Nodeworks

August 28, 2020

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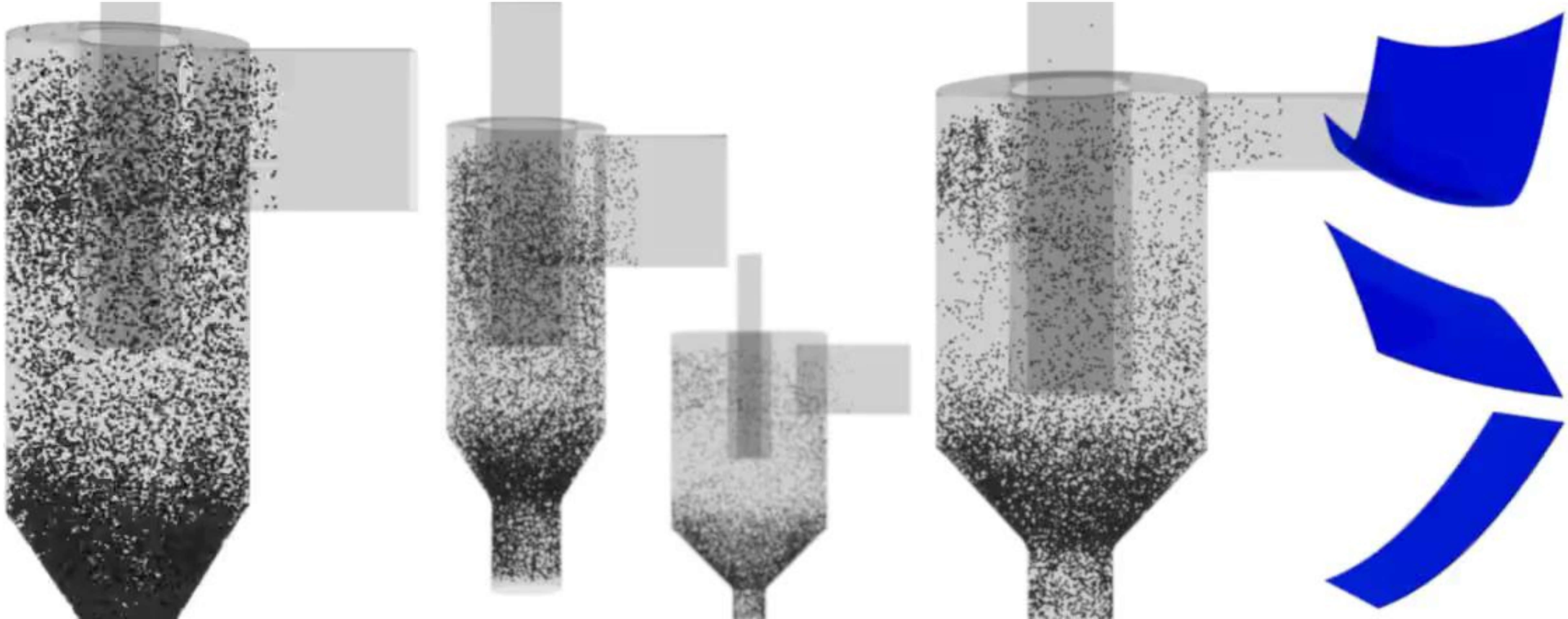
NETL | *Alpemi, LLC* | *LLNL*



So many options!

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Galaxy

Next Generation Workflow (NGW)

Luigi

nextflow

PLYNX

Themis

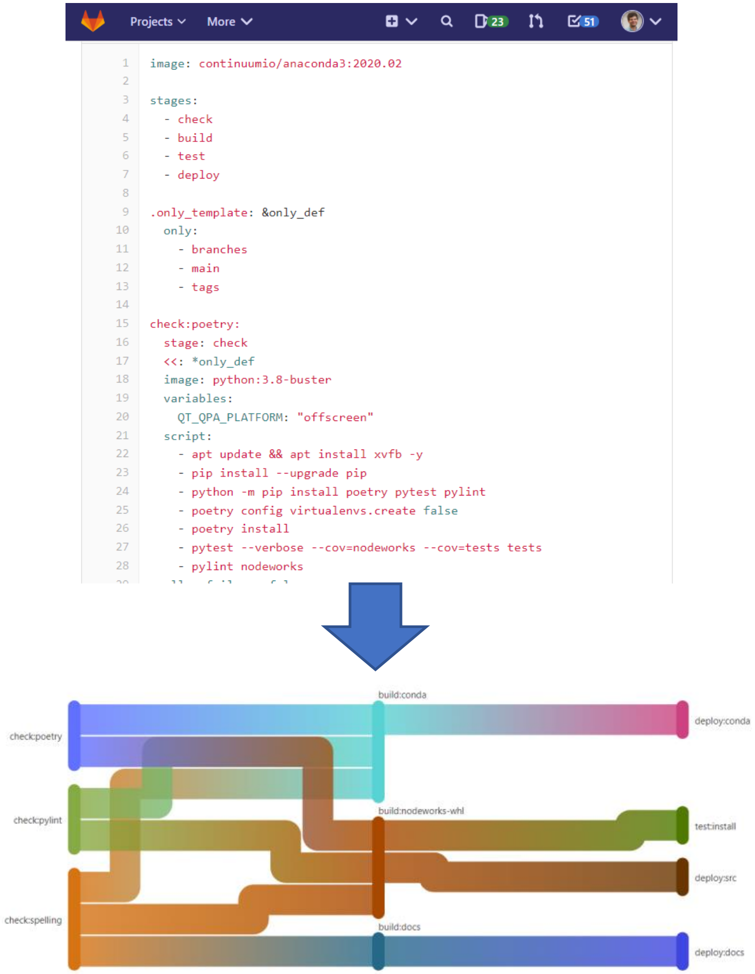
Pegasus

funcX

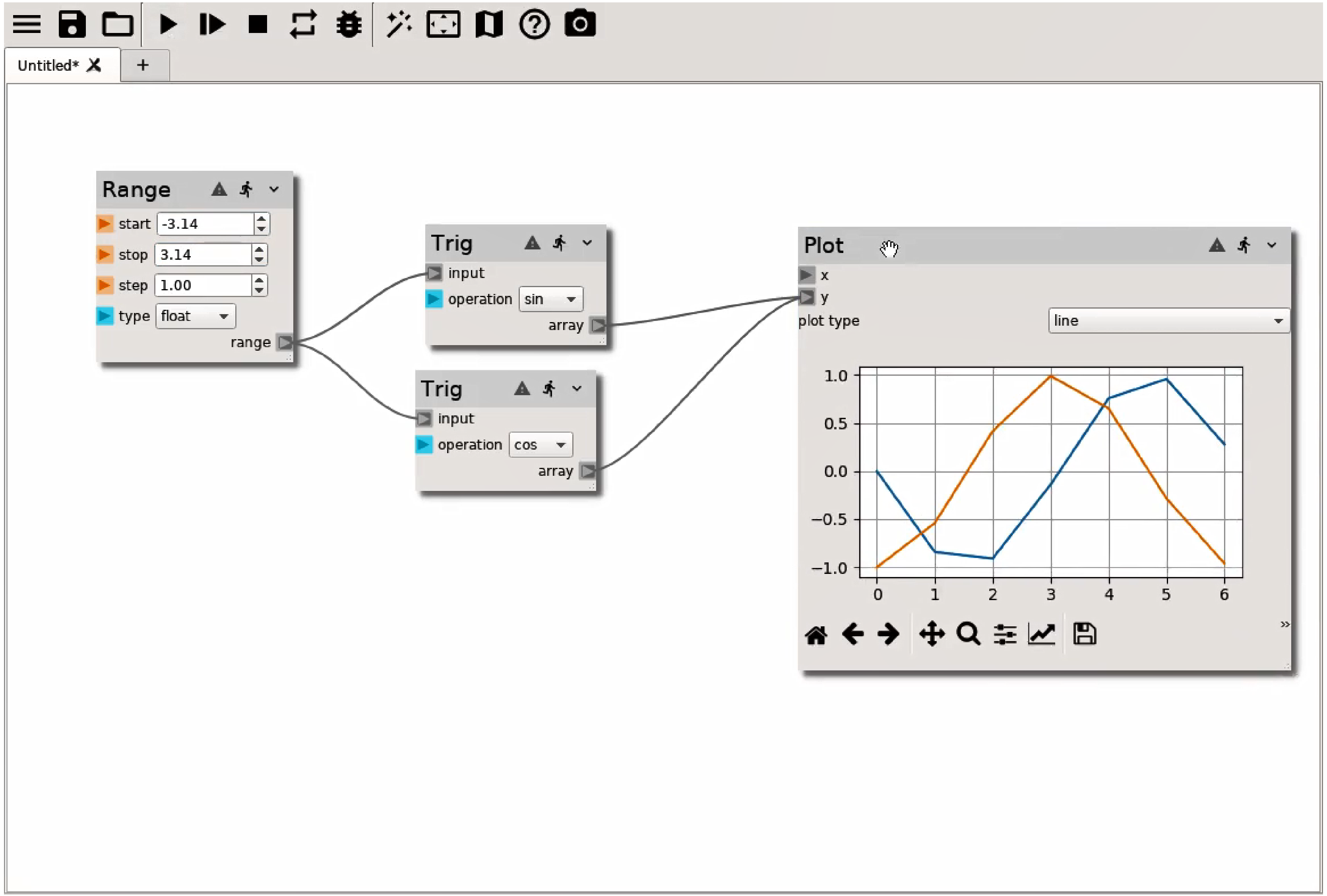
Apache Airflow

BEE

Low-Code/No-Code

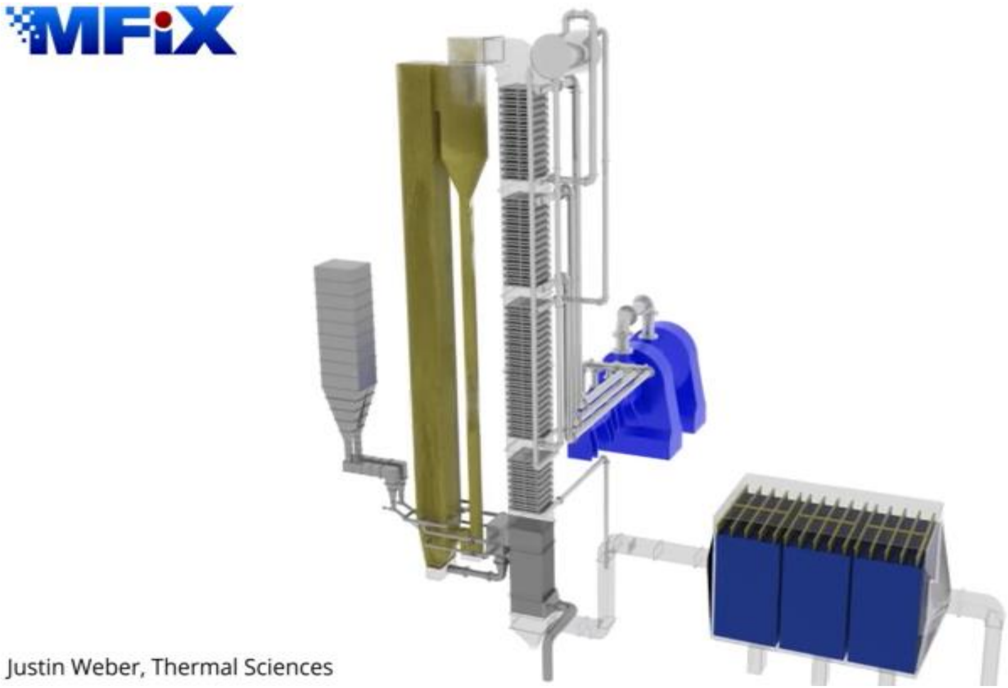


What is Nodeworks?



Application and framework for workflows

Why did you make this?



Justin Weber, Thermal Sciences

Parameter sweep → Run models → Optimize

Why did you make this?

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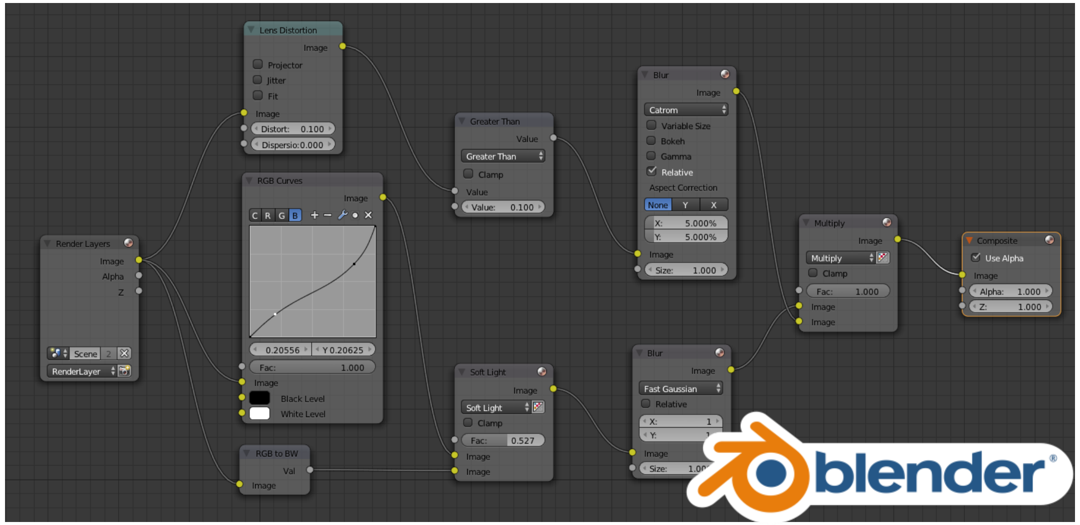

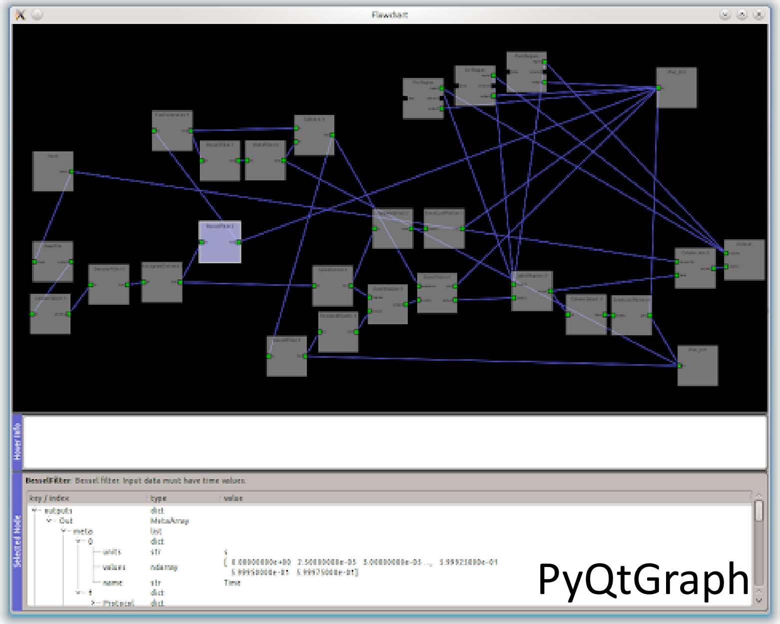

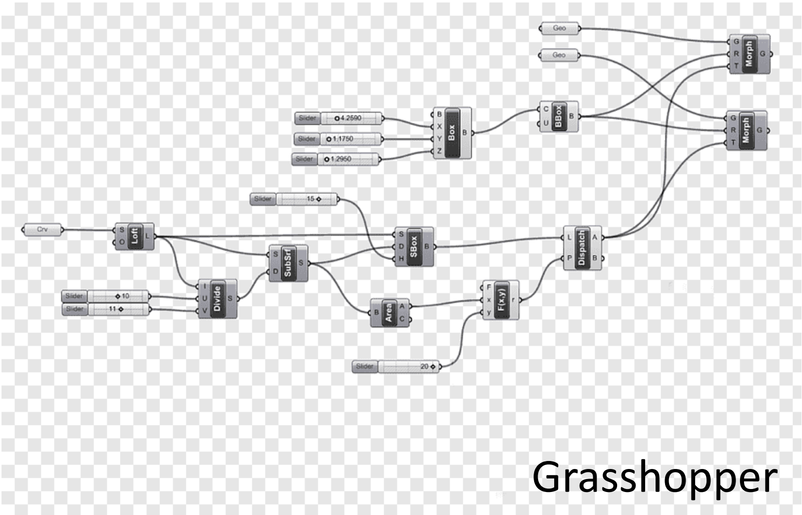

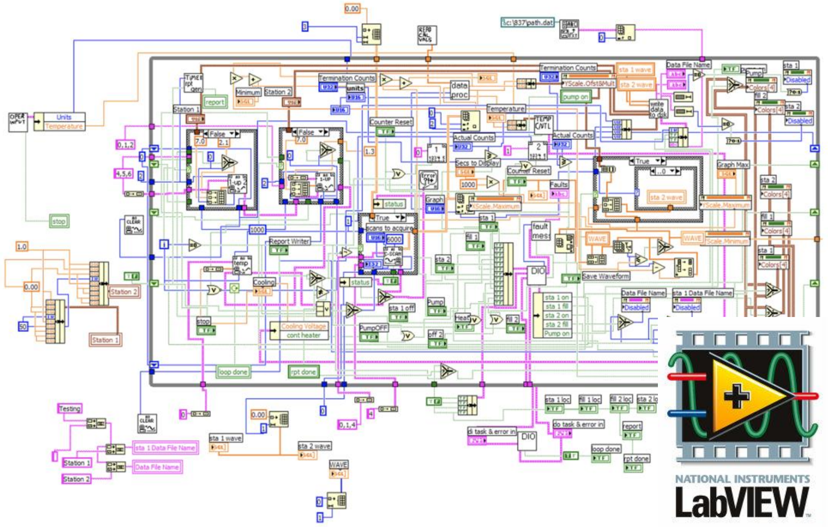

PLYNX

How is it constructed?

