# **POEM**

# Release 0.1

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## INTRODUCTION

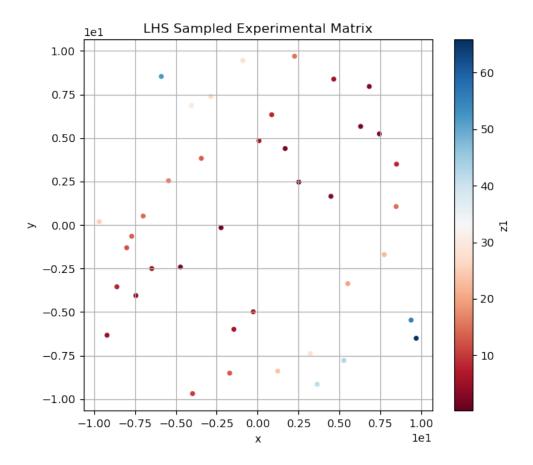
## 1.1 What Is POEM?

POEM is a platform for optimal experiment management, powered with automated machine learning to accelerate the discovery of optimal solutions and to automatically guide the design of experiments to be evaluated. POEM currently supports (1) random model explorations for experiment design, (2) sparse grid model explorations with the Gaussian polynomial chaos surrogate model to accelerate experiment design, (3) time-dependent model sensitivity and uncertainty analyses to identify importance features for experiment design, (4) model calibrations via Bayesian inference to integrate experiments in order to improve model performance, and (5) Bayesian optimization for optimal experimental design. POEM is also intended to simplify the experimental design process for users, enabling them to analyze the data with minimal human intervention, while also improving the technological output from research activities.

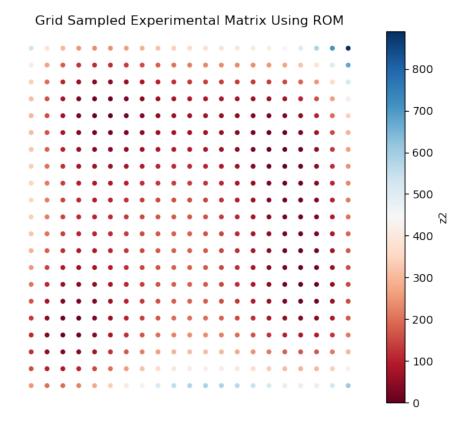
POEM leverages the Risk Analysis Virtual Environment (RAVEN), which is a robust platform that supports model explorations and decision making, to enable large scalability, reduce computational costs, and provide access to complex physical models when performing optimal experimental design.

# 1.2 Capabilities

- · Random model explorations for experiment design
  - See Monte Carlo Sampling
  - See Latin Hypercube Sampling

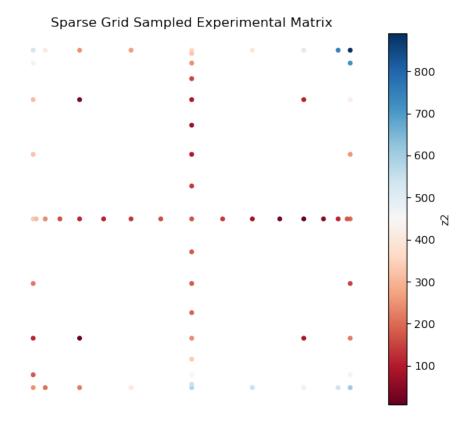


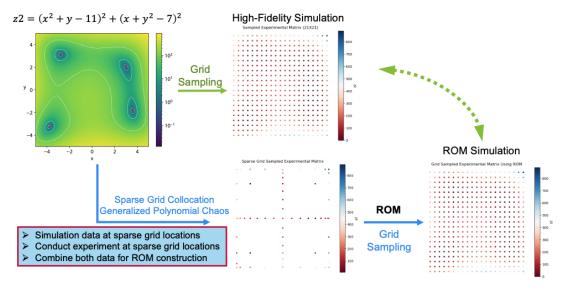
- Machine-learning-aided parameter space exploration
  - See Train ROM



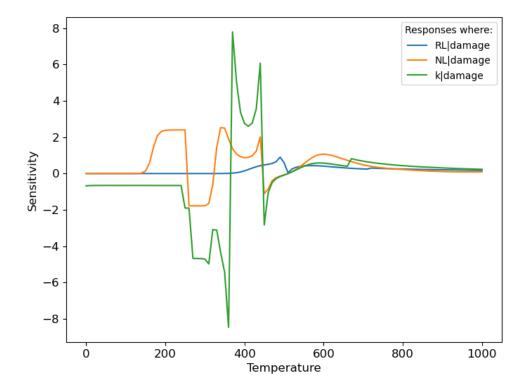
- Sparse grid stochastic collocation with Gaussian polynomial chaos expansion models to accelerate experimental design
  - See Generate Sparse Grid Locations

1.2. Capabilities 3

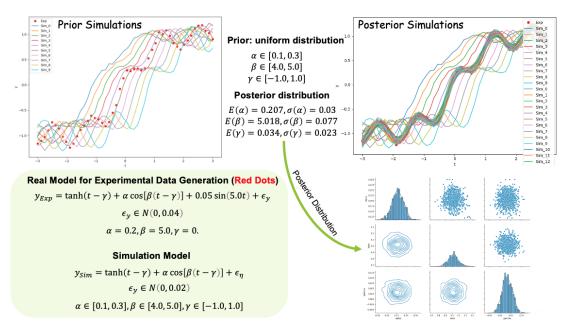




- Dynamic sensitivity and uncertainty analysis
  - See Sensitivity Analysis

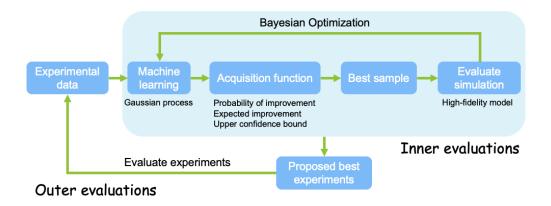


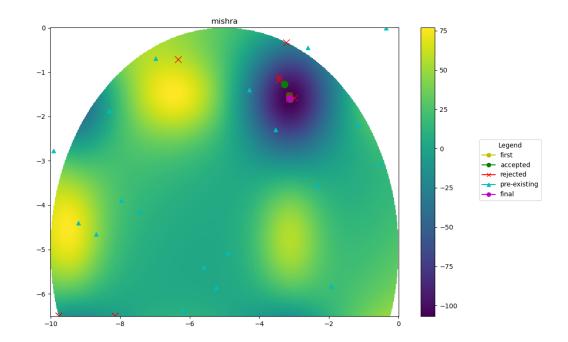
- Model calibration through Bayesian inference
  - See Model Calibration



