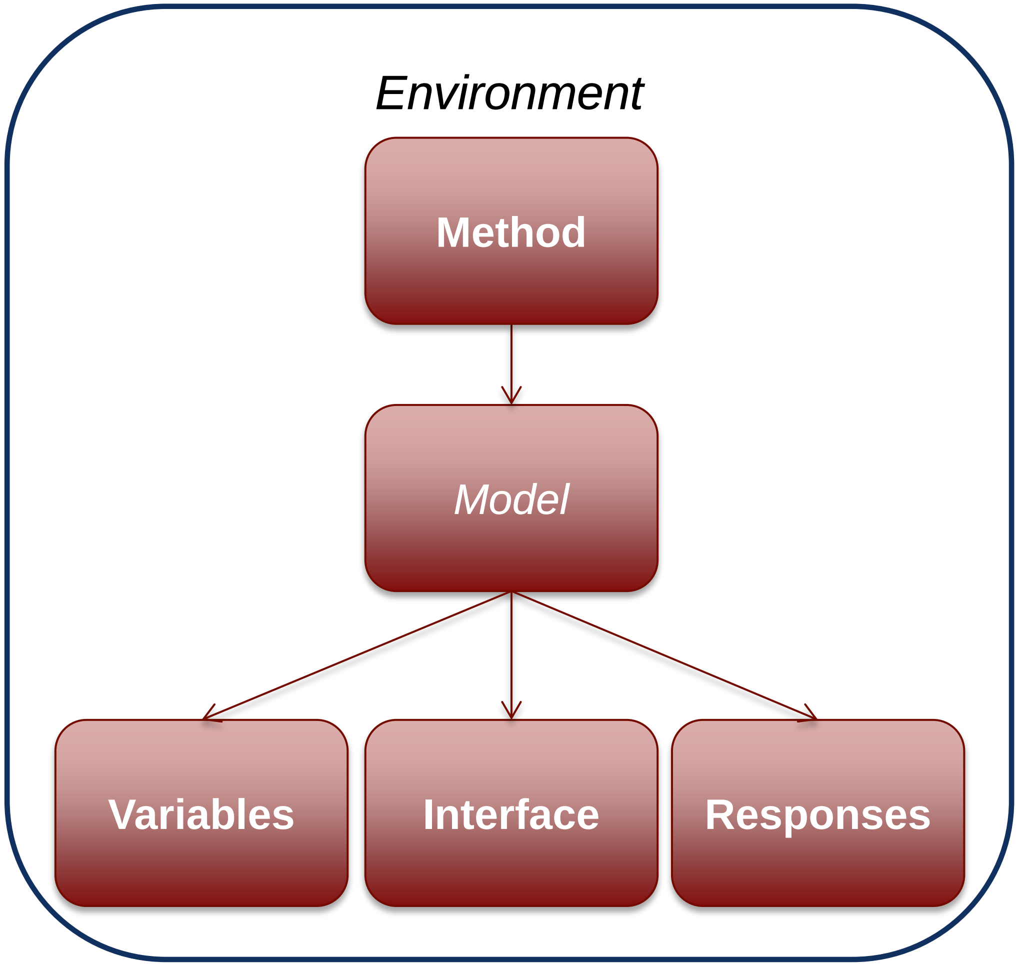


Dakota Input and Components

DAKOTA INPUT FILE

Dakota Input

```
environment
    tabular_data output_precision 1e-16

method
  centered_parameter_study
    step_vector 0.1 0.1 2.0 10. 1e5 5. 10.
    steps_per_variable 2

model
  single

variables
  active all
  continuous_design = 3
    initial_point  1.0     1.0     20.0
    descriptors    'w'     't'      'L'
  continuous_state = 4
    initial_state  500.0 29.E+6  50. 100.
    descriptors    'p'    'E'    'X'  'Y'

interface
  fork analysis_drivers = 'driver.sh'

responses
  response_functions = 3
  descriptors = 'area' 'stress' 'displacement'
  no_gradients no_hessians
```