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python

Qt

Tested operating systems:
- Linux (Centos @ Joule)
- OSX
- Windows

Deploy
- Conda
- Poetry
- Pyinstaller?

SciPy

scikit learn

NumPy

seaborn

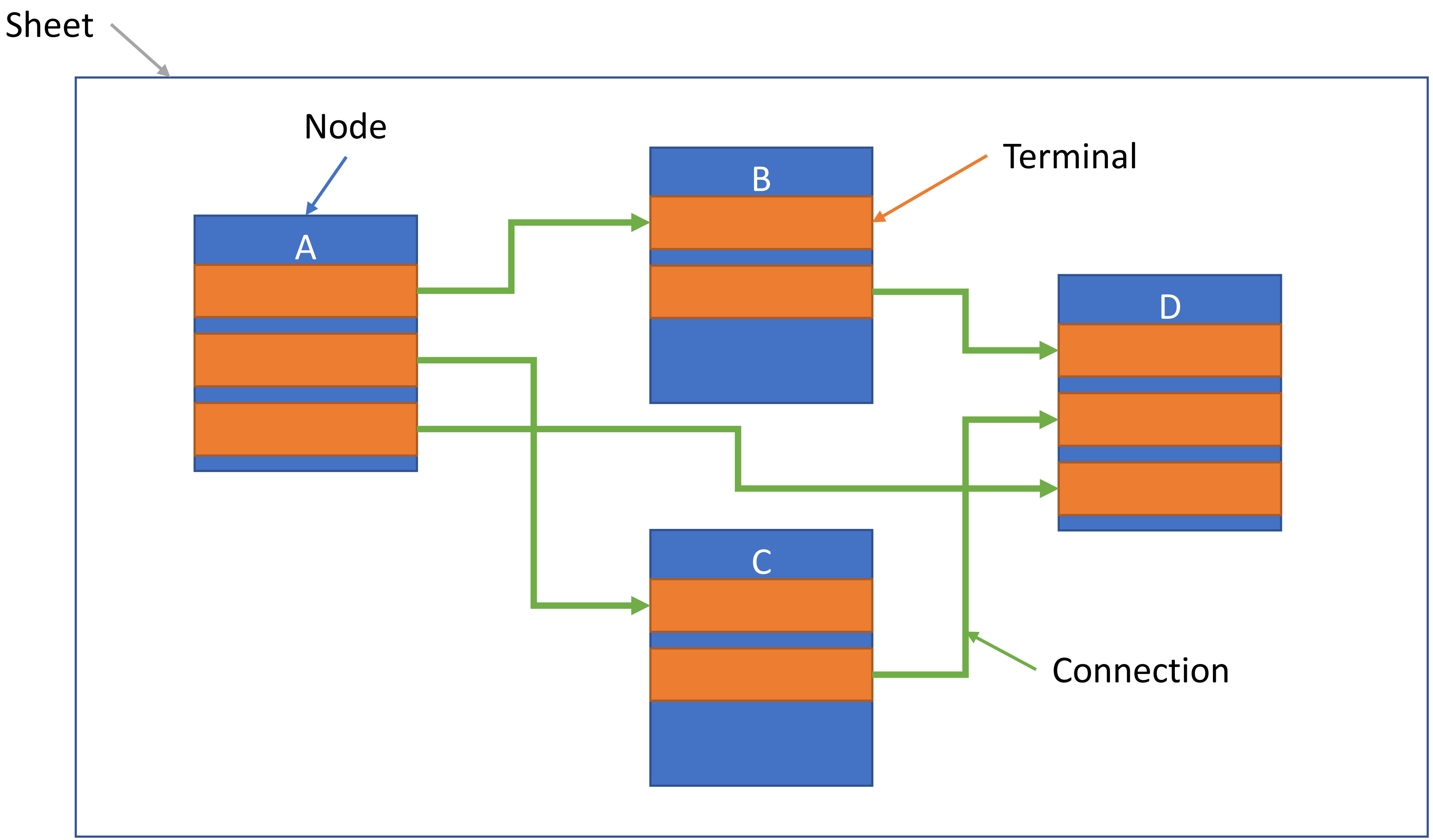
pandas

PyTorch

TensorFlow

matplotlib

How does it work?



Topological sort

1. A
2. B, C
3. D

Super easy to make your own nodes!

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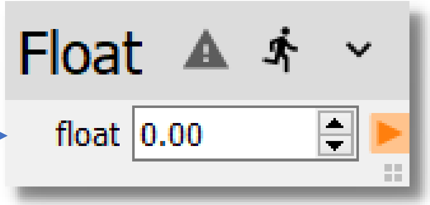
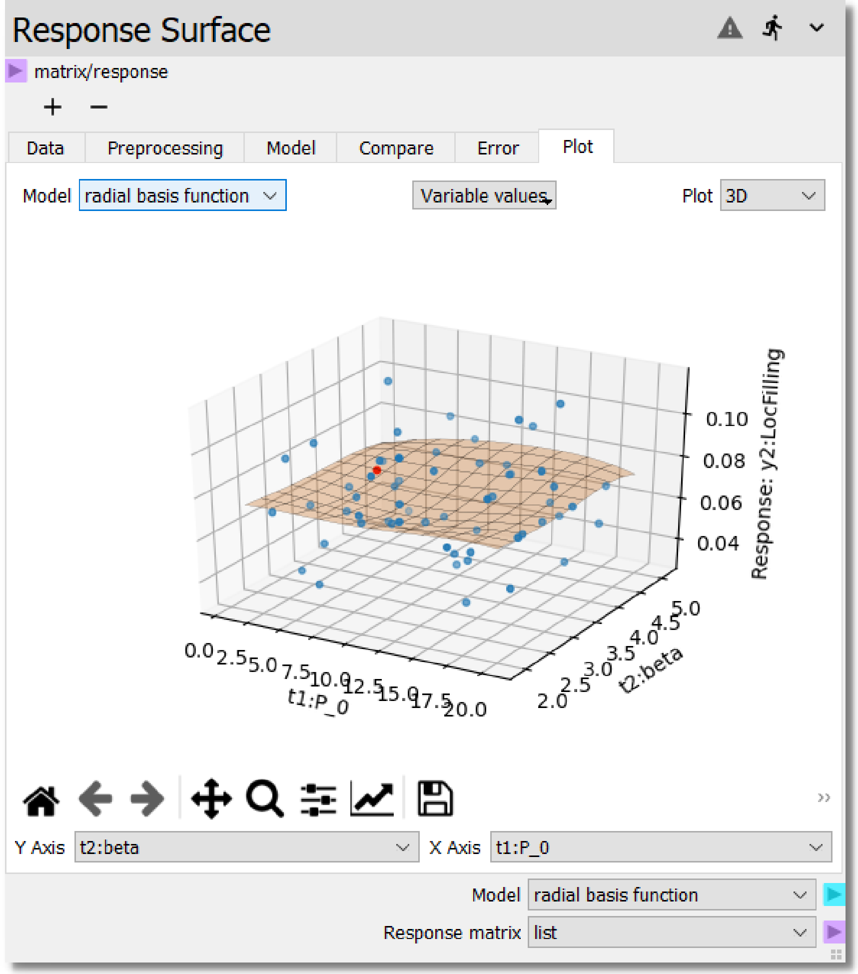
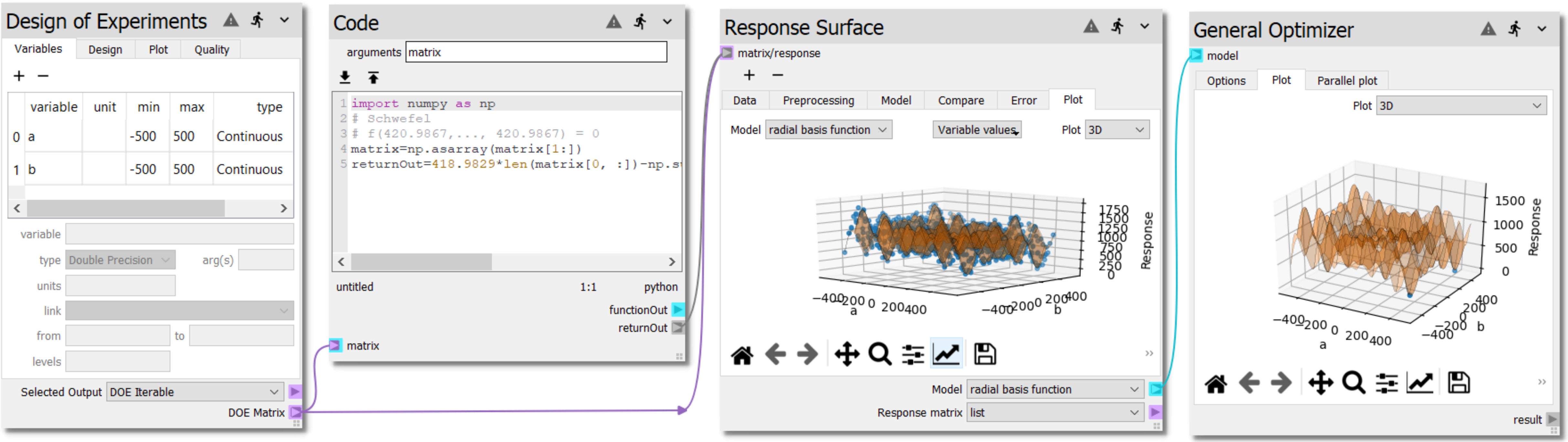
```python
class FloatNode(Node):
    '''
    Float Type

    Output Terminals
    ----------------
    (float):
        the float value of the spinbox
    '''
    name = 'Float'

    def __init__(self):
        self.terminalOpts = {
            'float': {'widget': 'doublespinbox',
                      'out':     True,
                      'dtype':   float, },
                      }
        Node.__init__(self)
```





Surrogate modeling and analysis toolset

Design of Experiments → Model evaluation → Response Surface Construction → Optimization / Sensitivity / Forward Propagation



Design of Experiments

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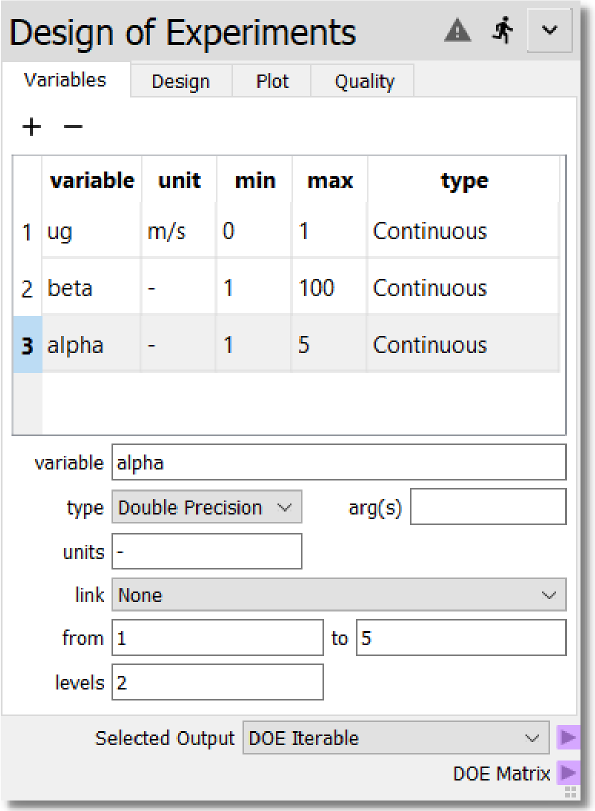
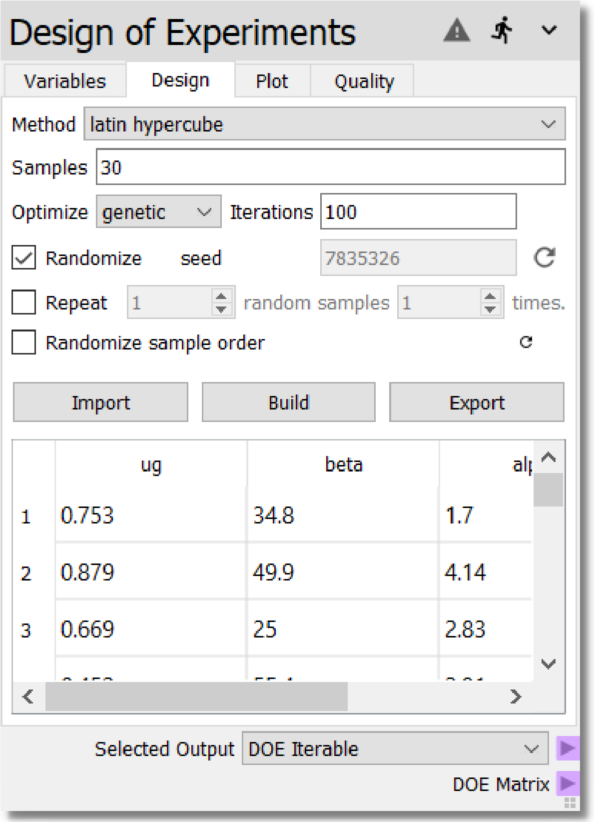
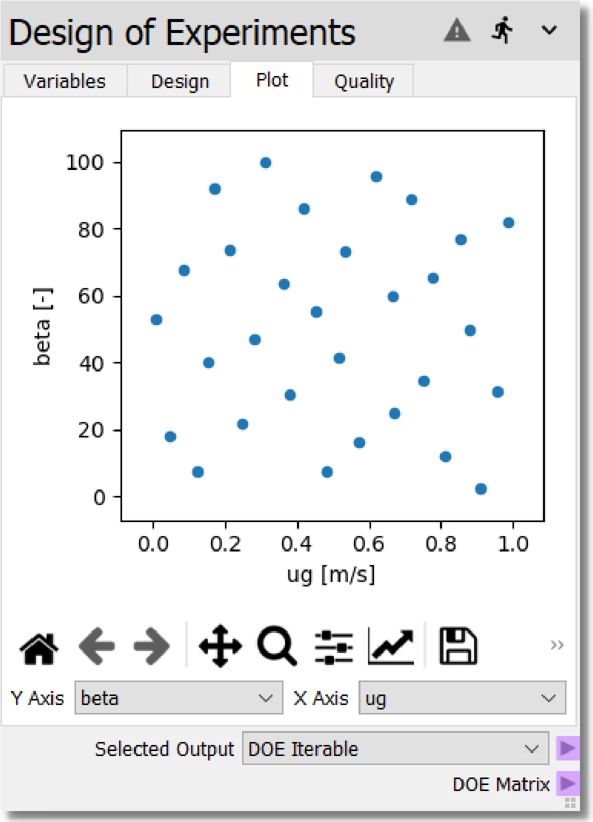