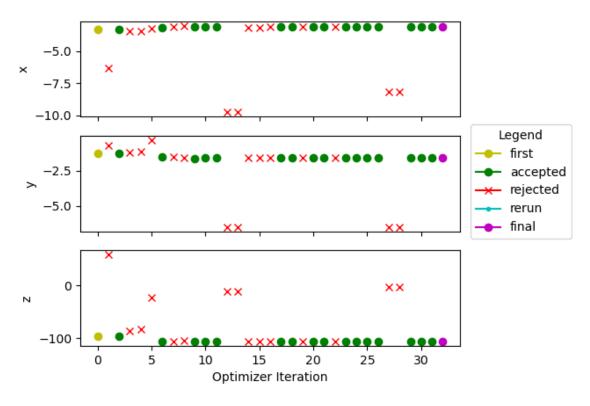
- Bayesian optimization for optimal experimental design
  - See Bayesian Optimization

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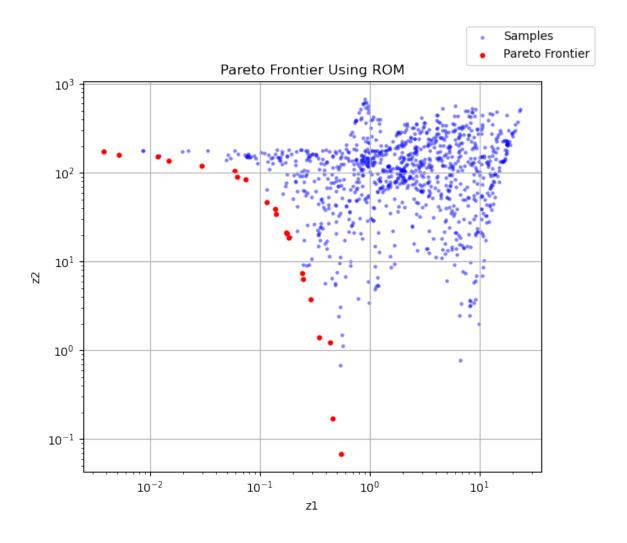


# Optimization Path



• Pareto frontier to guide the design of the experiment to be evaluated

1.2. Capabilities 7



**TWO** 

# **INSTALLATION**

## 2.1 How Is POEM Installed?

## 2.1.1 Installation

conda create -n poem\_libs python=3.10
conda activate poem\_libs
pip install poem-ravenframework

## 2.1.2 Clone

git clone git@github.com:idaholab/POEM.git

## 2.1.3 Test

cd POEM/tests
poem -i lhs\_sampling.xml

**THREE** 

# **QUICK START**

# 3.1 Input Structure

POEM utilizes XML to define its input structure. The main input blocks are covered in the following sections.

## 3.1.1 Simulation block

The root node containing the entire input, all of the following blocks fit inside the Simulation block.

```
<Simulation>
  <RunInfo>
    . . .
  </RunInfo>
 <GlobalSettings>
 </GlobalSettings>
  <Distributions>
  </Distributions>
  <Models>
  </Models>
  <Files>
  </Files>
  <Functions>
 </Functions>
  <LikelihoodModel>
  </LikelihoodModel>
</Simulation>
```

### 3.1.2 GlobalSettings block

This block specifies the global settings for the calculations. For example:

```
<GlobalSettings>
  <!-- Required Nodes -->
  <AnalysisType>LHS</AnalysisType>
  limit>10</limit>
  <Inputs>x, y</Inputs>
  <Outputs>OutputPlaceHolder</Outputs>

  <!-- Optional Nodes -->
  <pivot>time</pivot>
  <dynamic>True</dynamic>

  <!-- Optional Nodes, uses for certain analysis -->
  <SparseGridData>path/to/data.csv</SparseGridData>
  <data>path/to/data.csv</data>
  <InitialInputs>0.1, 4.0, -1.0</InitialInputs>
  <PolynomialOrder>3</PolynomialOrder>
  </GlobalSettings>
```

#### In general, this block accepts the following subnodes:

- · Required Nodes
  - AnalysisType: The type of analysis, it accepts the following keywords:
    - \* mc: Simple Monte Carlo analysis for a given model. See *Monte Carlo Sampling*.
    - \* 1hs: Sample the given model by using a Latin hypercube sampling (LHS) strategy. See *Latin Hypercube Sampling*.
    - \* sensitivity: Perform sensitivity analysis for the given model. The mean, variance, 95/95 percentile, correlation, Spearman correlation, sensitivity coefficients, etc. will be computed. See *Sensitivity Analysis*.
    - \* sparse\_grid\_construction: Generate sparse grid locations to guide experiments. These locations can be used to efficiently construct a high-order Gaussian polynomial chaos surrogate model. See *Generate Sparse Grid Locations*.
    - \* sparse\_grid\_rom: Train a multivariate high-order Gaussian polynomial chaos reduced-order model (ROM)/surrogate based on user-provided experimental data. See *Train ROM*.
    - \* train\_rom: Train a Gaussian process ROM based on user-provided data. See *Train ROM*.
    - \* bayesian\_optimization: Perform Bayesian optimization based on user-provided data and the simulation model. See *Bayesian Optimization*.
    - \* model\_calibration: Perform model calibration by utilizing Bayesian inference, based on user-provided data and the simulation model. See *Model Calibration*.
  - limit: The total number of model executions or the number of samples to generate
  - Inputs: List of input variables
  - Outputs: List of output variables (if no output variables exist, OutputPlaceHolder can be used)
- · Optional Nodes
  - dynamic: True if the user wants to perform a type of time-dependent analysis such as time-dependent ROM construction, sensitivity analysis, or model calibration

- pivot: Required if dynamic is True. The pivot variable for dynamic analysis (the default is time).
- Optional Nodes for Certain Analysis
  - SparseGridData: The experimental data usable for training the Gaussian polynomial chaos ROM (only used by sparse\_grid\_construction and sparse\_grid\_rom)
  - PolynomialOrder: The highest order for the Gaussian polynomial chaos ROM (only used by sparse\_grid\_construction and sparse\_grid\_rom)
  - data: The experimental data usable to train the Gaussian process chaos ROM. Only used by train\_rom and bayesian\_optimization
  - InitialInputs: The initial values for the input variables listed by <Inputs> in <GlobalSettings>.

#### 3.1.3 RunInfo block

This block specifies the calculation settings (e.g., working directory and number of parallel simulations).

```
<RunInfo>
    <WorkingDir>LHS</WorkingDir>
    <batchSize>1</batchSize>
</RunInfo>
```

#### In general, this block accepts the following subnodes:

- WorkingDir: Specifies the absolute or relative path to a directory that will store all the calculation results
- batchSize: Specifies the number of parallel executed simultaneously
- JobName: Specifies the name to use for the job when submitting to a PBS queue.