Input Formatting

See the Input Spec section of the Reference Manual

```
environment
  tabular_data output_precision 1e-16

method
  centered_parameter_study
    step_vector 0.1 0.1 2.0
                10 1.e5 5. 10.
    steps_per_variable 2

variables
  active all
  continuous_design = 3
    initial_point  1.0     1.0    20.0
    descriptors    "w"     "t"     "L"
  continuous_state = 4
    initial_state  500. 29.E+6 50. 100.
    descriptors    'p'    'E'    'X'   'Y'

interface
  fork
    analysis_driver = 'driver.sh'

responses
  response_functions = 3
  descriptors = 'area'
                'stress'
                'displacement'
  no_gradients no_hessians
```

Rules

- "Flat" text only
- Whitespace is ignored
- Comments begin with # and continue to the end of the line
- Keyword order largely unimportant as long as major sections are respected and there is no ambiguity
- Equal signs are optional
- Strings surrounded by single or double quotes (beware of "fancy" quotes)
- Scientific notation is fine
- Shortcuts to be used with care
  - Repeated values in lists: N*Value
  - Ranges: Lower:Step:Upper (Range will include the upper bound)
  - Unambiguous abbreviations (BUT..)

Input Best Practice: Block Pointers and IDs

```
environment
    tabular_data output_precision 1e-16

method
  id_method 'pstudy'
  model_pointer 'pstudy_model'
  centered_parameter_study
    step_vector 0.1 0.1 2.0 10. 1e5 5. 10.
    steps_per_variable 2

model
  id_model 'pstudy_model'
  variables_pointer 'cantilever_vars'
  interface_pointer 'cantilever_inf'
  responses_pointer 'cantilever_resp'
  single

variables
  id_variables 'cantilever_vars'
  active all
  continuous_design = 3
    initial_point  1.0     1.0     20.0
    descriptors    'w'     't'      'L'
  continuous_state = 4
    initial_state  500.0 29.E+6  50.  100.
    descriptors    'p'     'E'    'X'   'Y'

interface
  id_interface 'cantilever_inf'
  fork analysis_drivers = 'driver.sh'

responses
  id_responses 'cantilever_resp'
  response_functions = 3
  descriptors = 'area' 'stress' 'displacement'
  no_gradients no_hessians
```

- Block pointers and IDs enable explicit tracking
  - To which model a method is applied
  - Which variables, interface, responses comprise a model
- Best practice for simple Dakota input
- Critical for complex Dakota input

Dakota Input and Components

DAKOTA REFERENCE MANUAL

Dakota Reference Manual

- All permitted Dakota keywords are documented in the Dakota Reference Manual
- The Keywords section of the manual is organized hierarchically and contains
  - Keyword descriptions
  - Usage examples
  - Defaults
  - .. and more
- Let’s take a tour… https://dakota.sandia.gov/content/manuals

Exercise

Goal: Convert a centered parameter study to a different kind of parameter study

1. Copy the example files located in `~/exercises/input/` to a new working directory.
2. Using your favorite text editor, open the copy of `dakota_cantilever_centered.in` that you made. Change it to a different kind of parameter study
   1. **Hint 1:** *Use the Reference Manual!*
   2. **Hint 2:** *You may also have to change the variables block! Check the example on the Reference Manual page!*
3. Run Dakota using your modified input file:

```
dakota -i dakota_cantilever_centered.in
```