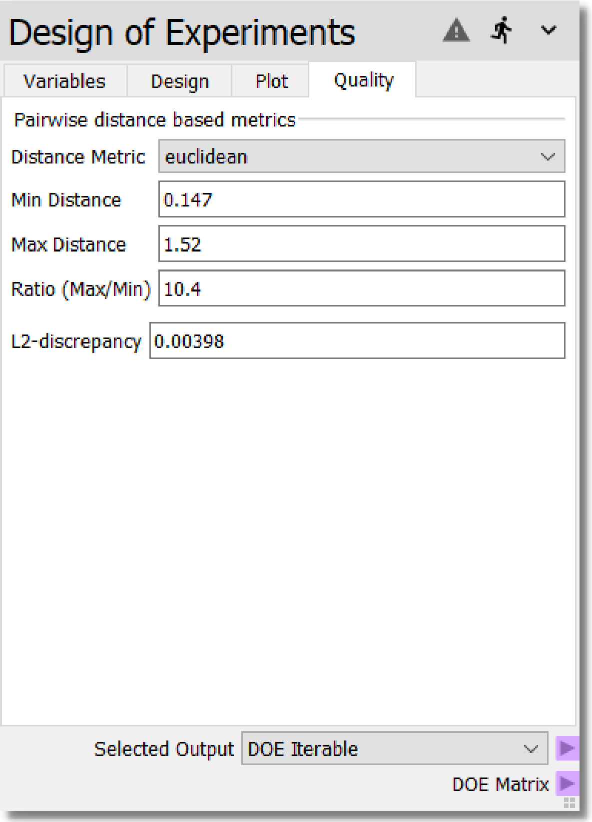
Factorial
Covary



Montecarlo
Latin hypercube



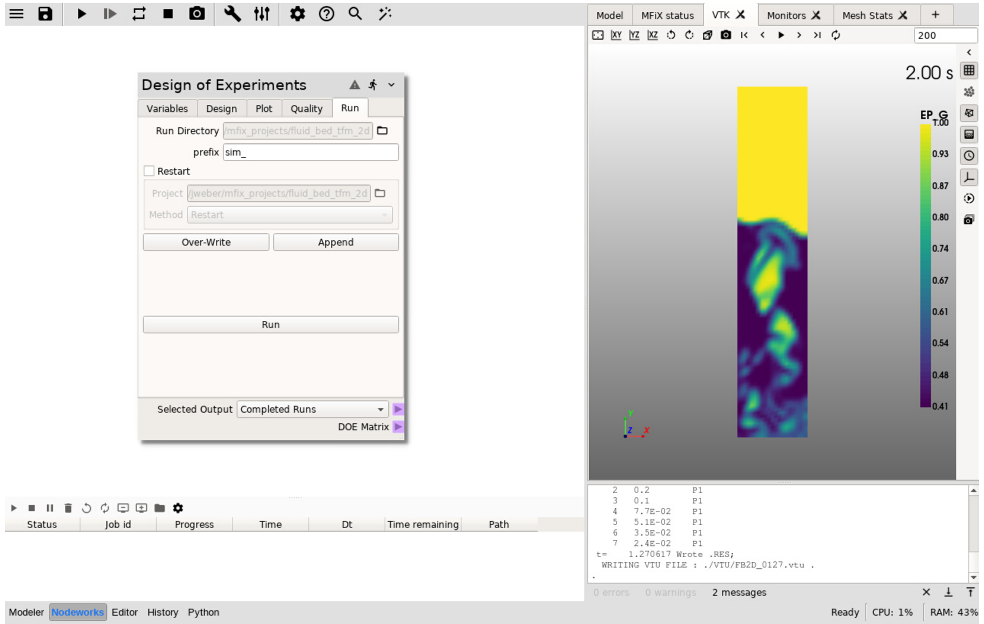
Central composite
Sobol



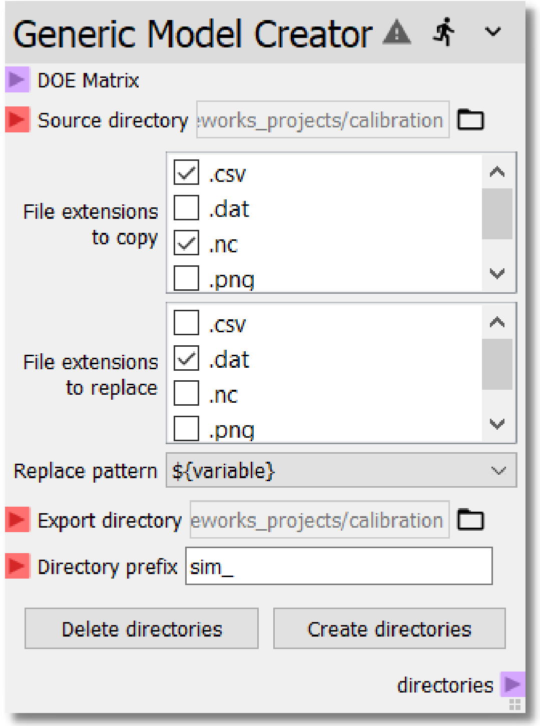
Hammersly
Halton

Building the models

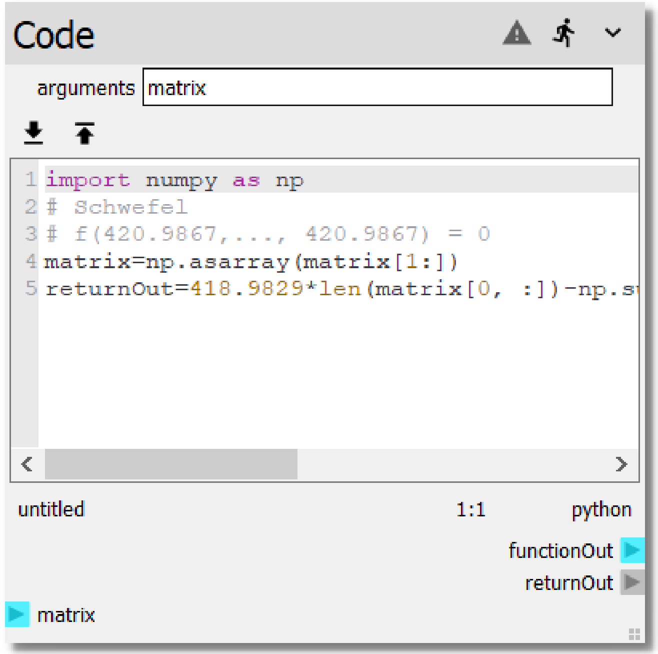
From within the MFiX GUI



Search/replace text

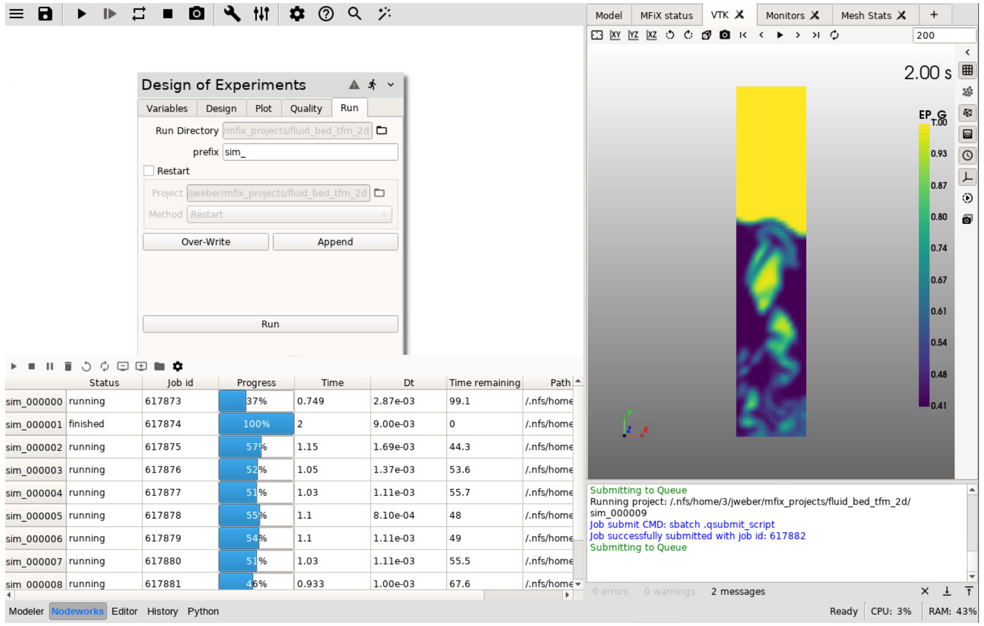


Custom python script

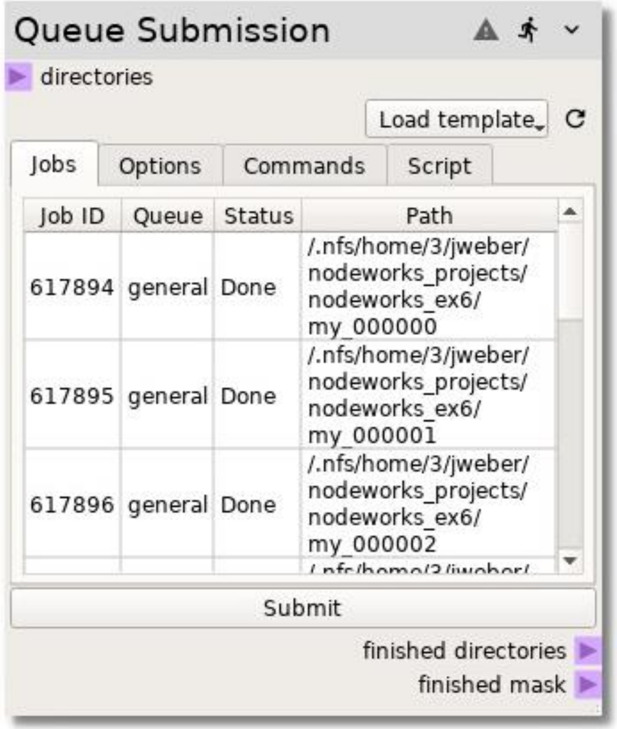


Running the models

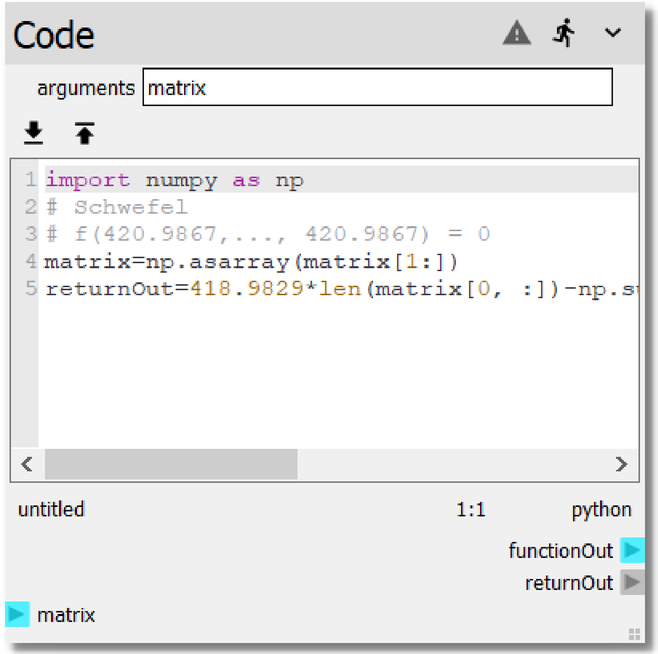
From within the MFiX GUI



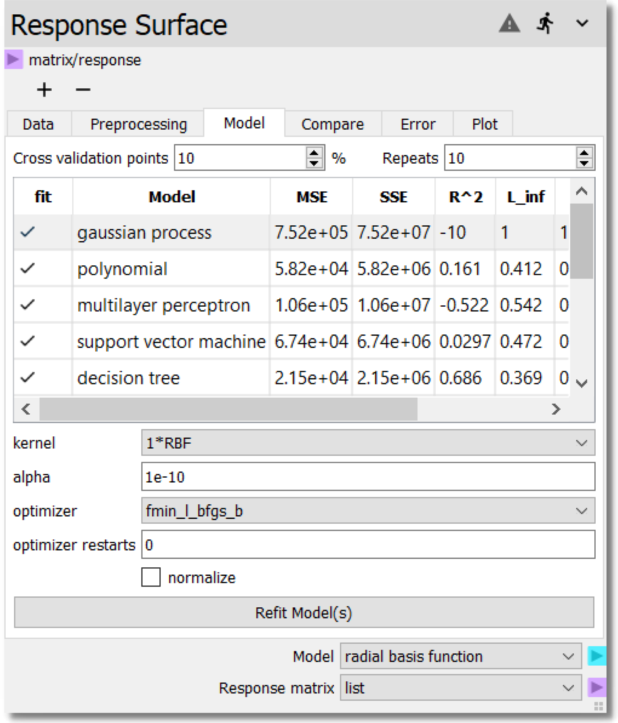
Queue submission

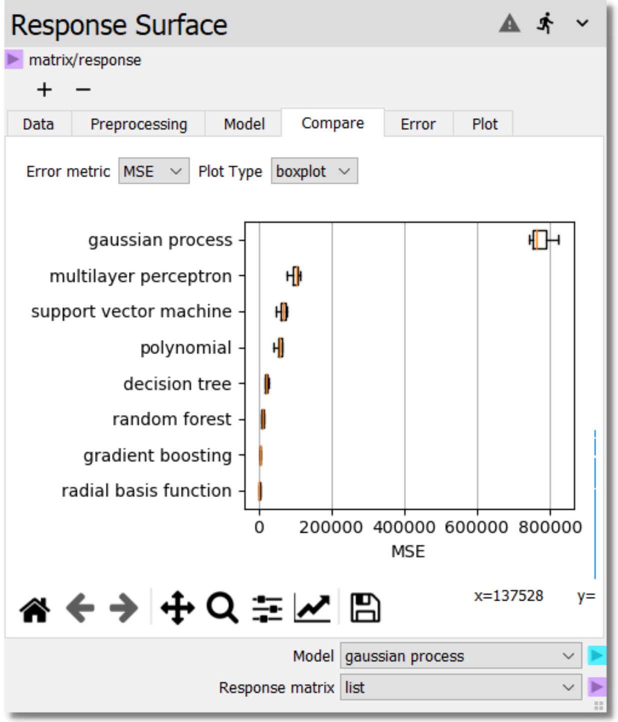


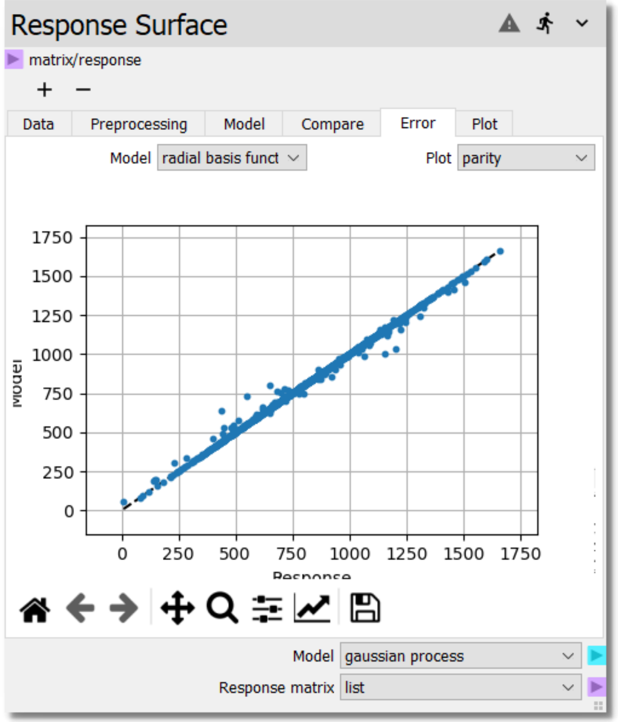
Custom python script

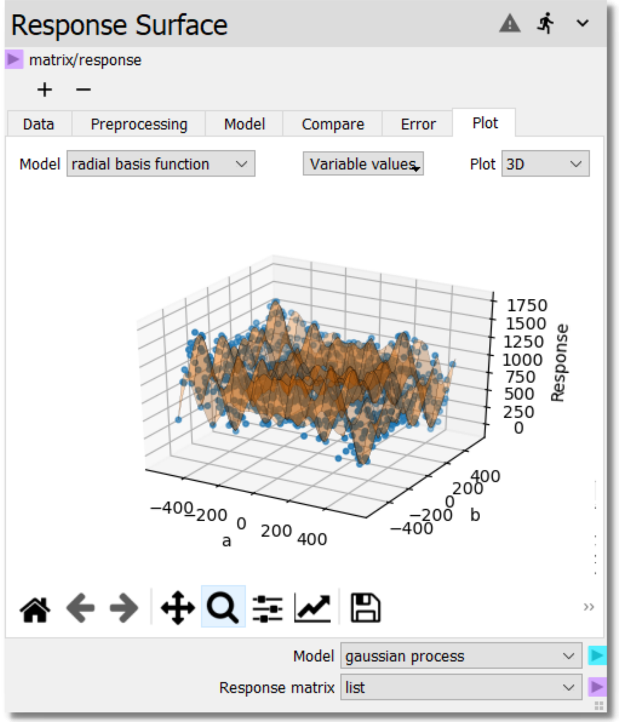