#### RunInfo for Cluster Usage

3.1. Input Structure 13

#### 3.1.4 Files block

This block specifies the files to be used as input for the <Models> block. Users can specify as many input files as they need, and utilize the <Input> node to specify the name and path/to/file.

```
<Files>
     <Input name="sauq" type="">../../models/sauq.m</Input>
     <Input name="rt" type="">../../models/RateTheory.m</Input>
     <Input name="kc" type="">../../models/KlemensCallawayModel.m</Input>
</Files>
```

#### 3.1.5 Distributions block

POEM leverages the RAVEN (https://github.com/idaholab/raven) input structure to build customized workflows for model explorations and optimal experimental design. In this case, POEM provides support for all the probability distributions available in RAVEN. The following is an example for the <Distributions> block:

In this block, users must define the distribution for each variable listed in the GlobalSettings Inputs node, and the name for the distribution should match the variable name listed under <GlobalSettings><Inputs>VariableList</Inputs></GlobalSettings>.

#### 3.1.6 Models block

As with the <Distributions> block, POEM leverages the RAVEN (https://github.com/idaholab/raven) <Models> input structure. In this case, POEM provides support for all the models available in RAVEN. The following is an example for the <Models> block.

As its name suggests, an external model is an entity that is embedded at run time. This object allows the user to create a Python module that will be treated as a predefined internal model object.

The specifications of an external model must be defined within the XML block <ExternalModel>. This blocks accepts the following subnodes:

• inputs: Each variable name must match a variable used/defined in the external Python model.

outputs: Each variable name must match a variable used/defined in the external Python model.

Each variable defined in the <ExternalModel>, <inputs>, and <outputs> blocks is available in the module (each method implemented) as a Python self. member.

#### 3.1.7 Functions block

POEM leverages the RAVEN (https://github.com/idaholab/raven) <Functions> input structure. In this case, POEM provides support for using user-defined external functions. These functions are Python modules, with a format automatically interpretable by RAVEN software.

The following is an example for the <Functions> block:

```
<Functions>
  <External file="../../models/mishraBirdConstrained.py" name="constraint1">
        <variables>x,y</variables>
        </External>
  </Functions>
```

In this section, the XML input syntax and the format of the accepted functions are fully specified. The specifications of an external function must be defined within the XML <external> block. This XML node requires the following attributes:

- name: User-defined name of this function
- file: Absolute or relative path specifying the code associated with this function.

To make the code aware of the variables the user will manipulate/use in their own Python function, the variables must be specified in the <variables> subnode input block. Within this block, the user must input only the variables directly used by the external function.

When the external function variables are defined, the code will initialize them at runtime and keep track of their values throughout the simulation. Each variable defined in the <variables> block is available in the function as a Python self. member. Below, an example of a user-defined external function is reported; the method evaluate needs to be defined in the function file:

```
def evaluate(self):
   return self.a * self.c
```

#### 3.1.8 LikelihoodModel block for model calibration

This node is only used for model calibration analysis. The following is an example:

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The <LikelihoodModel> node accepts the following subnodes:

- simTargets: Targets of simulations used in the calibration.
- expTargets: Targets of experiments used in the calibration. Either variables or list of values. This node accepts the following attributes:
  - shape: Determines the number of targets and number of experimental observations for each target. For example, shape="3,2" indicates two targets, with three observations for each; whereas shape="10" indicates one target with 10 observations. Omitting this optional attribute will instead result in a single target with multiple observations.
  - computeCov: Indicates whether the experiment covariance matrix is provided or is instead computed based
    on the given experiment observations. If True, we will compute the covariance based on the given observations; otherwise, the user must provide the covariance matrix.
  - correlation: Indicates whether the targets are correlated. If True, and compute is True, we will compute the covariance matrix. If False, but compute is True, we will only compute the variance of each target.
- expCov: Experiment covariance (i.e., measurement noise). This node accepts the following attribute:
  - diag: If True, only the variance for each target must be provided; otherwise, the user needs to provide the full covariance matrix.
- biasTargets: Models uncertainty/discrepancy/bias/error in Targets that are used in calibration.
- biasCov: Models covariance, model bias/discrepancy, or model inadequacy caused by missing physics or numerical approximation. This node accepts the following attribute:
  - diag: If True, only the variance for each target must be provided; otherwise, the user needs to provide the full covariance matrix.
- romCov: Models uncertainty caused by the surrogate model, such as interpolation. This node accepts the following attribute:
  - diag: If True, only the variance for each target must be provided; otherwise, the user needs to provide the full covariance matrix.
- reduction: Allows reduction on likelihood model construction. This node accepts the following attributes:
  - type: This is the reduction method, and its default is **PCA**.
  - basis: User-provided basis vector for reduction.
  - shape: Determines the basis vectors for reduction. For example, shape="10,2" indicates two basis vectors with dimension 10.

**FOUR** 

## MONTE CARLO SAMPLING

Monte Carlo sampling was utilized to perform random model explorations for experiment design. For this analysis, set <AnalysisType>MC</AnalysisType>. For example, the following input utilizes Monte Carlo sampling to generate 10 random samples of input variables x, y with associated Uniform distributions.

```
<?xml version="1.0" ?>
<Simulation>
 <RunInfo>
   <WorkingDir>MC</WorkingDir>
    <batchSize>1</batchSize>
 </RunInfo>
 <GlobalSettings>
   <AnalysisType>MC</AnalysisType>
   t>10</limit>
   <Inputs>x, y</Inputs>
    <Outputs>OutputPlaceHolder
 </GlobalSettings>
 <Distributions>
   <Uniform name='x'>
     <le><lowerBound>-10</le>
      <upperBound>0</upperBound>
   </Uniform>
   <Uniform name='v'>
     <lowerBound>-6.5</lowerBound>
      <upperBound>0</upperBound>
   </Uniform>
 </Distributions>
</Simulation>
```

When a dynamic model is provided, the users need to set the pivot> and <dynamic> nodes in <GlobalSettings>, as illustrated in the following example:

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```
<GlobalSettings>
    <AnalysisType>MC</AnalysisType>
   <limit>10</limit>
   <Inputs>x0, y0, z0</Inputs>
    <pivot>time</pivot>
    <dynamic>True</dynamic>
    <0utputs>x,y,z
  </GlobalSettings>
  <Distributions>
   <Normal name="x0">
     <mean>4</mean>
      <sigma>1</sigma>
    </Normal>
   <Normal name="y0">
      <mean>4</mean>
      <sigma>1</sigma>
    </Normal>
   <Normal name="z0">
      <mean>4</mean>
      <sigma>1</sigma>
    </Normal>
  </Distributions>
  <Models>
    <ExternalModel ModuleToLoad="../models/lorentzAttractor.py" name="lorentzAttractor"_</pre>
→subType="">
     <inputs>inputGroup</inputs>
      <outputs>outputGroup
    </ExternalModel>
  </Models>
</Simulation>
```

Users can can also employ inputGroup and outputGroup to represent the input and output variable lists, respectively, as illustrated in the example <ExternalModel> node above.

## LATIN HYPERCUBE SAMPLING

LHS was utilized to perform random model explorations for experiment design. For this analysis, set <AnalysisType>LHS</AnalysisType>. For example, the following input utilizes LHS to generate 10 random LHS samples of input variables x,y with associated Uniform distributions:

```
<?xml version="1.0" ?>
<Simulation>
  <RunInfo>
    <WorkingDir>LHS_mishra</WorkingDir>
    <batchSize>1</batchSize>
  </RunInfo>
  <GlobalSettings>
    <AnalysisType>LHS</AnalysisType>
    t>10</limit>
    <Inputs>x, y</Inputs>
    <Outputs>z</Outputs>
  </GlobalSettings>
  <Distributions>
    <Uniform name='x'>
      <le><lowerBound>-10</le>
      <upperBound>0</upperBound>
    </Uniform>
    <Uniform name='y'>
      <lowerBound>-6.5</lowerBound>
      <upperBound>0</upperBound>
    </Uniform>
  </Distributions>
  <Models>
   <ExternalModel ModuleToLoad="../../models/mishraBirdConstrained" name="mishra"__</pre>
⇒subType="">
      <inputs>x, y</inputs>
      <outputs>z</outputs>
    </ExternalModel>
  </Models>
</Simulation>
```

When a dynamic model is provided, the users need to set the pivot> and <dynamic> node in <GlobalSettings>, as illustrated in the following example:

```
<?xml version="1.0" ?>
<Simulation>
  <RunInfo>
    <WorkingDir>LHS</WorkingDir>
    <batchSize>1</batchSize>
  </RunInfo>
  <GlobalSettings>
   <AnalysisType>LHS</AnalysisType>
    limit>10</limit>
   <Inputs>x0, y0, z0</Inputs>
    <pivot>time</pivot>
    <dynamic>True</dynamic>
    <0utputs>x,y,z</0utputs>
  </GlobalSettings>
  <Distributions>
    <Normal name="x0">
      <mean>4</mean>
      <sigma>1</sigma>
   </Normal>
    <Normal name="v0">
      <mean>4</mean>
      <sigma>1</sigma>
    </Normal>
    <Normal name="z0">
      <mean>4</mean>
      <sigma>1</sigma>
    </Normal>
  </Distributions>
  <Models>
    <ExternalModel ModuleToLoad="../models/lorentzAttractor.py" name="lorentzAttractor"_</pre>
→subType="">
      <inputs>inputGroup</inputs>
      <outputs>outputGroup
    </ExternalModel>
  </Models>
</Simulation>
```

Users can also employ inputGroup and outputGroup to represent the input and output variable lists, respectively, as illustrated in the example <ExternalModel> node above.

SIX

## TRAIN ROM

ROMs or machine learning models can be trained based on experiment data or a mix of experiment data and simulation data.

## 6.1 Train Gaussian Process Model

For this analysis, set <AnalysisType>train\_rom</AnalysisType>. For example, the following input utilizes data provided by the <data> node to train the Gaussian process model. After training, the Gaussian process model inputs will be sampled via an LHS algorithm, along with their associated distributions, and the number of samples will be equal to the value of limit>.

```
<?xml version="1.0" ?>
<Simulation>
  <RunInfo>
    <WorkingDir>GP</WorkingDir>
    <batchSize>1</batchSize>
  </RunInfo>
  <GlobalSettings>
   <AnalysisType>train_rom</AnalysisType>
   <data>../LHS/sampling_dump.csv</data>
    t>10</limit>
    <Inputs>x, y</Inputs>
    <0utputs>z1</0utputs>
  </GlobalSettings>
  <Distributions>
    <Uniform name='x'>
      <le><lowerBound>-10</lowerBound>
      <upperBound>0</upperBound>
    </Uniform>
    <Uniform name='y'>
      <lowerBound>-6.5</lowerBound>
      <upperBound>0</upperBound>
    </Uniform>
  </Distributions>
</Simulation>
```

# 6.2 Train the Dynamic Gaussian Process Model

When a dynamic model is provided, the users need to set the pivot> and <dynamic> nodes in <GlobalSettings>,
as illustrated in the example below. In addition, set <AnalysisType>train\_rom</AnalysisType>. For example,
the following input will utilize data provided by the <data> node to train the Gaussian process model. After training,
the Gaussian process model inputs will be sampled via an LHS algorithm, along with their associated distributions,
and the number of samples will be equal to the value of

```
<?xml version="1.0" ?>
<Simulation>
 <RunInfo>
    <WorkingDir>GP_dynamic</WorkingDir>
    <batchSize>1</batchSize>
 </RunInfo>
 <GlobalSettings>
   <AnalysisType>train_rom</AnalysisType>
   <data>../LHS/sampling_dynamic_dump.csv</data>
   <limit>10</limit>
   <Inputs>x0, y0, z0</Inputs>
   <pivot>time</pivot>
   <dynamic>True</dynamic>
    <0utputs>x,y,z</0utputs>
 </GlobalSettings>
 <Distributions>
   <Normal name="x0">
      <mean>4</mean>
      <sigma>1</sigma>
   </Normal>
   <Normal name="y0">
      <mean>4</mean>
      <sigma>1</sigma>
    </Normal>
    <Normal name="z0">
      <mean>4</mean>
      <sigma>1</sigma>
   </Normal>
 </Distributions>
 <Models>
   <ExternalModel ModuleToLoad="../models/lorentzAttractor.py" name="lorentzAttractor"
</pre>
→subType="">
      <inputs>inputGroup</inputs>
      <outputs>outputGroup
   </ExternalModel>
 </Models>
</Simulation>
```

# 6.3 Train Gaussian Polynomial Chaos Model with Sparse Grid

For this analysis, set <AnalysisType>sparse\_grid\_rom</AnalysisType>. As an example, the following input utilizes data provided by the <SparseGridData> node to train a Gaussian polynomial chaos model. After training, the Gaussian process model inputs will be sampled via a Monte Carlo sampling algorithm, along with their associated distributions, and the number of samples will be equal to the value of 1imit>.

```
<?xml version="1.0" ?>
<Simulation>
  <GlobalSettings>
    <AnalysisType>sparse_grid_rom</AnalysisType>
    <Inputs>x, y</Inputs>
    <0utputs>z1</0utputs>
    <PolynomialOrder>2</PolynomialOrder>
    limit>10</limit>
    <SparseGridData>dump_SparseGrid.csv</SparseGridData>
  </GlobalSettings>
  <Distributions>
    <Uniform name="x">
      <le><lowerBound>-10</le>
      <upperBound>10</upperBound>
    </Uniform>
    <Uniform name="y">
      <le><lowerBound>-10</le>
      <upperBound>10</upperBound>
    </Uniform>
  </Distributions>
  <Models>
    < External Model Module To Load = ".../models/matyas" name = "external Model" sub Type = "">
      <inputs>x, y</inputs>
      <outputs>z1</outputs>
    </ExternalModel>
  </Models>
</Simulation>
```

For this ROM, users can also set the highest order of the Gaussian polynomial chaos expansions by simply setting <PolynomialOrder> in <GlobalSettings>.

# 6.4 Train Dynamic Gaussian Polynomial Chaos Model with Sparse Grid

When a dynamic model is provided, the users need to set the pivot> and <dynamic> nodes in <GlobalSettings>,
as illustrated in the example below. For this analysis, set <AnalysisType>sparse\_grid\_rom</AnalysisType>. As
an example, the following input utilizes data provided by the <SparseGridData> node to train a Gaussian polynomial
chaos model. After training, the Gaussian process model inputs will be sampled via a Monte Carlo sampling algorithm,
along with their associated distributions, and the number of samples will be equal to the value of limit>.