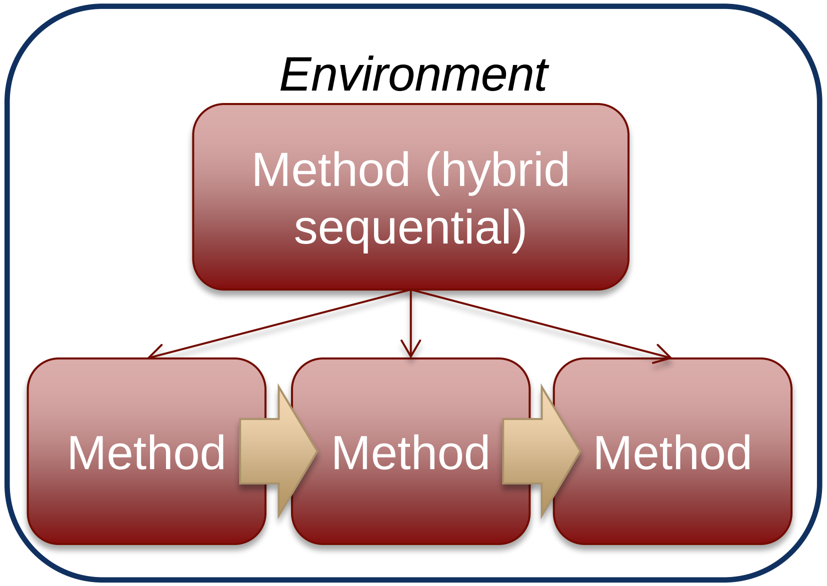
Does it do what you expect based on the method description in the Reference Manual? Discuss any challenges with your neighbor.

Dakota Input and Components

ADVANCED DAKOTA INPUT (TIME PERMITTING)

Multiple Methods: Sequential Hybrid Example

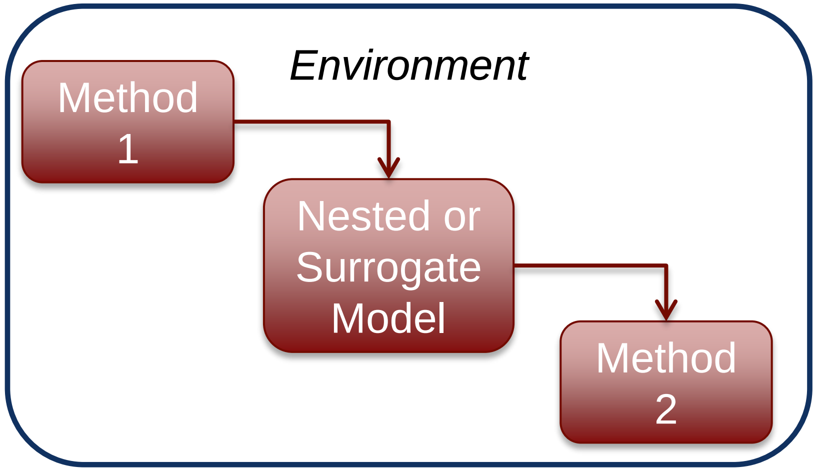
- Multiple methods may be specified, e.g., to apply a sequence of methods to a problem
- Environment block is required in this case to identify top-level method
- Block pointers and IDs are critical to identify execution order



```
environment
  top_method_pointer = 'HS'

method
  id_method = 'HS'
  hybrid sequential
    method_pointer_list = 'GA' 'PS' 'NLP'

method
  id_method = 'GA'
  model_pointer = 'M1'
  coliny_ea

method
  id_method = 'PS'
  model_pointer = 'M1'
  coliny_pattern_search

method
  id_method = 'NLP'
  model_pointer = 'M1'
  optpp_newton

model
  id_model 'M1'
  variables_pointer 'cantilever_vars'
  interface_pointer 'cantilever_inf'
  responses_pointer 'cantilever_resp'
  single
```

Multiple Models: Surrogate Example

- Multiple models (and multiple methods) may be specified for complex analyses, e.g., surrogate-based approaches
- Block pointers and IDs are critical to identify top-level method and which methods are applied to which models
- More on this in surrogate module



```
environment
  method_pointer = 'METHOD_ON_SURR'

method
  id_method = 'METHOD_ON_SURR'
  sampling
  sample_type lhs
  samples = 100
  seed = 3487
  model_pointer = 'SURR_MODEL'

model
  id_model = 'SURR_MODEL'
  surrogate global
  dace_method_pointer = 'DACE'
  polynomial linear

method
  id_method = 'DACE'
  model_pointer = 'DACE_M'
  sampling
  samples = 20
  seed = 3492

model
  id_model = 'DACE_M'
  single
  interface_pointer = 'I1'
  variables_pointer = 'V1'
  responses_pointer = 'R1'
```