Response Surface

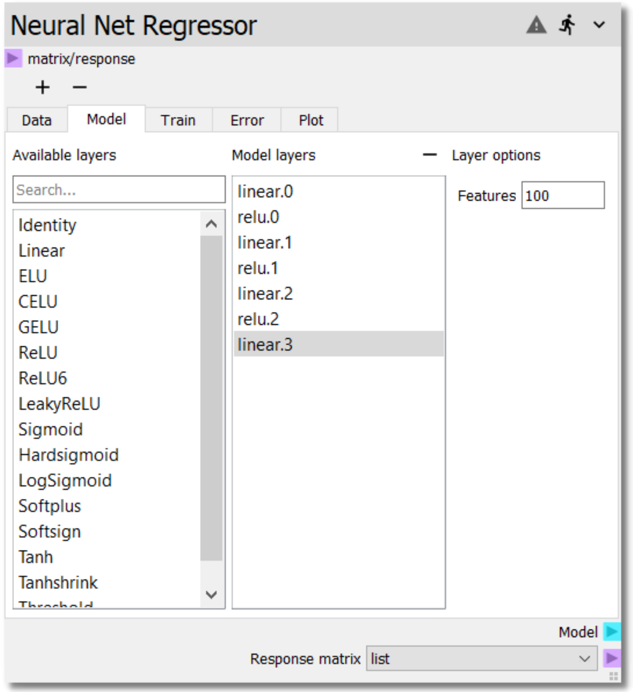


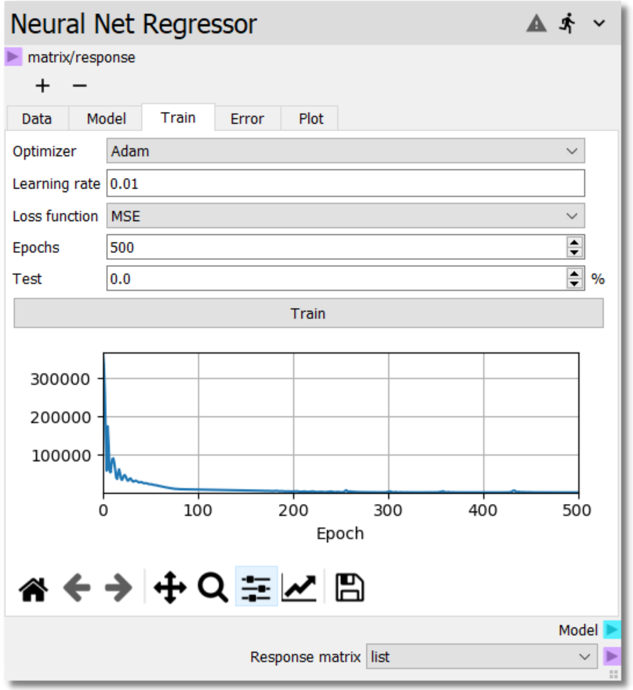


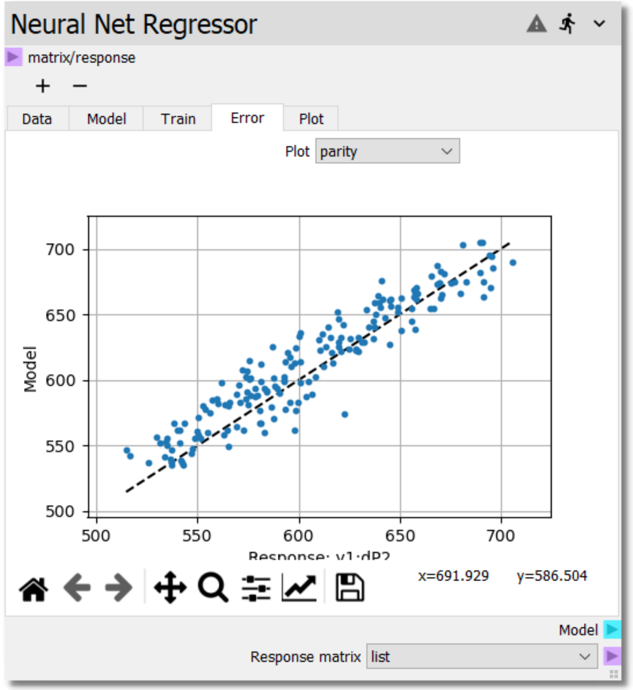


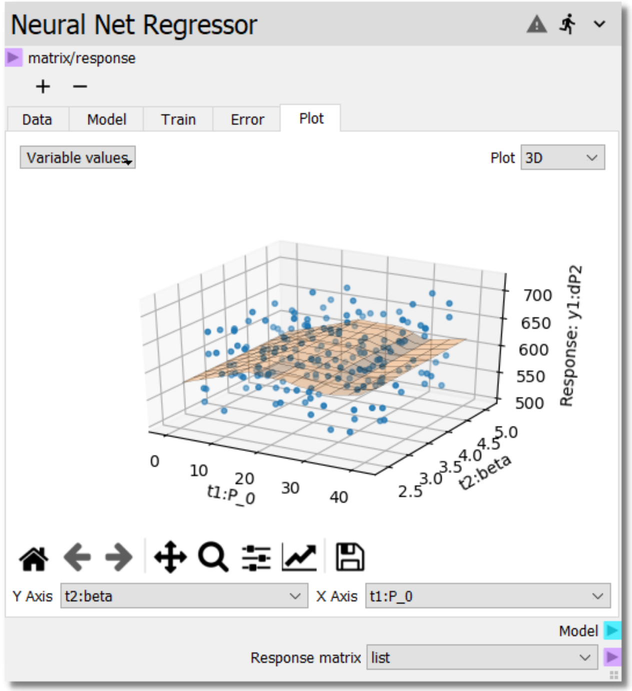


Neural Net Regressor



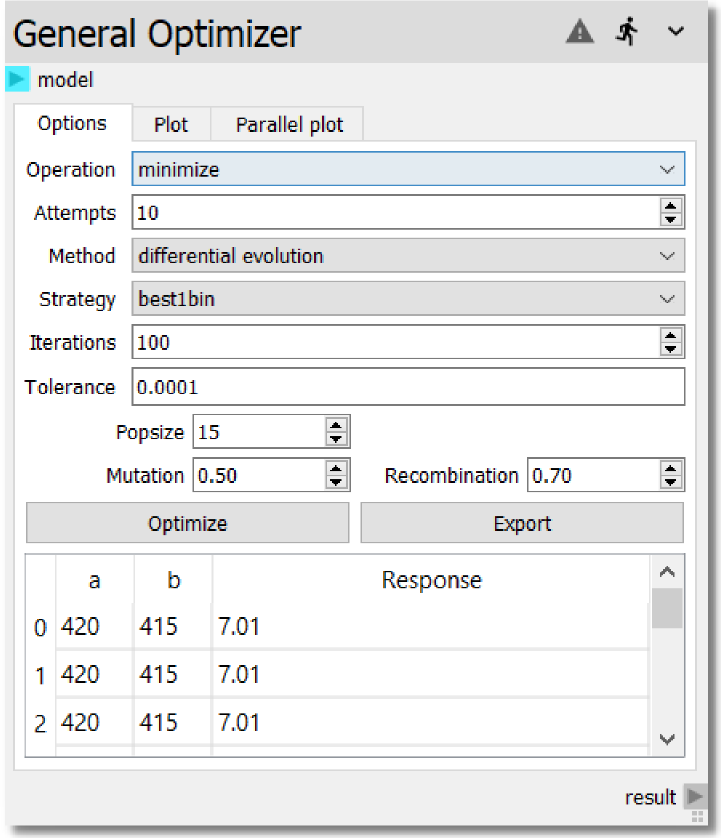


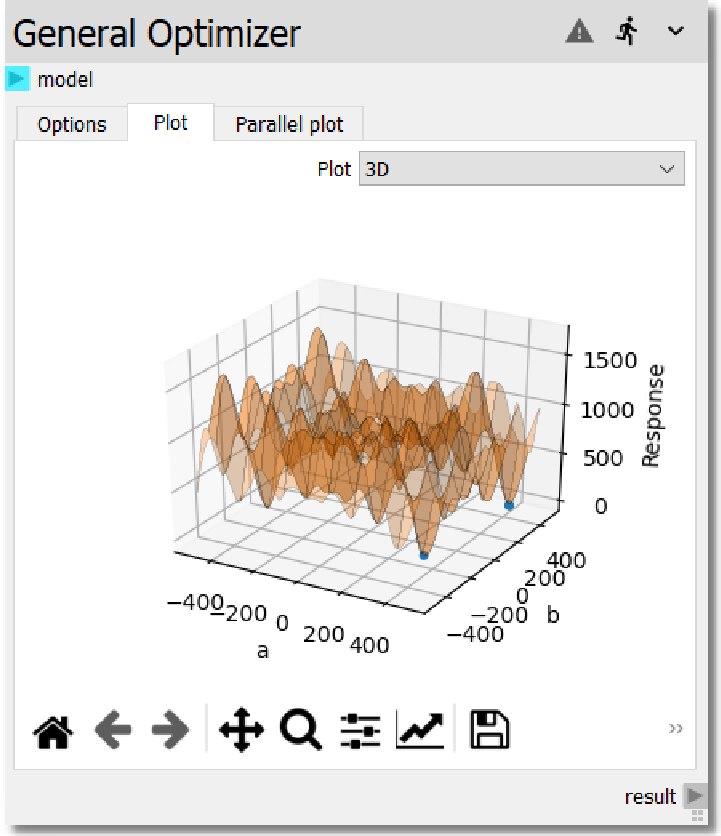


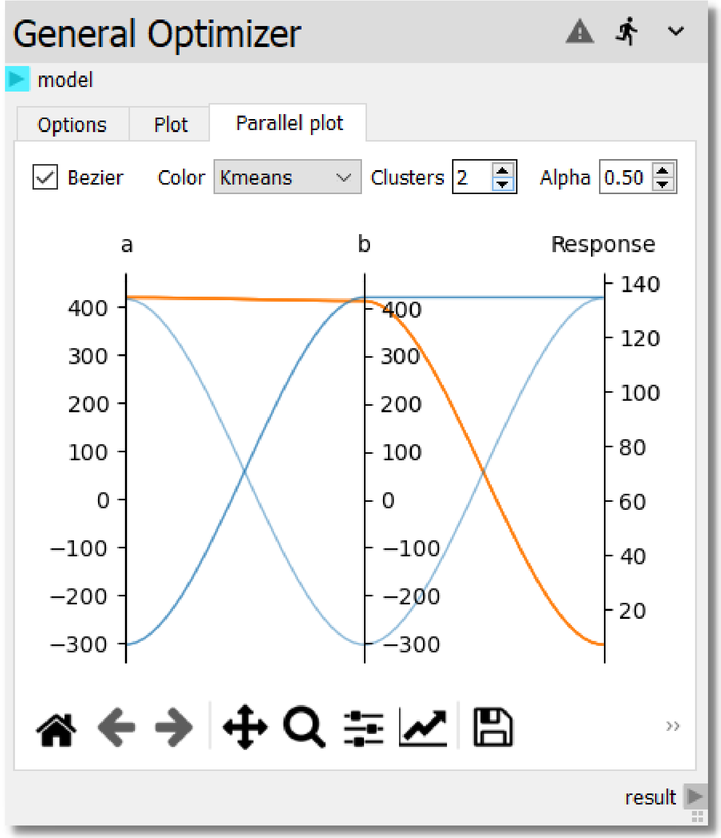


PyTorch

Optimization







Differential evolution
Basin hopping
SHGO - simplicial homology global optimization
Dual annealing

Schwefel function $f(420.99, 420.99) = 0$

Sensitivity Analysis

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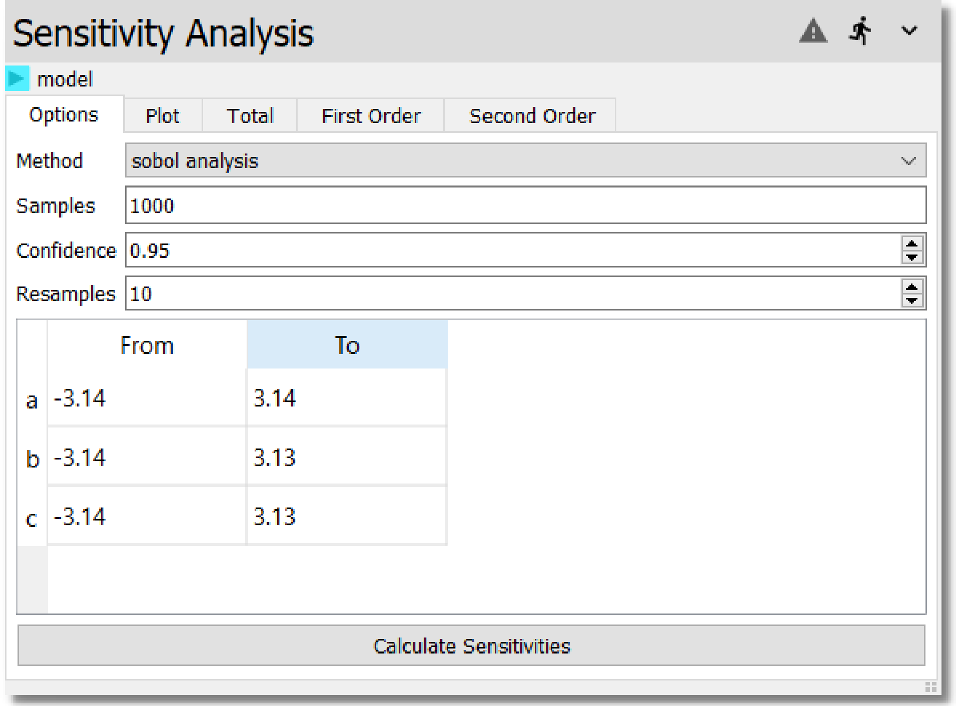
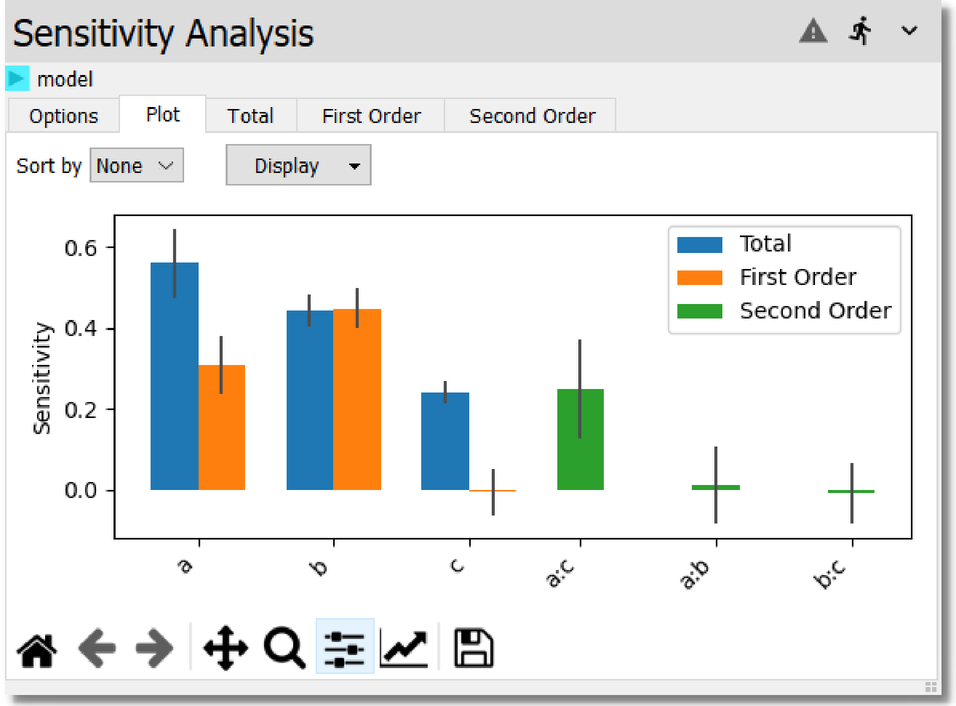
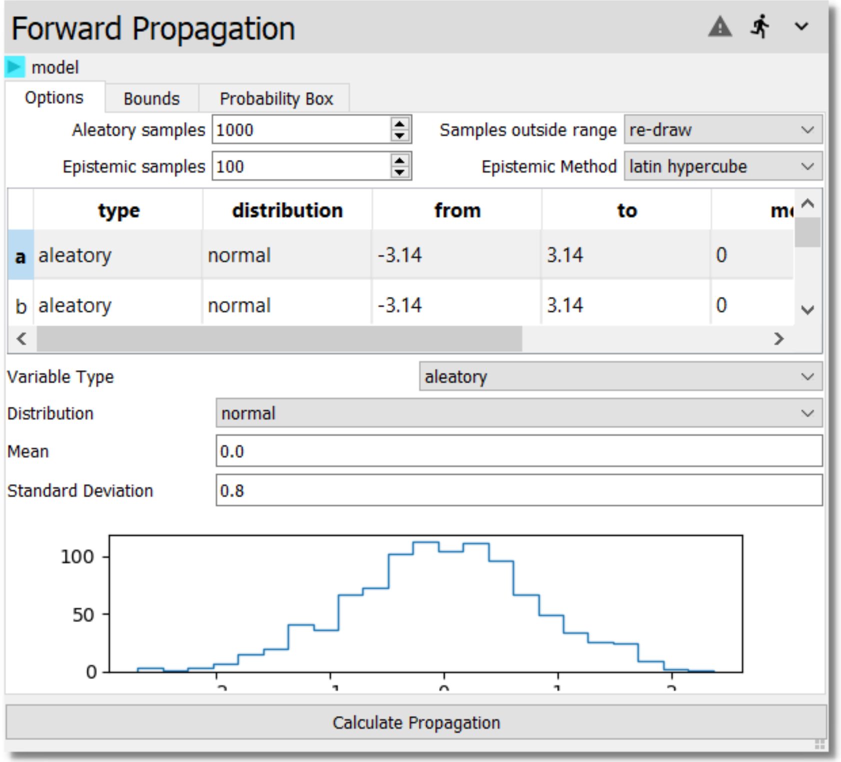