```
<?xml version="1.0" ?>
<Simulation>
  <RunInfo>
    <WorkingDir>SparseGridDynamic</WorkingDir>
    <batchSize>1</batchSize>
  </RunInfo>
  <GlobalSettings>
    <AnalysisType>sparse_grid_rom</AnalysisType>
    <Inputs>x0, y0, z0</Inputs>
    <pivot>time</pivot>
    <dynamic>True</dynamic>
   <0utputs>x,y,z</0utputs>
   <PolynomialOrder>2</PolynomialOrder>
   <limit>10</limit>
    <SparseGridData>../SparseGrid/SparseGrid_dynamic_dump.csv</SparseGridData>
  </GlobalSettings>
  <Distributions>
    <Normal name="x0">
      <mean>4</mean>
      <sigma>1</sigma>
    </Normal>
    <Normal name="v0">
      <mean>4</mean>
      <sigma>1</sigma>
    </Normal>
    <Normal name="z0">
      <mean>4</mean>
      <sigma>1</sigma>
    </Normal>
  </Distributions>
  <Models>
    <ExternalModel ModuleToLoad="../models/lorentzAttractor.py" name="lorentzAttractor"_</pre>
→subType="">
      <inputs>inputGroup</inputs>
      <outputs>outputGroup
    </ExternalModel>
  </Models>
</Simulation>
```

For this ROM, the users can also set the highest order of the Gaussian polynomial chaos expansions by simply setting <PolynomialOrder> in <GlobalSettings>.

## GENERATE SPARSE GRID LOCATIONS

Sparse grid model explorations can be performed with a Gaussian polynomial chaos surrogate model so as to accelerate the experiment design.

When generating sparse grid locations, users can also set the highest order of the Gaussian polynomial chaos expansions by simply setting <PolynomialOrder> in <GlobalSettings>. The higher the polynomial order, the more sparse grid locations will be generated.

Once the experiment data are generated at the given sparse grid locations, the Gaussian polynomial chaos surrogate model can automatically be constructed. See the Train ROM section of this document for how to train the Gaussian polynomial chaos surrogate model.

## 7.1 Static Model

```
<Simulation>
  <RunInfo>
    <WorkingDir>SparseGrid</WorkingDir>
    <Sequence>SparseGridSampler, print
    <batchSize>1</batchSize>
  </RunInfo>
  <GlobalSettings>
    <AnalysisType>sparse_grid_construction</AnalysisType>
    <Inputs>x, y</Inputs>
    <0utputs>z1</0utputs>
    <PolynomialOrder>3</PolynomialOrder>
  </GlobalSettings>
  <Distributions>
    <Uniform name="x">
      <le><lowerBound>-10</lowerBound>
      <upperBound>10</upperBound>
    </Uniform>
    <Uniform name="y">
      <le><lowerBound>-10</lowerBound>
      <upperBound>10</upperBound>
    </Uniform>
  </Distributions>
  <Models>
```

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# 7.2 Dynamic Model

When a dynamic model is provided, the users need to set the pivot> and <dynamic> nodes in <GlobalSettings>, as illustrated in the following example:

```
<?xml version="1.0" ?>
<Simulation>
  <RunInfo>
    <WorkingDir>SparseGrid</WorkingDir>
    <Sequence>SparseGridSampler, print</Sequence>
    <batchSize>1</batchSize>
  </RunInfo>
  <GlobalSettings>
    <AnalysisType>sparse_grid_construction</AnalysisType>
    <Inputs>x0, y0, z0</Inputs>
    <pivot>time</pivot>
    <dynamic>True</dynamic>
    <0utputs>x,y,z</0utputs>
    <PolynomialOrder>3</PolynomialOrder>
  </GlobalSettings>
  <Distributions>
    <Normal name="x0">
      <mean>4</mean>
      <sigma>1</sigma>
    </Normal>
    <Normal name="v0">
      <mean>4</mean>
      <sigma>1</sigma>
    </Normal>
    <Normal name="z0">
      <mean>4</mean>
      <sigma>1</sigma>
    </Normal>
  </Distributions>
  <Models>
    < External Model Module To Load = "../models/lorentz Attractor.py" name = "lorentz Attractor"
→subTvpe="">
      <inputs>inputGroup</inputs>
      <outputs>outputGroup
                                                                             (continues on next page)
```

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```
</ExternalModel>
</Models>
</Simulation>
```

7.2. Dynamic Model 27

## SENSITIVITY ANALYSIS

# 8.1 Static Sensitivity Analysis

For this analysis, set <AnalysisType>sensitivity</AnalysisType>. A Monte Carlo method will be utilized to sample the given model with limit number.

```
<?xml version="1.0" ?>
<Simulation>
  <RunInfo>
    <JobName>sauq</JobName>
    <WorkingDir>sauq_runs</workingDir>
    <batchSize>1</batchSize>
  </RunInfo>
  <GlobalSettings>
    <AnalysisType>sensitivity</AnalysisType>
    <limit>10</limit>
    <Inputs>x, y</Inputs>
    <0utputs>z1</0utputs>
  </GlobalSettings>
  <Distributions>
    <Uniform name='x'>
      <le><lowerBound>-10</le>
      <upperBound>0</upperBound>
    </Uniform>
    <Uniform name='y'>
      <le><lowerBound>-6.5</le>
      <upperBound>0</upperBound>
    </Uniform>
  </Distributions>
  <Models>
   <ExternalModel ModuleToLoad="../models/matyas" name="externalModel" subType="">
      <inputs>x, y</inputs>
      <outputs>z1</outputs>
    </ExternalModel>
 </Models>
</Simulation>
```

# 8.2 Dynamic Sensitivity Analysis

Time-dependent model sensitivity and uncertainty analyses will be employed to identify the importance features for experiment design. For this analysis, set <AnalysisType>sensitivity</AnalysisType>. A Monte Carlo method will be utilized to sample the given model with limit number. When a dynamic model is provided, the users need to set the epivot> and <dynamic> nodes in the <GlobalSettings>, as illustrated in the following example:

```
<?xml version="1.0" ?>
<Simulation>
  <RunInfo>
    <JobName>sauq</JobName>
    <WorkingDir>sauq_dynamic_external</WorkingDir>
    <batchSize>1</batchSize>
  </RunInfo>
  <GlobalSettings>
    <AnalysisType>sensitivity</AnalysisType>
    t>10</limit>
    <Inputs>x0, y0, z0</Inputs>
    <pivot>time</pivot>
    <dynamic>True</dynamic>
    <0utputs>x,y,z</0utputs>
  </GlobalSettings>
  <Distributions>
    <Normal name="x0">
      <mean>4</mean>
      <sigma>1</sigma>
    </Normal>
    <Normal name="y0">
      <mean>4</mean>
      <sigma>1</sigma>
    </Normal>
    <Normal name="z0">
      <mean>4</mean>
      <sigma>1</sigma>
    </Normal>
  </Distributions>
  <Models>
    <ExternalModel ModuleToLoad="../models/lorentzAttractor.py" name="lorentzAttractor"_</pre>
→subType="">
      <inputs>inputGroup</inputs>
      <outputs>outputGroup
    </ExternalModel>
  </Models>
</Simulation>
```

NINE

## **BAYESIAN OPTIMIZATION**

This chapter covers Bayesian optimization for optimal experimental design.

## 9.1 Example

For this analysis, set <AnalysisType>bayesian\_optimization</AnalysisType>. The existing experiment data can be provided through <data> in <GlobalSettings>. For example:

```
<?xml version="1.0" ?>
<Simulation verbosity="debug">
  <RunInfo>
    <WorkingDir>Optimization</WorkingDir>
    <batchSize>1</batchSize>
  </RunInfo>
  <GlobalSettings>
    <AnalysisType>bayesian_optimization</AnalysisType>
    <data>../LHS_mishra/sampling_dump.csv</data>
    limit>10</limit>
    <Inputs>x, y</Inputs>
    <0utputs>z</0utputs>
  </GlobalSettings>
  <Distributions>
    <Uniform name='x'>
      <le><lowerBound>-10</lowerBound>
      <upperBound>0</upperBound>
    </Uniform>
    <Uniform name='y'>
      <lowerBound>-6.5</lowerBound>
      <upperBound>0</upperBound>
    </Uniform>
  </Distributions>
  <Models>
    <ExternalModel ModuleToLoad="../../models/mishraBirdConstrained.py" name="mishra"_</pre>
→subType="">
      <inputs>x, y</inputs>
      <outputs>z</outputs>
    </ExternalModel>
```

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# 9.2 Python External Model and Constrain

```
import numpy as np
def evaluate(x,y):
             Evaluates Mishra bird function.
             @ In, x, float, value
             @ In, y, float, value
             @ Out, evaluate, value at x, y
       evaluate = np.sin(y)*np.exp(1.-np.cos(x))**2 + np.cos(x)*np.exp(1.-np.sin(y))**2 + (x-p.sin(y))**2 +
 \hookrightarrowy)**2
      return evaluate
def constraint(x,y):
             Evaluates the constraint function @ a given point (x,y)
             @ In, x, float, value of the design variable x
             @ In, y, float, value of the design variable y
              @ Out, g(x,y), float, g(x, y) = 25 - ((x+5.)**2 + (y+5.)**2)$
                                          the constraint is designed such that
                                          the constraint function must be \geq = 0,
                                         so if:
                                          1) f(x,y) >= 0 then g = f
                                          2) f(x,y) >= a then g = f - a
                                         3) f(x,y) \le b then g = b - f
                                          4) f(x,y) = c then g = 0.001 - (f(x,y) - c)
       condition = 25.
       g = condition - ((x+5.)**2 + (y+5.)**2)
      return g
###
# RAVEN hooks
def run(self,Inputs):
```

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# MODEL CALIBRATION

Model calibrations are performed via Bayesian inference to integrate experiments so as to improve model performance. For this analysis, set <AnalysisType>model\_calibration</AnalysisType>. When a dynamic model is provided, the users need to set the pivot> and <dynamic> nodes in <GlobalSettings>, as illustrated in the below example. In addition, the initial values for the input variables can be provided via <InitialInputs>.

```
<?xml version="1.0" ?>
<Simulation verbosity="debug">
 <RunInfo>
    <WorkingDir>calibration_dynamic</WorkingDir>
    <batchSize>1</batchSize>
 </RunInfo>
 <GlobalSettings>
    <AnalysisType>model_calibration</AnalysisType>
    <pivot>time</pivot>
    <dynamic>True</dynamic>
    <limit>100</limit>
    <Inputs>alpha, beta, gamma</Inputs>
    <InitialInputs>0.1, 4.0, -1.0</InitialInputs>
    <Outputs>eta</Outputs>
 </GlobalSettings>
 <LikelihoodModel>
    <simTargets>eta</simTargets>
    <expTargets shape="1,50" computeCov='False' correlation='False'>
      -1.16074224 -1.10303445 -1.02830511 -0.89782965 -0.73765453 -0.7989537
      -0.86163706 \ -1.02209944 \ -1.12444044 \ -1.23657398 \ -1.16081758 \ -1.01219869
                  -0.80444122 -0.70893668 -0.61012531 -0.65670863 -0.6768583
      -0.74732441 \ -0.81448647 \ -0.73232671 \ -0.54989334 \ -0.39796749 \ -0.07894291
        0.13067378  0.28999998  0.27418965  0.313329
                                                          0.32306704 0.2885684
        0.32736775 \quad 0.52458854 \quad 0.69446572 \quad 0.82419521 \quad 1.04393683 \quad 1.00435818
        1.0810376
                    0.97245373  0.82406522  0.76067559  0.70145544  0.79479965
        0.88035895  0.97750307  1.11524353  1.17159017  1.18299222  1.07255006
        1.02835909 0.90784132
    </expTargets>
    <expCov diag="True">
        0.02, 0.02, 0.02, 0.02, 0.02, 0.02, 0.02, 0.02, 0.02, 0.02, 0.02, 0.02,
        0.02, 0.02, 0.02, 0.02, 0.02, 0.02, 0.02, 0.02, 0.02, 0.02, 0.02,
        0.02, 0.02, 0.02, 0.02, 0.02, 0.02, 0.02, 0.02, 0.02, 0.02, 0.02, 0.02,
```