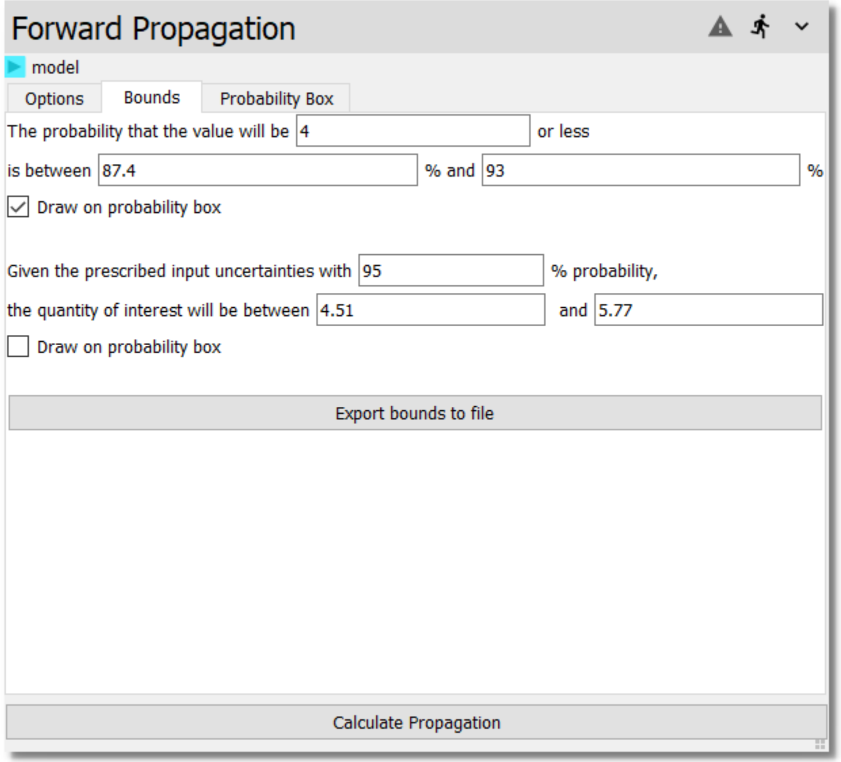


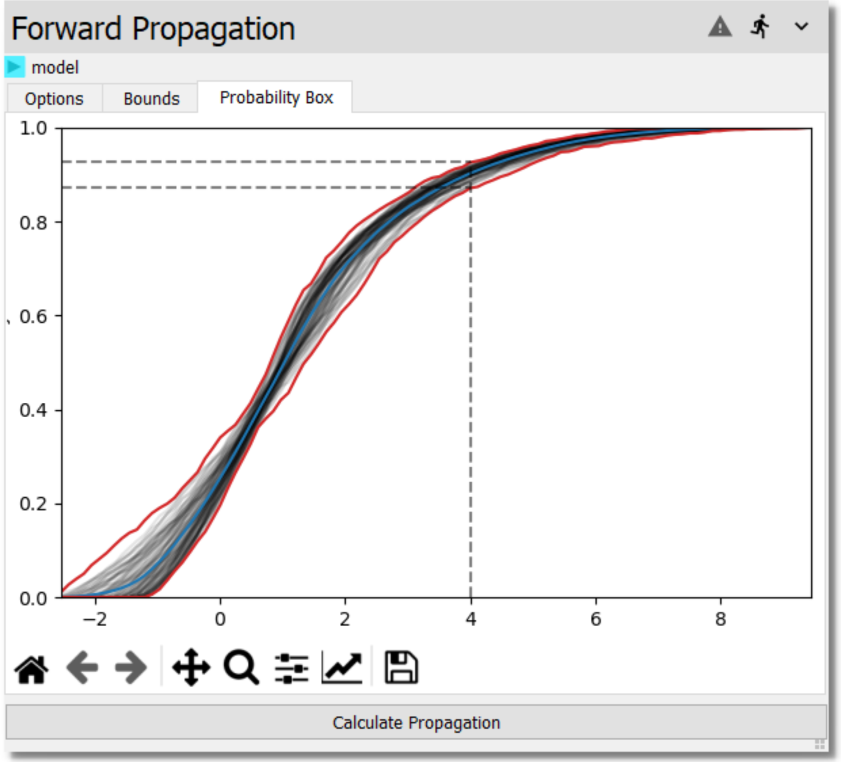
Sobol
Method of Morris
Fourier amplitude sensitivity test
Delta moment-independent measure
Random balance designs Fourier applicated sensitivity test

SALib

Forward Propagation



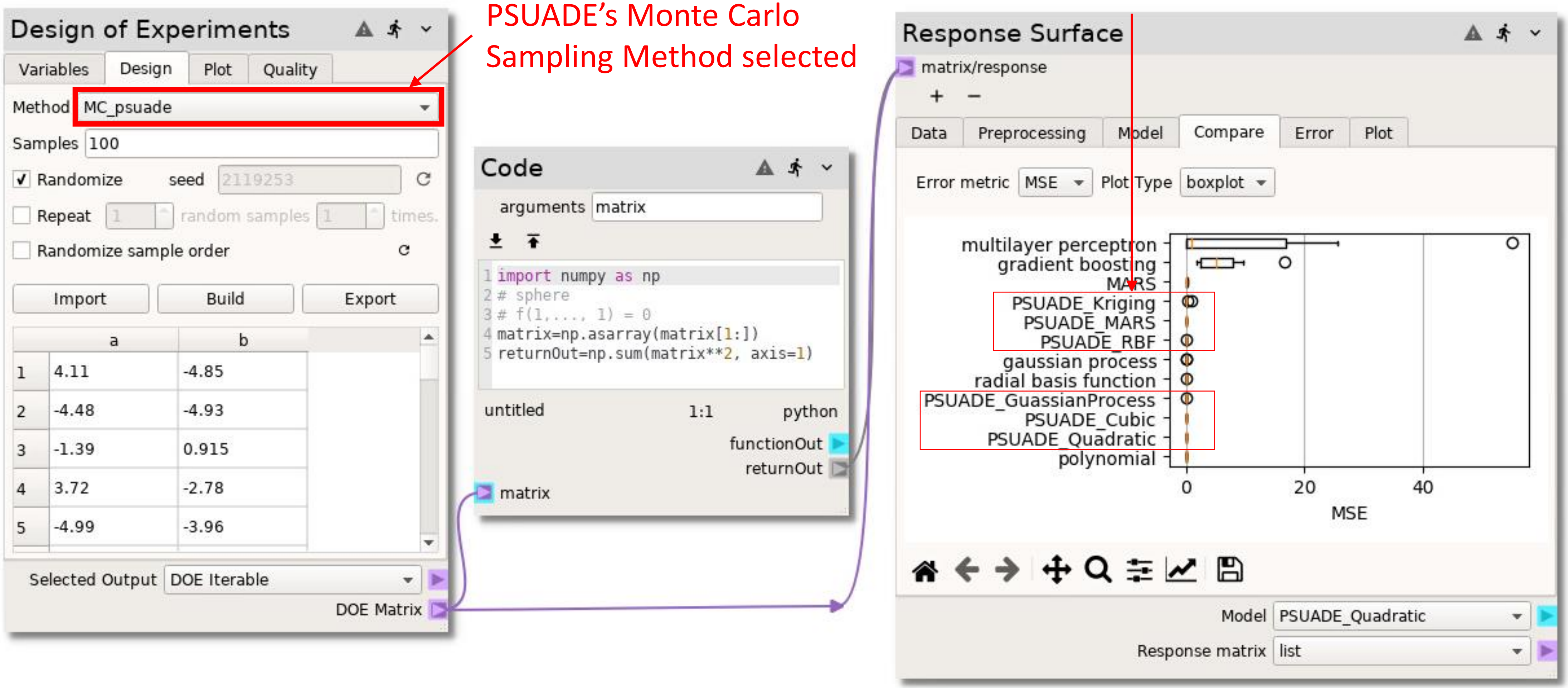




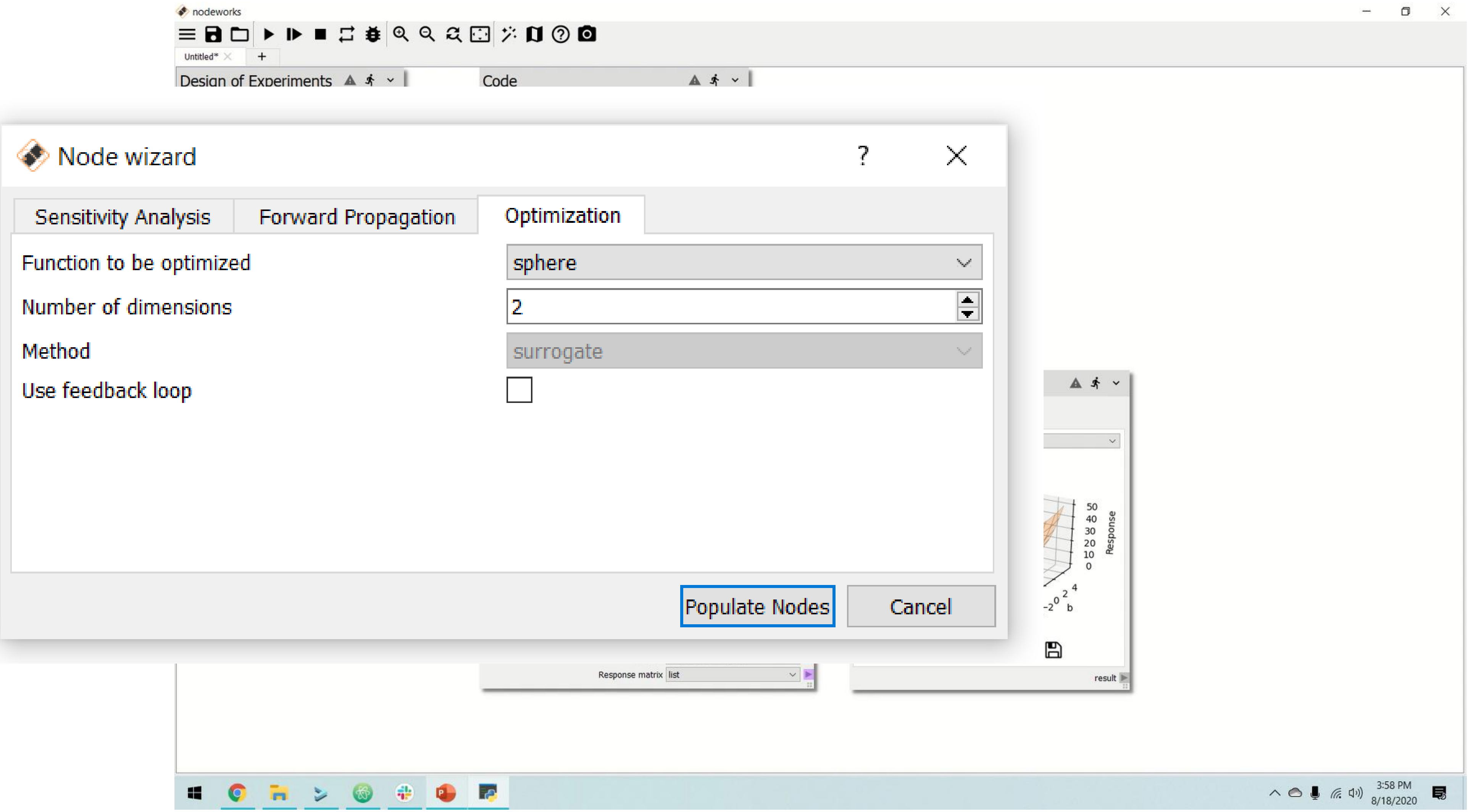
Integration with PSUADE UQ Toolkit from LLNL

PSUADE's Response Surface Methods also tested

PSUADE's Monte Carlo Sampling Method selected

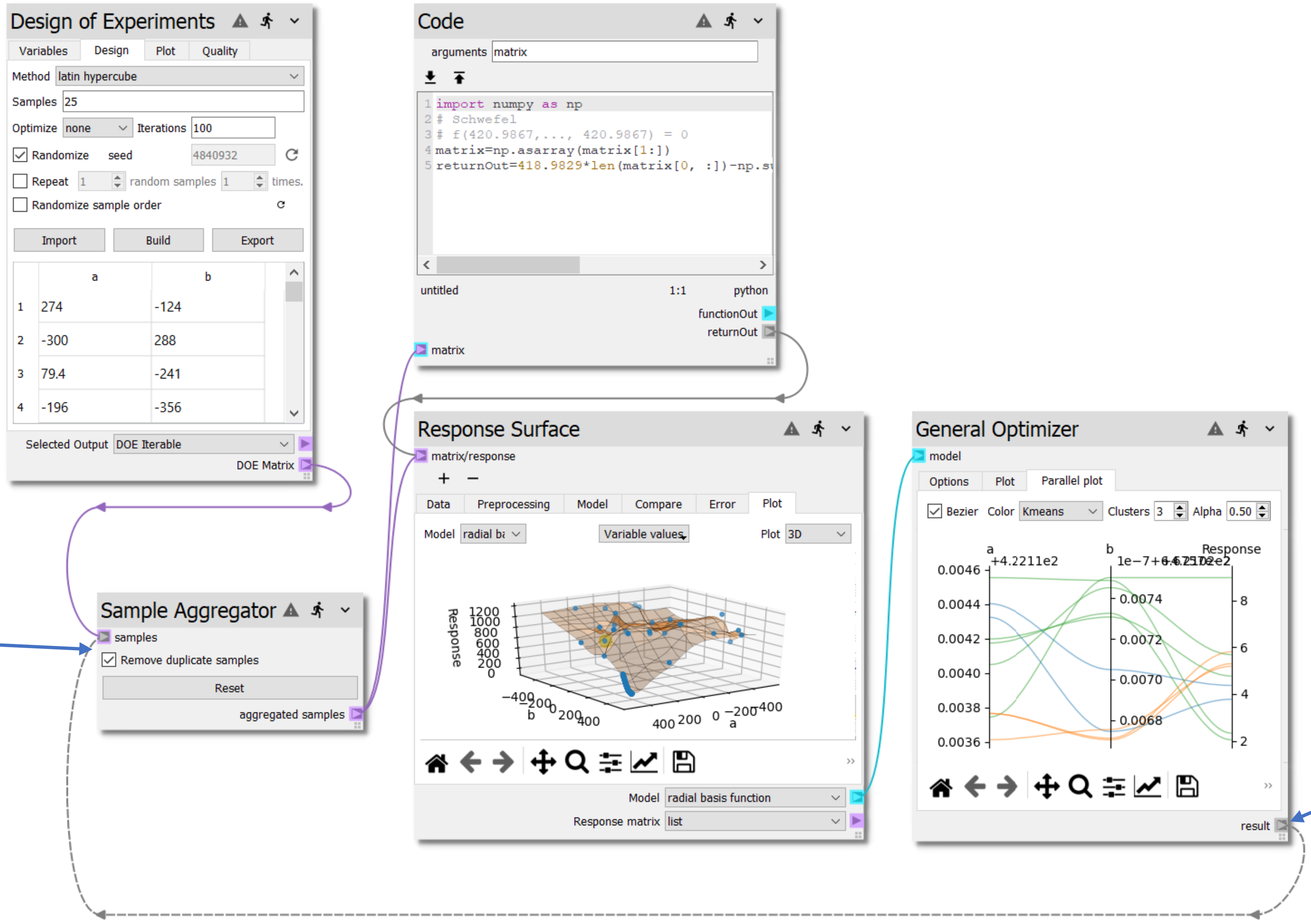


Wizard for Quick Setup of Workflow Templates



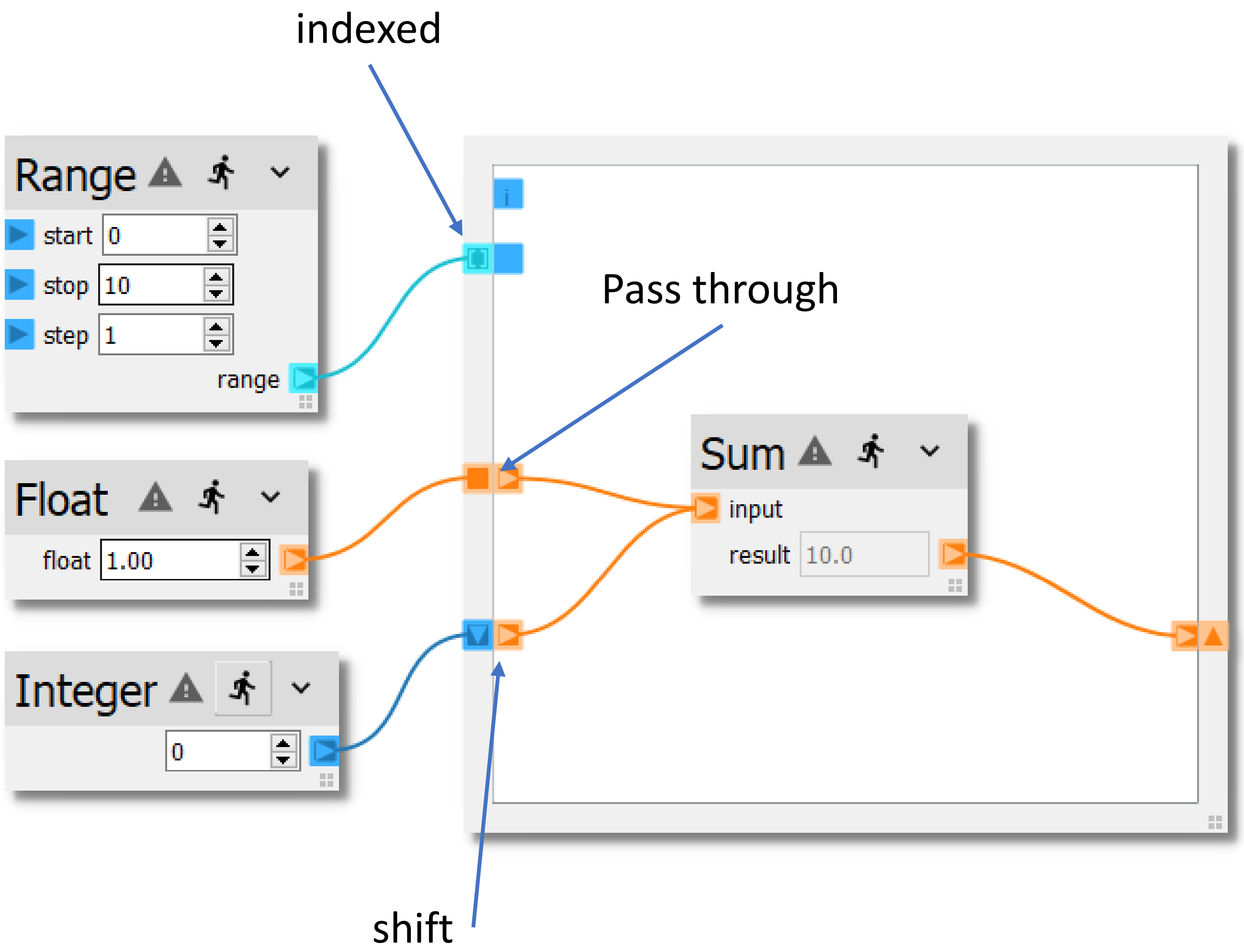
Feedback

Append new samples



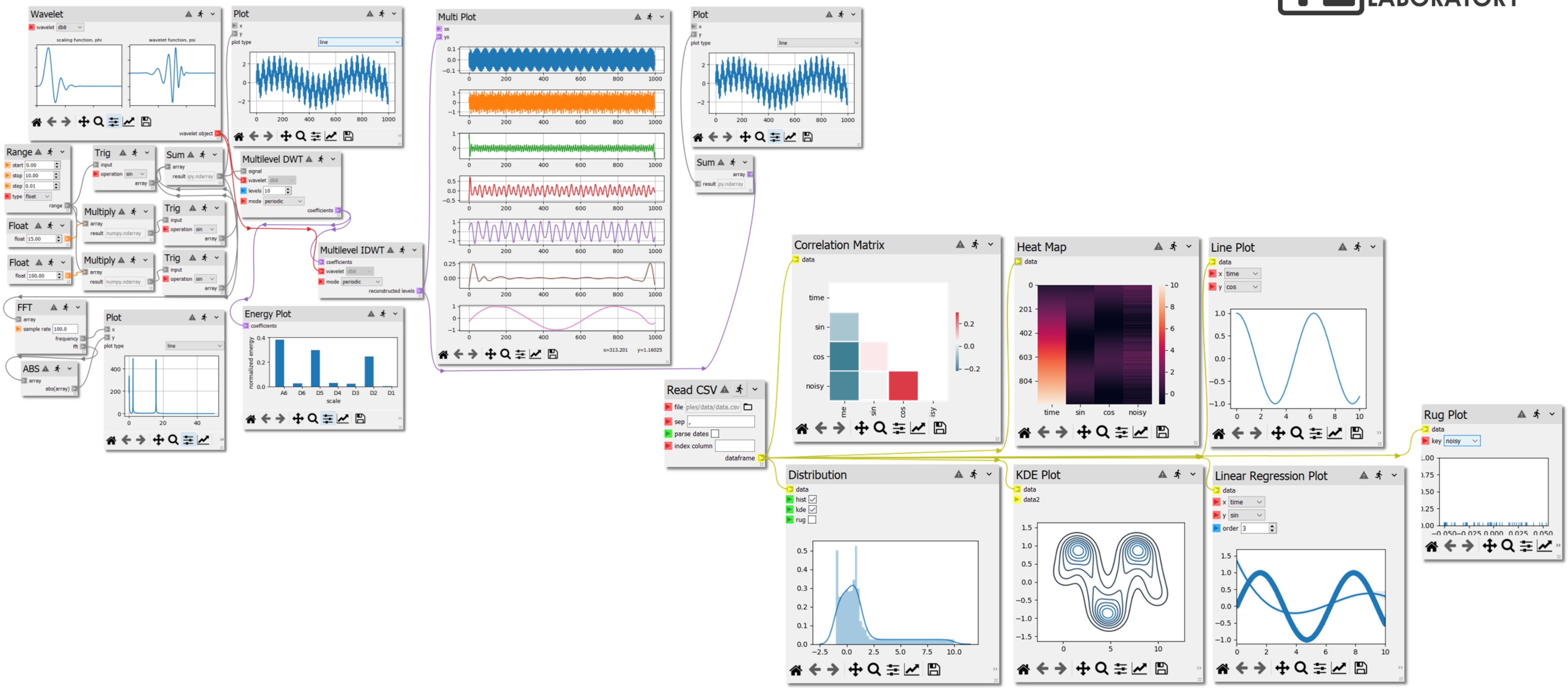
Return "optimal" points for evaluation

Loops



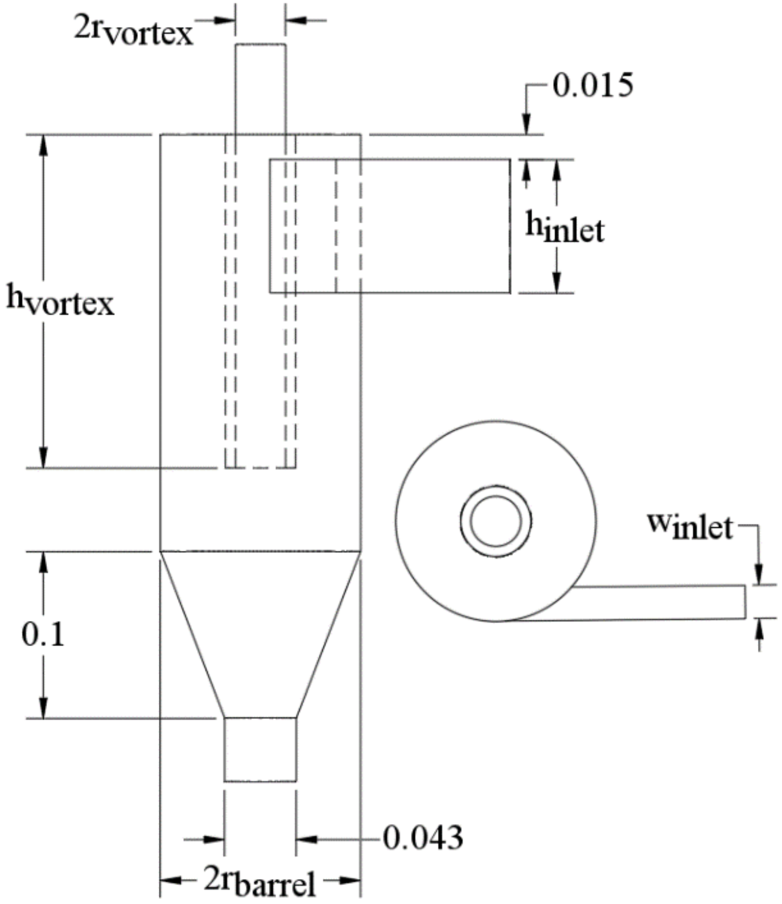
indexed
Pass through
shift
Range
start 0
stop 10
step 1
range
Float
float 1.00
Integer
0
i
Sum
input
result 10.0

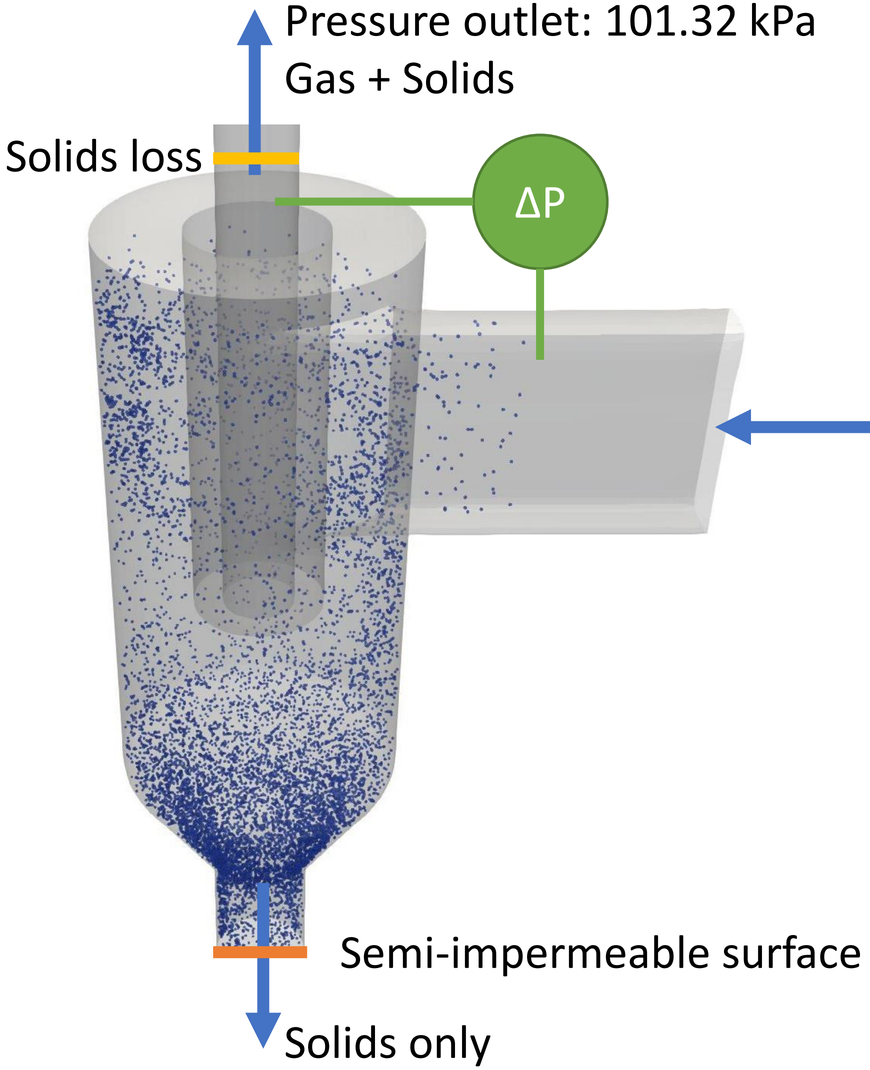
Other nodes


Wavelet
Plot
Multi Plot
Range
Trig
Sum
Multilevel DWT
Float
Multiply
Multilevel IDWT
FFT
ABS
Energy Plot
Read CSV
Correlation Matrix
Heat Map
Line Plot
Rug Plot
Distribution
KDE Plot
Linear Regression Plot

Examples

Example 1 | Cyclone Optimization





Cell size 5 x 5 x 5 mm, uniform

Gas	0.02 kg/s
Solids	0.08 kg/s

HDPE

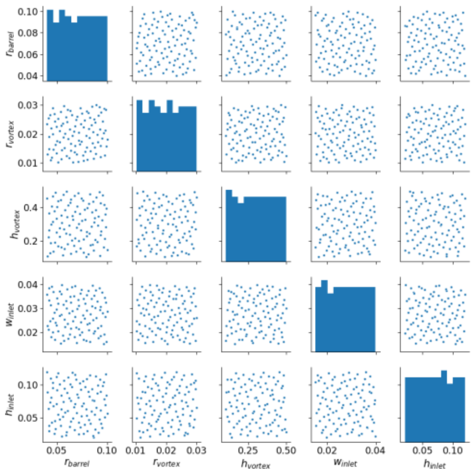
Diameter: 871 μm

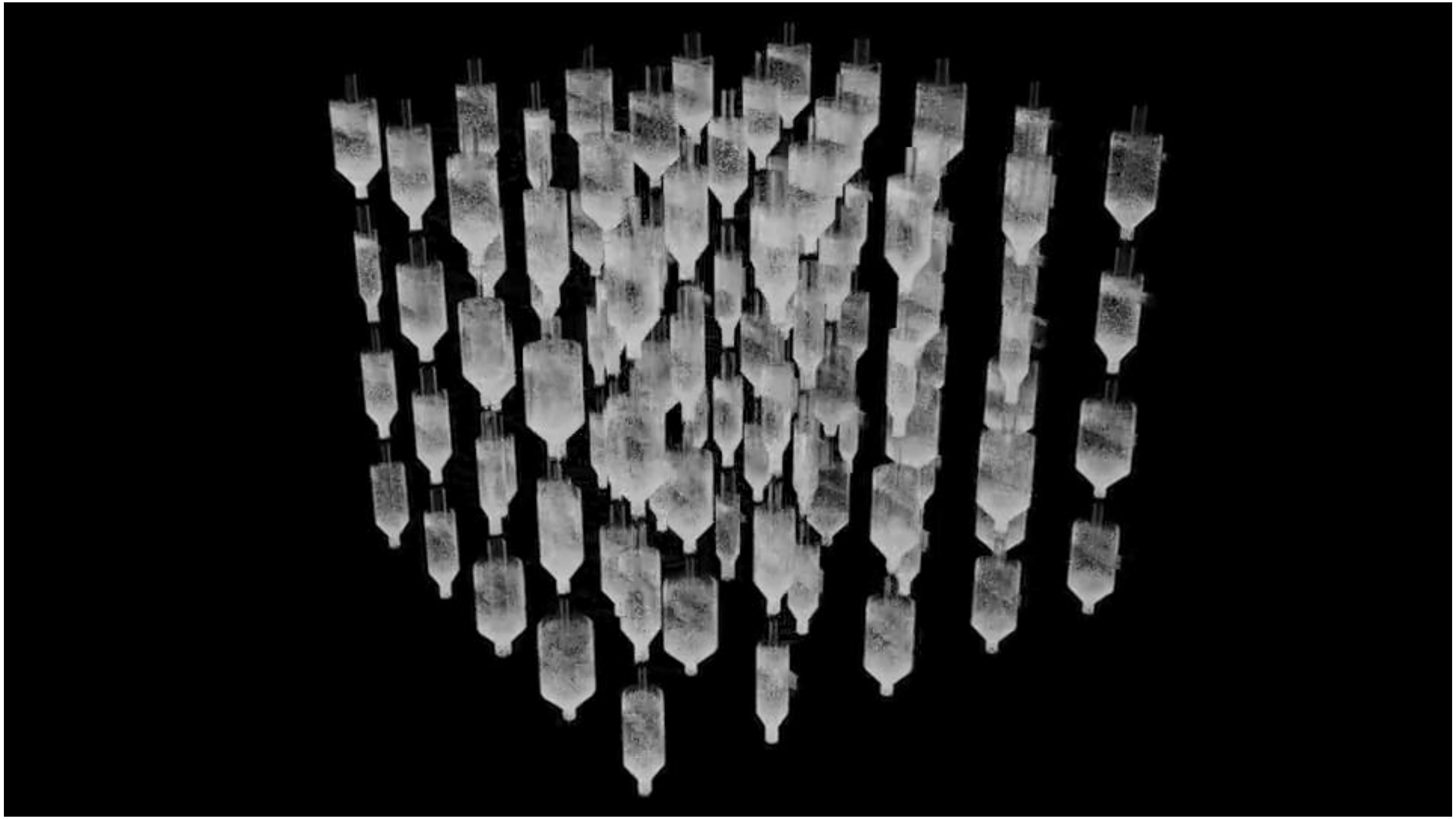
Density: 860 kg/m^3

~1 particles/parcel

Example 1 | Run the models!

- All models ran simultaneously
- Took 21 minutes to 7 hours per model
- Cell count varied from 40,320 to 169,764
- Three models failed (6%), due to bad mesh