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```
0.02, 0.02, 0.02, 0.02, 0.02, 0.02, 0.02, 0.02, 0.02, 0.02, 0.02,
       0.02, 0.02, 0.02, 0.02, 0.02, 0.02
   </expCov>
   <!-- <biasTargets></biasTargets>
   <biasCov diag="False"></biasCov> -->
    <!-- <romCov diag="True"></romCov> -->
  </LikelihoodModel>
  <Distributions>
   <Uniform name='alpha'>
      <lowerBound>0.1</lowerBound>
      <upperBound>0.3</upperBound>
   </Uniform>
    <Uniform name='beta'>
      <le><lowerBound>4</lowerBound>
      <upperBound>6</upperBound>
   </Uniform>
   <Uniform name='gamma'>
      <le><lowerBound>-1</le>
      <upperBound>1</upperBound>
    </Uniform>
  </Distributions>
  <Models>
   <ExternalModel ModuleToLoad="../models/model_cal" name="model" subType="">
      <inputs>inputGroup</inputs>
      <outputs>outputGroup
   </ExternalModel>
  </Models>
</Simulation>
```

**CHAPTER** 

# **ELEVEN**

# **SUPPORT**

The easiest way to get help with the project is to open an issue on Github.

The mailing list at  $\dots$  is also available for support.

# 11.1 Developer

• Congjian, Wang: congjian.wang@inl.gov

# 11.2 Copyright

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CHAPTER	
TWELVE	

# **CONTRIBUTORS**

**CHAPTER** 

# **THIRTEEN**

# **API REFERENCE**

This page contains auto-generated API reference documentation<sup>1</sup>.

# 13.1 src

# 13.1.1 Subpackages

13.1.1.1 src.poem

**Subpackages** 

src.poem.templates

# Attributes

configFileName

path

templateConfig

# **Package Contents**

```
src.poem.templates.configFileName = 'config.toml'
src.poem.templates.path
src.poem.templates.templateConfig
```

<sup>1</sup> created with sphinx-autoapi

#### **Submodules**

#### src.poem.PoemTemplate

Created on April 1, 2024 @author: wangc

This module inherits from the base Template class for Input Templates, which use an established input template as an accelerated way to write new RAVEN workflows.

#### **Attributes**

```
RAVEN_FRAMEWORK_LOC

logger
```

#### **Classes**

PoemTemplate POEM: Template Class

#### **Module Contents**

```
src.poem.PoemTemplate.RAVEN_FRAMEWORK_LOC
src.poem.PoemTemplate.logger

class src.poem.PoemTemplate.PoemTemplate
    Bases: ravenframework.InputTemplates.TemplateBaseClass.Template
    POEM: Template Class
    _validEntities = ['RumInfo', 'Files', 'Models', 'Distributions', 'Samplers', 'Optimizers', 'DataObjects',...

loadTemplate(filename)
    Loads template file statefully. @ In, filename, str, name of file to load (xml) @ Out, None.
    createWorkflow(inputs, miscDict)
```

Creates a new RAVEN workflow based on the information in dicitonary "inputs." @ In, inputs, dict, dictionary that contains XML node info that needs to be appended (i.e., {RavenXMLNodeTag: ListOfNodes}). @ In, miscDict, dict, dictionary that contains XML node text info that needs to be updated (i.e., {RavenXMLNodeTag: value}) @ Out, xml.etree.ElementTree.Element, modified copy of template ready to run.

```
writeWorkflow(template, destination, run=False)
```

Writes a template to file. @ In, template, xml.etree.ElementTree.Element, file to write @ In, destination, str, path and filename to write to @ In, run, bool, optional, if True then run the workflow after writing? good idea? @ Out, errors, int, 0 if successfully wrote [and run] and non-zero if there was a problem.

### runWorkflow(destination)

Runs the workflow at the destination @ In, destination, str, path and filename of RAVEN input file @ Out, res, int, system results of running the code.

# src.poem.PoemTemplateInterface

Created on April 1, 2024 @author: wangc

This module is the POEM template interface, which uses the user-provided input XML file to construct the corresponding RAVEN workflows (i.e., the RAVEN input XML file).

# **Attributes**

logger

fh

formatter

ravenFrameworkPath

#### **Classes**

_	_
DoomTomn	lateInterface
- ruemi emu i	alenneriace

lhExternalModelNode

POEM Template Interface

# **Module Contents**

```
src.poem.PoemTemplateInterface.logger
src.poem.PoemTemplateInterface.fh
src.poem.PoemTemplateInterface.formatter
src.poem.PoemTemplateInterface.ravenFrameworkPath
class src.poem.PoemTemplateInterface.PoemTemplateInterface(filename)
    Bases: object
    POEM Template Interface
    uniformDistNode
    samplerVarNode
    externalModelNode
```

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```
lhModelNode
reductionNode
basisNode
validAnalysis = ['sensitivity', 'sparse_grid_construction', 'sparse_grid_rom',
'lhs', 'mc', 'train_rom',...
analysisRequired
analysisOptions
_inputFile
_filenameRoot
_inputVarList = []
_outputVarList = []
_externalModelList = []
_externalModelInputDict
_externalModelOutputDict
_distList = []
_samplerList = []
_ensembleModelList = []
_dsList = []
_printList = []
_variableGroupsList = []
_inputDict
_pivot = 'time'
_{limit} = 1000
_initSamples = 20
_templateFile = None
_analysisType = None
_ravenNodeDict
_statsPrefix = ['skewness', 'variationCoefficient', 'mean', 'kurtosis', 'median',
'max', 'min', 'var', 'sigma']
_statsVectorPrefix = ['nsen', 'sen', 'pearson', 'cov', 'vsen', 'spearman']
_polynomialOrder = '2'
```

```
_sparseGridData = None
_data = None
_expTargets = None
_expCov = None
_dynamic = False
_initInputs = None
_globalSettings
_miscDict
getTemplateFile()
getOutput()
```

Obtains the processed outputs from this class: PoemTemplateInterface @ In, None @ Out, (outputDict, miscDict), tuple, first dictionary contains the whole element that needs to be appended in the templated input, while the second dictionary contains only the values that need to be replaced.

## readInput()

Reads the POEM input files and constructs corresponding ET elements @ In, None @ Out, None.

### readGlobalSettings(xmlNode)

Reads the RunInfo XML node from the input root @ In, xmlNode, xml.etree.ElementTree.Element, the input root xml @ Out, None.

# checkInput()

Checks the consistency of user-provided inputs @ In, None @ Out, None.

# static buildPointSet(name, inputs, outputs)

Builds a single PointSet XML node @ In, name, str, the name for the PointSet @ In, inputs, str, string that contains the list of input variables @ In, outputs, str, string that contains the list of output variables @ out, pointSet, xml.etree.ElementTree.Element, the constructed PointSet XML node.

# static buildHistorySet(name, inputs, outputs, pivot='time')

Builds a single HistorySet XML node @ In, name, str, the name for the PointSet @ In, inputs, str, string that contains the list of input variables @ In, outputs, str, string that contains the list of output variables @ out, historySet, xml.etree.ElementTree.Element, the constructed HistorySet XML node.

#### static buildPrint(name, source)

Builds a single OutStream Print XML node @ In, name, str, the name for the PointSet @ In, source, str, string that contains name of Data Object @ out, printObj, xml.etree.ElementTree.Element, the constructed print XML node.

# buildSamplerVariable(inputs, distNode, limit=20, grid=False, init=None)

Builds the sampler variable block.

```
static buildSparseGridSampler(name='SparseGrid')
static buildMonteCarloSampler(name, limit)
static buildWariableGroup(name, varList)
```

Builds the variable group node @ In, name, str, the name for the variable group @ In, varList, list, list of variables @ out, group, xml.etree.ElementTree.Element, the constructed variable group XML node.

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#### buildStatsGroup(name, inputs, outputs)

Builds the basic statistic variable group node @ In, name, str, the name for the variable group @ In, inputs, list, list of input variables @ In, outputs, list, list of output variables @ out, group, xml.etree.ElementTree.Element, the constructed variable group XML node.

#### static findRequiredNode(xmlNode, nodeTag)

Finds the required XML node @ In, xmlNode, xml.etree.ElementTree.Element, xml element node @ In, nodeTag, str, node tag that is used to find the node @ Out, subnode, xml.etree.ElementTree.Element, xml element node.

# src.poem.plotUtils

#### **Attributes**

```
markerMap
markers
```

### **Functions**

```
addPoint(ax, x, y, accepted)

plotFunction(fig, title, method, constraint, xscale, ...)  Plots a 2D function as a colormap. Returns parameters suitable to plotting in a pcolormesh call.

animate(n, ax, x, y, a)

animatePlot(x, y, a, fig, title, method, constraint, ...)

optPath(x, y, a, fig, title, method, constraint, ...)
```

#### **Module Contents**

Plots a 2D function as a colormap. Returns parameters suitable to plotting in a pcolormesh call @ In, title, string, title name for figure @ In, method, function, method to call with x,y to get z result @ In, constraint, function, boolean method that determines acceptability @ In, xscale, tuple(float), low/hi value for x @ In, yscale, tuple(float), low/hi value for y @ In, cscale, tuple(float), optional, low and high values for the color map @ In, log, bool, optional, if False will not lognormalize the color map @ In, samps, int @ In, extData, pandas.Dataframe @ Out, X, np.array(np.array(float)), mesh grid of X values @ Out, Y, np.array(np.array(float)), mesh grid of Y values @ Out, Z, np.array(np.array(float)), mesh grid of Z (response) values.

src.poem.plotUtils.animate(n, ax, x, y, a)

src.poem.plotUtils.animatePlot(x, y, a, fig, title, method, constraint, xscale, yscale, cscale=None, log=False, samps=500, xp=None, yp=None)

src.poem.plotUtils.optPath(x, y, a, fig, title, method, constraint, xscale, yscale, cscale=None, log=False, samps=500, xp=None, yp=None)

#### src.poem.poemUtils

Created on April 1, 2024 @author: wangc

#### **Attributes**

logger

#### **Functions**

-	
<pre>convertNodeTextToList(nodeText[, sep])</pre>	Converts a space- or comma-separated string to list of string
<pre>convertNodeTextToFloatList(nodeText[, sep])</pre>	Converts a space- or comma-separated string to list of float
<pre>convertStringToFloat(xmlNode)</pre>	Converts XML node text to float
<pre>convertStringToInt(xmlNode)</pre>	Converts XML node text to integer
toString(s)	Method aimed at converting a string in type str
<pre>convertStringToBool(nodeText)</pre>	Converts string to bool

### **Module Contents**

src.poem.poemUtils.logger

src.poem.poemUtils.convertNodeTextToList(nodeText, sep=None)

Converts a space- or comma-separated string to list of string @ In, nodeText, str, string from XML node text @ Out, listData, list, list of strings.

src.poem.poemUtils.convertNodeTextToFloatList(nodeText, sep=None)

Converts a space- or comma-separated string to list of float @ In, nodeText, str, string from xml node text @ Out, listData, list, list of floats.

src.poem.poemUtils.convertStringToFloat(xmlNode)

Converts XML node text to float @ In, xmlNode, xml.etree.ElementTree.Element, xml element @ Out, val, float, value of xml element text.

src.poem.poemUtils.convertStringToInt(xmlNode)

Converts XML node text to integer @ In, xmlNode, xml.etree.ElementTree.Element, xml element @ Out, val, integer, value of xml element text.

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#### src.poem.poemUtils.toString(s)

Method aimed at converting a string in type str @ In, s, string, string to be converted @ Out, s, string, the casted value.

#### src.poem.poemUtils.convertStringToBool(nodeText)

Converts string to bool @ In, nodeText, str, string from XML node text @ Out, val, bool, True or False.

# 13.1.2 Submodules

# 13.1.2.1 src.\_utils

Utilities for use within POEM

#### **Attributes**

argvs

#### **Functions**

<pre>get_raven_loc()</pre>	Return	RAVEN	location:	read	from
	POEM/.ravenconfig.xml.				
<pre>get_plugin_loc(plugin[, raven_path])</pre>	Get plug	in location in	installed RAVE	EN.	

## **Module Contents**

#### src.\_utils.get\_raven\_loc()

Return RAVEN location: read from POEM/.ravenconfig.xml @ In, None @ Out, loc, string, absolute location of RAVEN.

## src.\_utils.get\_plugin\_loc(plugin, raven\_path=None)

Get plugin location in installed RAVEN @ In, plugin, string, the plugin name @ In, raven\_path, string, optional, if given then start with this path @ Out, plugin\_loc, string, location of plugin.

src.\_utils.argvs

### 13.1.2.2 src.main

Created on April 1, 2024 @author: wangc

This module is the POEM template interface, which uses the user-provided input XML file to construct the corresponding RAVEN workflows (i.e., RAVEN input XML file).

# **Attributes**

RAVEN\_FRAMEWORK\_LOC

logger

fh

formatter

#### **Functions**

runWorkflow(destination)	Runs the workflow at the destination.
main()	

# **Module Contents**

src.main.RAVEN\_FRAMEWORK\_LOC

src.main.logger

src.main.fh

src.main.formatter

src.main.runWorkflow(destination)

Runs the workflow at the destination @ In, destination, str, path and filename of RAVEN input file @ Out, res, int, system results of running the code.

src.main.main()

# 13.2 PoemTester

Tests by running an executable.

# 13.2.1 Attributes

POEM\_LOC

RAVEN\_FRAMEWORK\_LOC

TESTER\_LOC

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# 13.2.2 Classes

PoemRun

A POEM standalone test interface.

# 13.2.3 Module Contents

PoemTester.**POEM\_LOC** 

PoemTester.RAVEN\_FRAMEWORK\_LOC

 ${\tt PoemTester.} \textbf{TESTER\_LOC}$ 

class PoemTester.PoemRun(name, param)

Bases: RavenFramework.RavenFramework

A POEM standalone test interface.

# static get\_valid\_params()

Returns a list of valid parameters and their descriptions for this type of test @ In, None @ Out, params, \_ValidParameters, the parameters for this class.

### poem\_driver

# get\_command()

Returns the command this test will run @ In, None @ Out, cmd, string, command to run.

**CHAPTER** 

# **FOURTEEN**

# **CONTRIBUTIONS**

All contributions are welcome. You can help this project grow in multiple ways, from creating an issue, to reporting an improvement or a bug, to submitting a pull request to the development branch. The people who have been involved in the development of the package are listed on the *contributors page*.

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```