Example 1 | Workflow

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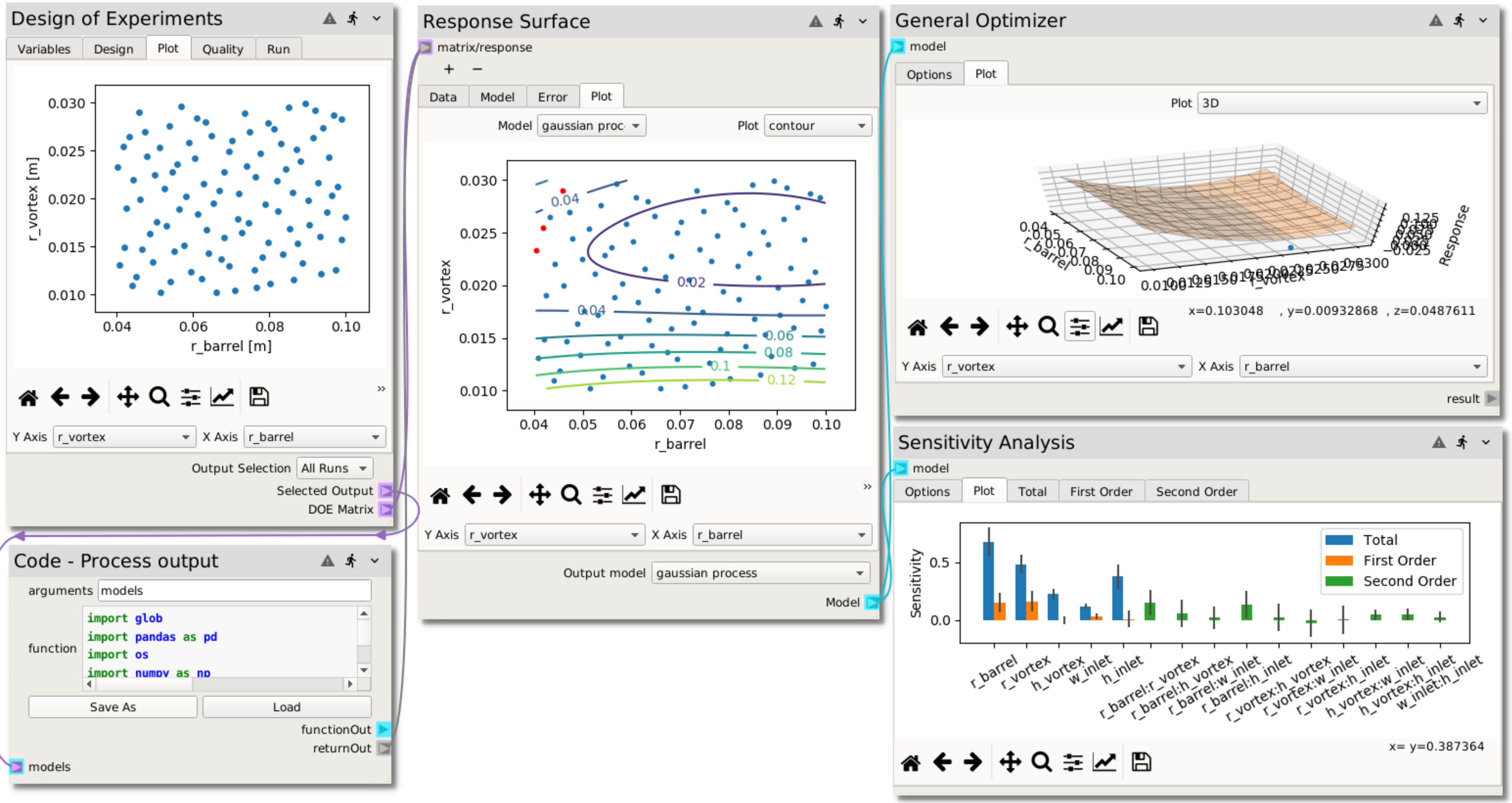
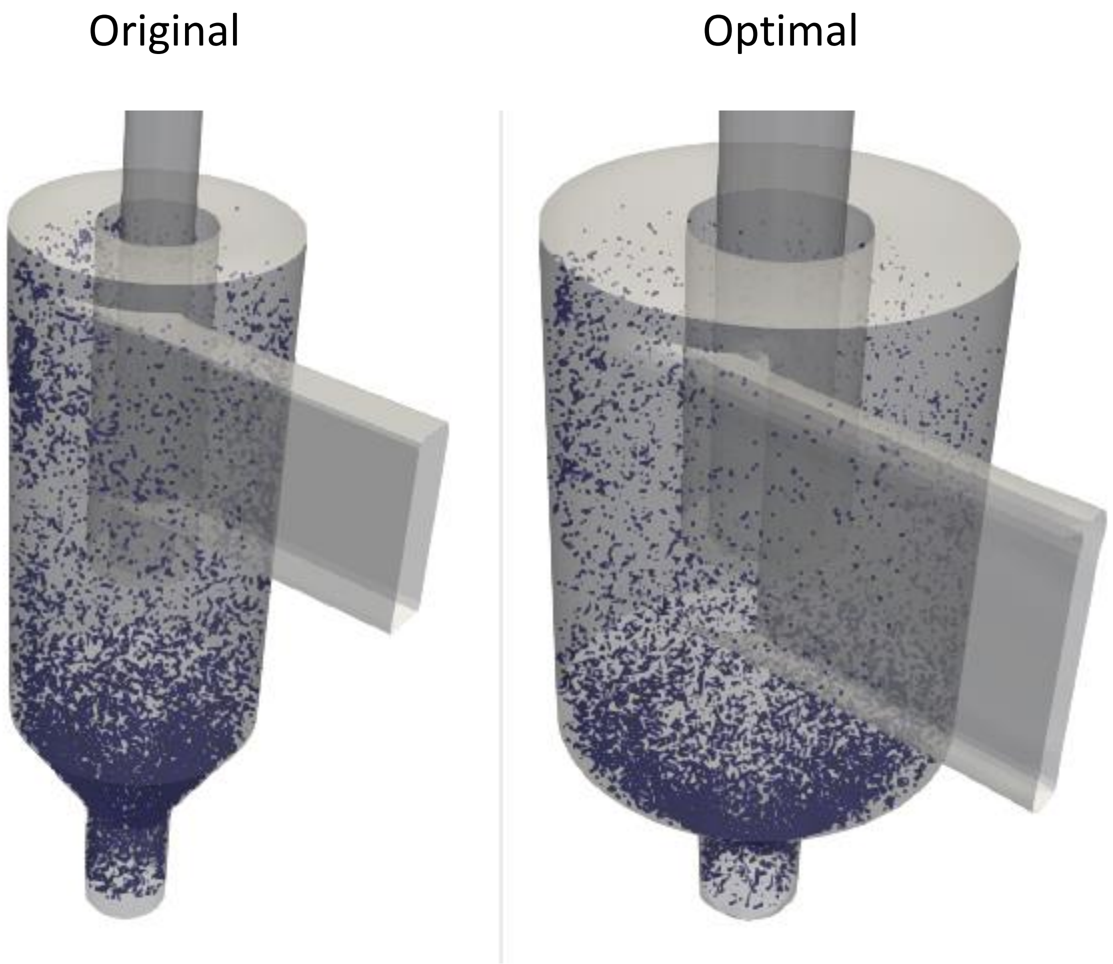


Example 1 | Optimization



Using differential evolution
- 11 times lower pressure drop
- 2.3 times lower mass loss

Variable	Original (m)	Optimal (m)
r_{barrel}	0.06	0.096
r_{vortex}	0.015	0.026
h_{vortex}	0.4	0.373
h_{inlet}	0.08	0.12
w_{inlet}	0.02	0.015

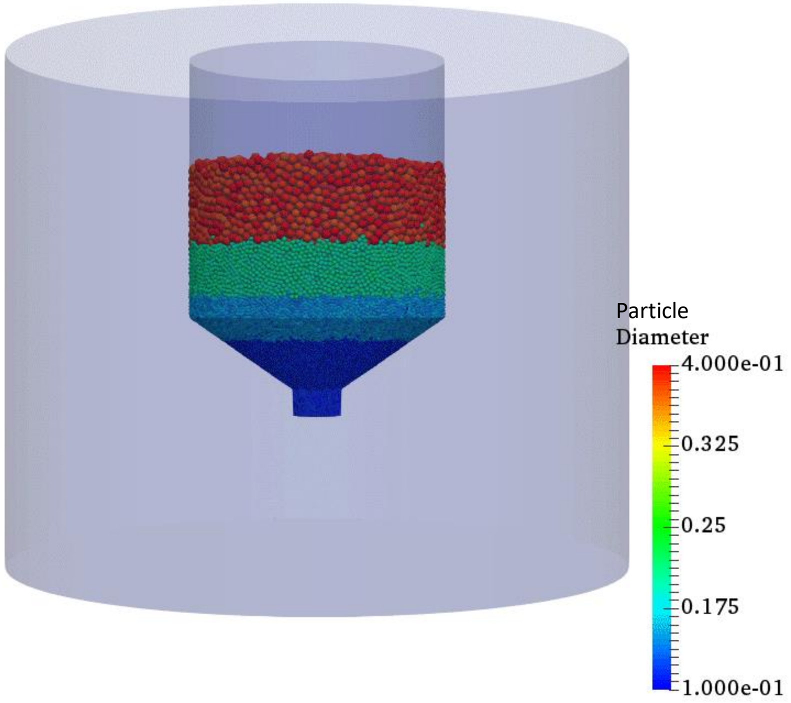
Edge of design space

Example 2 | Hopper Discharge Calibration

- Problem: Discharge of granular materials from a hopper.
- Frequently encountered setup in industrial settings.
- Typically design is based on empirical correlations, which doesn't necessarily always provide robust and efficient designs.
- Accurate modeling & simulation of granular material through Discrete Element Method (DEM) is critical for credible models.
- Use Nodeworks to perform model calibration (deterministic) for four modeling parameters in MFIX-DEM:

θ_1: Particle-Particle Friction Coefficient
θ_2: Particle-Wall Friction Coefficient
θ_3: Particle-Particle Restitution Coefficient
θ_4: Particle-Wall Restitution Coefficient

Example visualization of hopper discharge modeled with MFIX-DEM



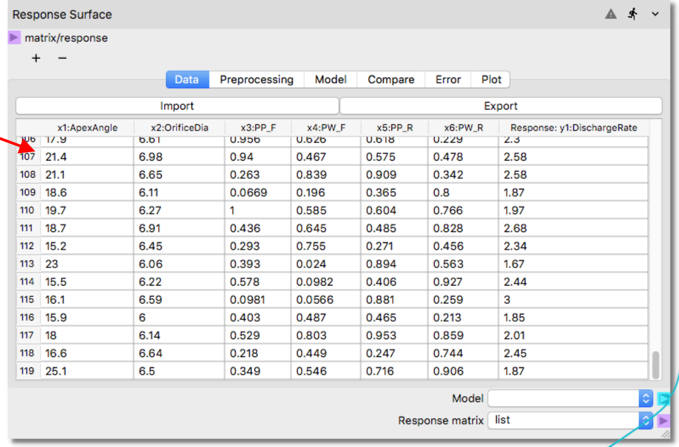
Source: Chen, Adep, Emady, Jiao, and Gel, "Enhancing the physical modeling capability of open-source MFIX-DEM Software for handling particle size polydispersity: Implementation and Validation" Powder Technology, 317 (2017) 117–125 doi: http://dx.doi.org/10.1016/j.powtec.2017.04.055

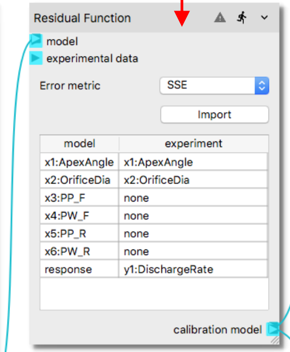
Example 2 | Hopper Discharge Calibration (cont'd)

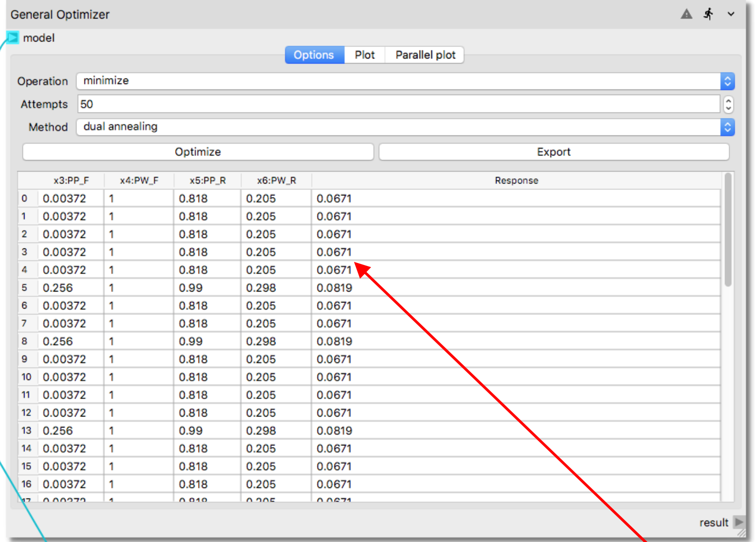
Deterministic Calibration

imports experimental data and evaluates the response surface at each set of model/experimental parameters, calculating a residual metric

.CSV directly imported







120 sample simulation campaign performed externally in batch mode for 7 parameters:

x_1: Apex Angle x_2: Orifice Diameter

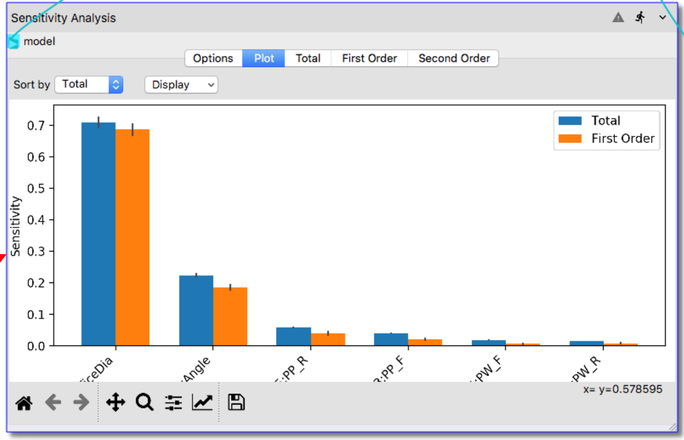
x_3: θ_1: Particle-Particle Friction Coefficient

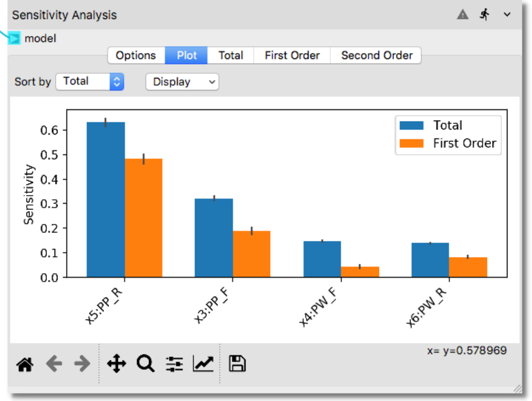
x_4: θ_2: Particle-Wall Friction Coefficient

x_5: θ_3: Particle-Particle Restitution Coefficient

x_6: θ_4: Particle-Wall Restitution Coefficient

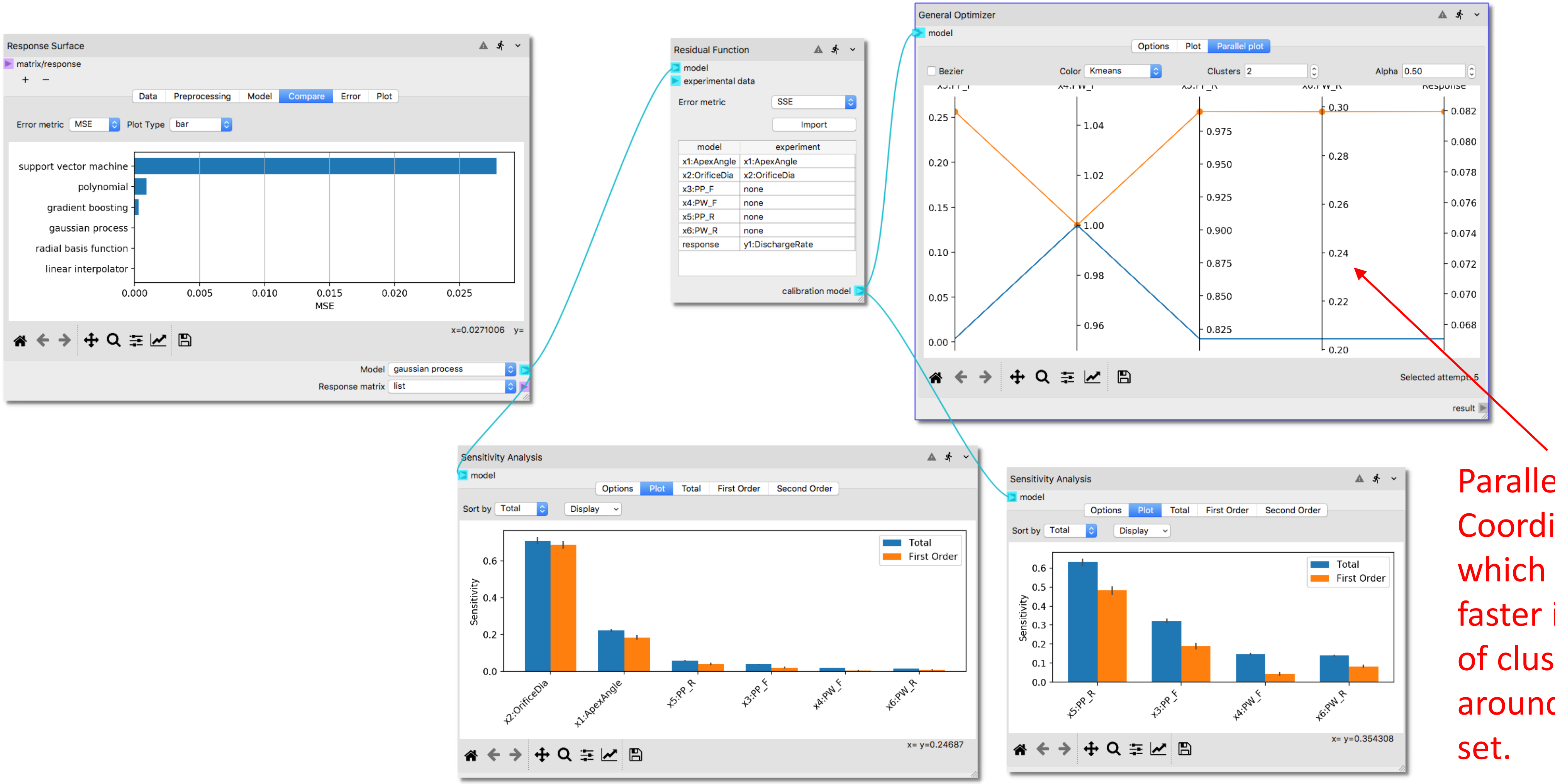
asses the sensitivity of the input parameters based on the simulation campaign results





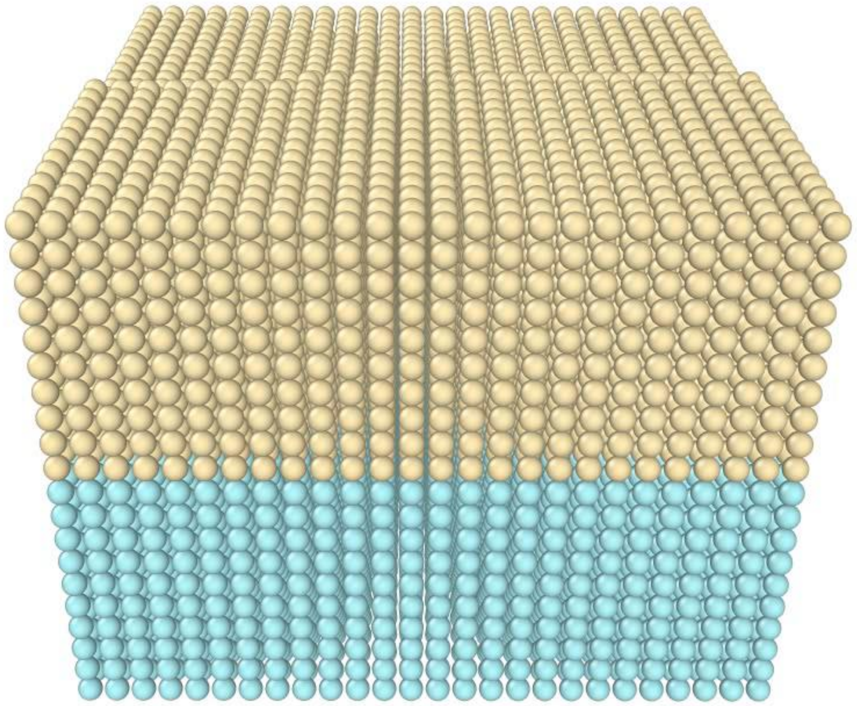
Minimize residual metric with multiple random starts, identifying optimal model inputs.

Example 2 | Hopper Discharge Calibration (cont'd)

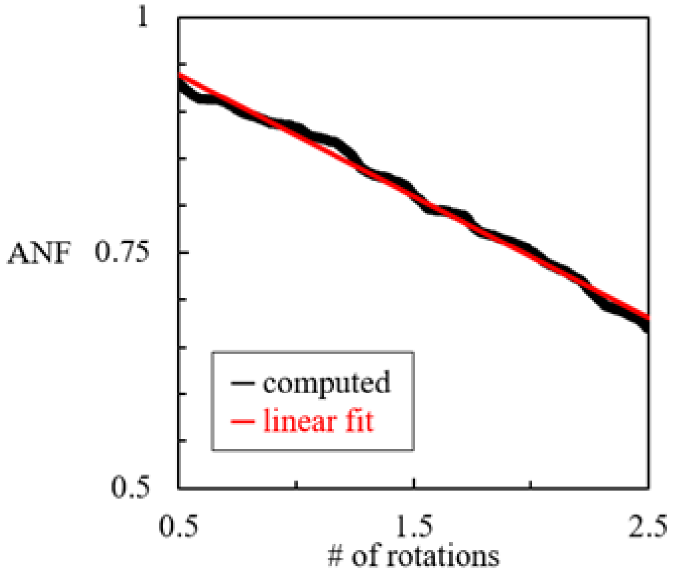


Parallel Coordinates Plot, which enables faster identification of clustering around solution set.

Example 3 | Discrete Element Method Mixing UQ



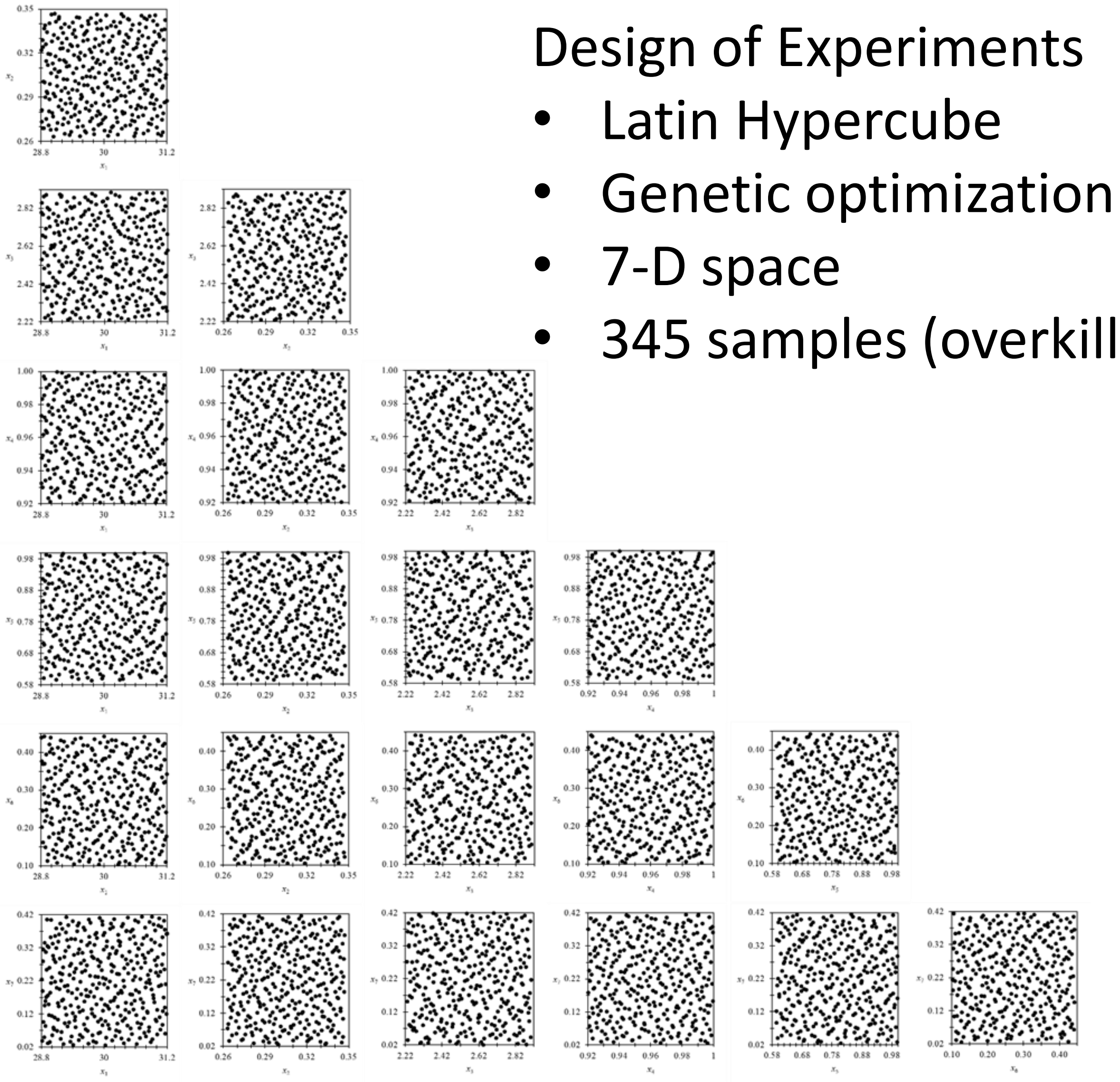
Quantify mixing as the rate of decay of the **A**like **N**eighbor **F**raction (ANF)



ANF = fraction of particles within $2.5r_p$-radius of a given particle with the same color (averaged over all particles)

Source: Fullmer, W. D.; Dahl, S.; Weber, J. *Surrogate Modeling Approach to Uncertainty Quantification for a DEM Model of a Rotating Cubic Tumbler*; NETL-TRS-5-2019; NETL Technical Report Series; U.S. Department of Energy, National Energy Technology Laboratory: Morgantown, WV, 2019, p 24. DOI: 10.18141/1514272.

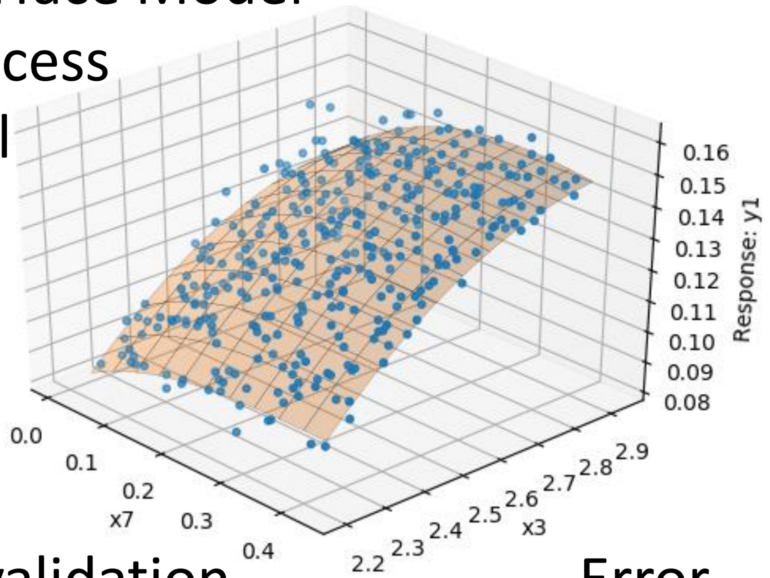
Example 3 | DOE → Simulations → Surrogate



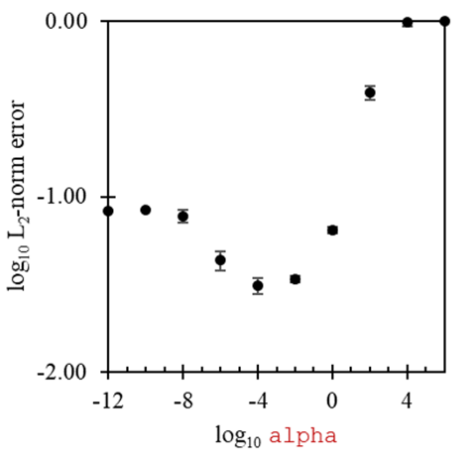
Design of Experiments
- Latin Hypercube
- Genetic optimization
- 7-D space
- 345 samples (overkill?)

Response Surface Model

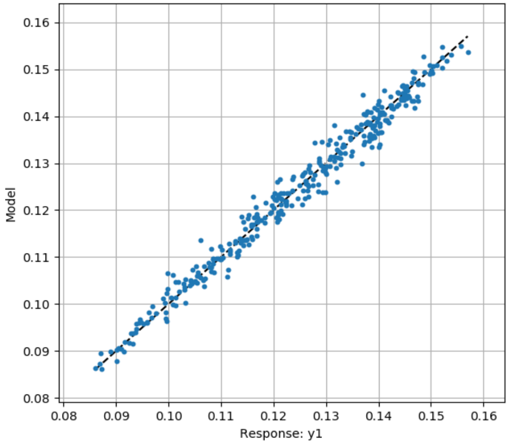
Gaussian Process
- RBF kernel



Cross-validation

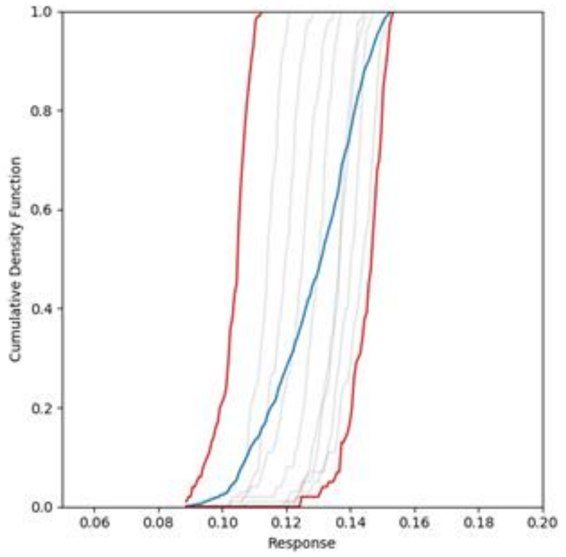


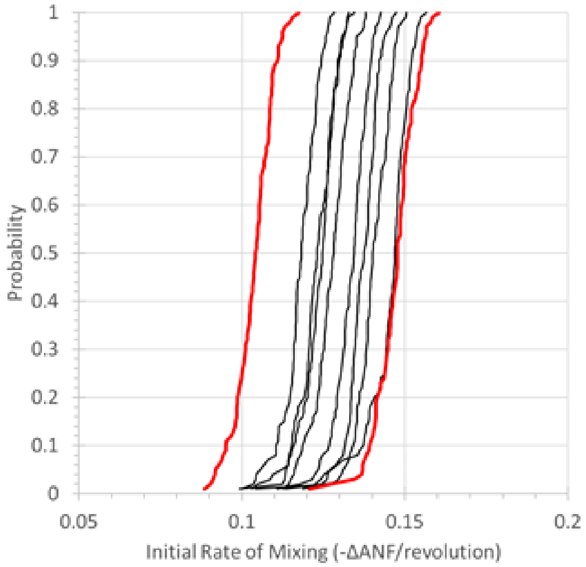
Error

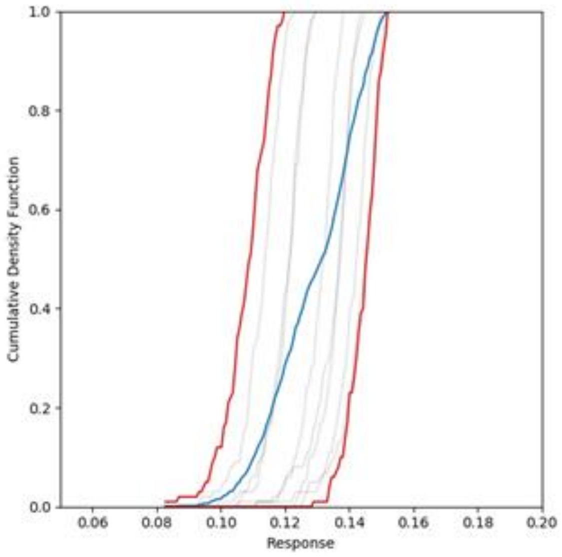


Example 3 | Forward Propagation

Hybrid/nested sampling approach of Roy & Obekampf
10 epistemic samples, each with 100 aleatory samples





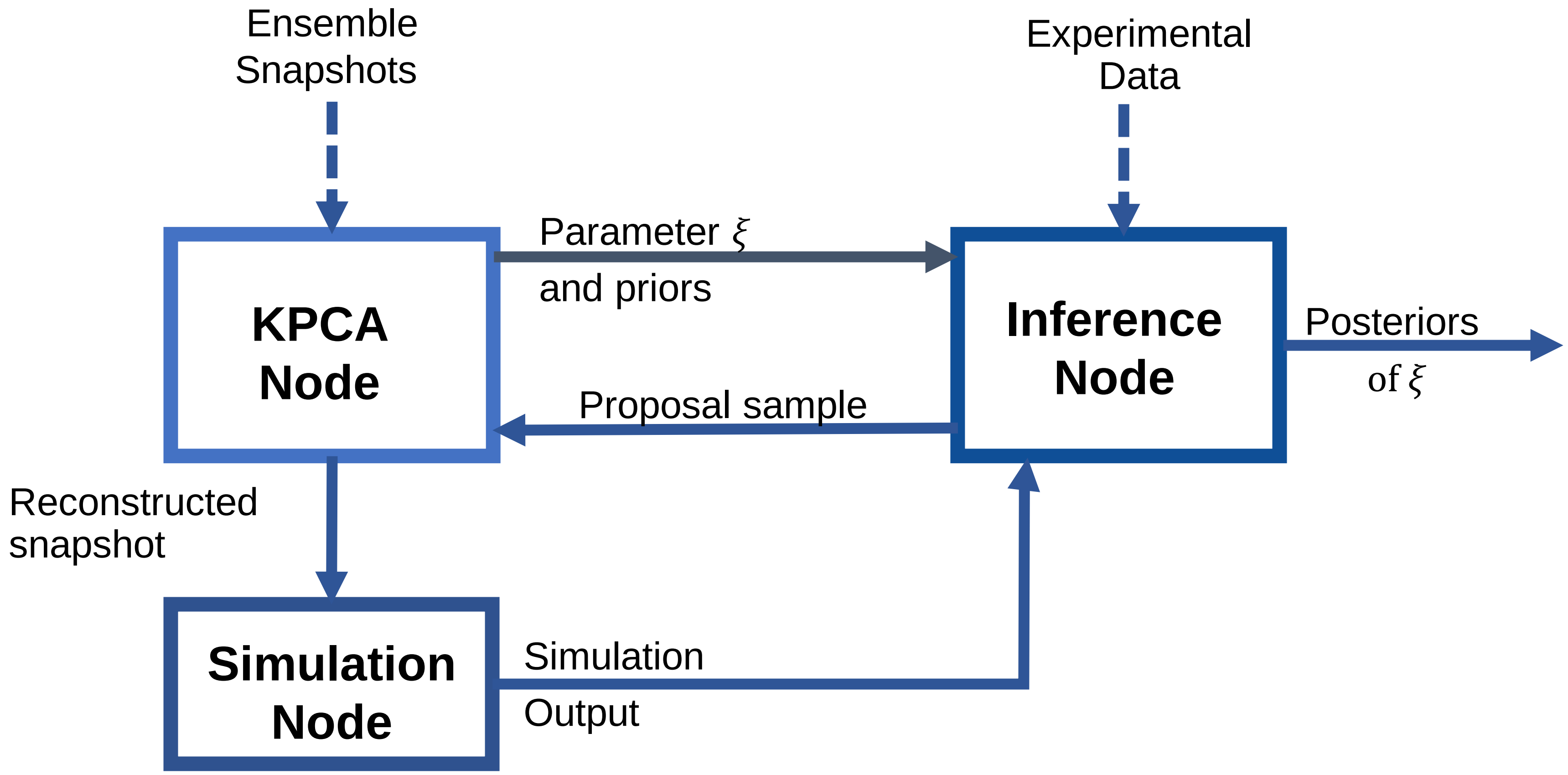


1000 CFD runs

Original direct sample p-box of Dahl et al (2019)

Examples of surrogate model propagated p-boxes

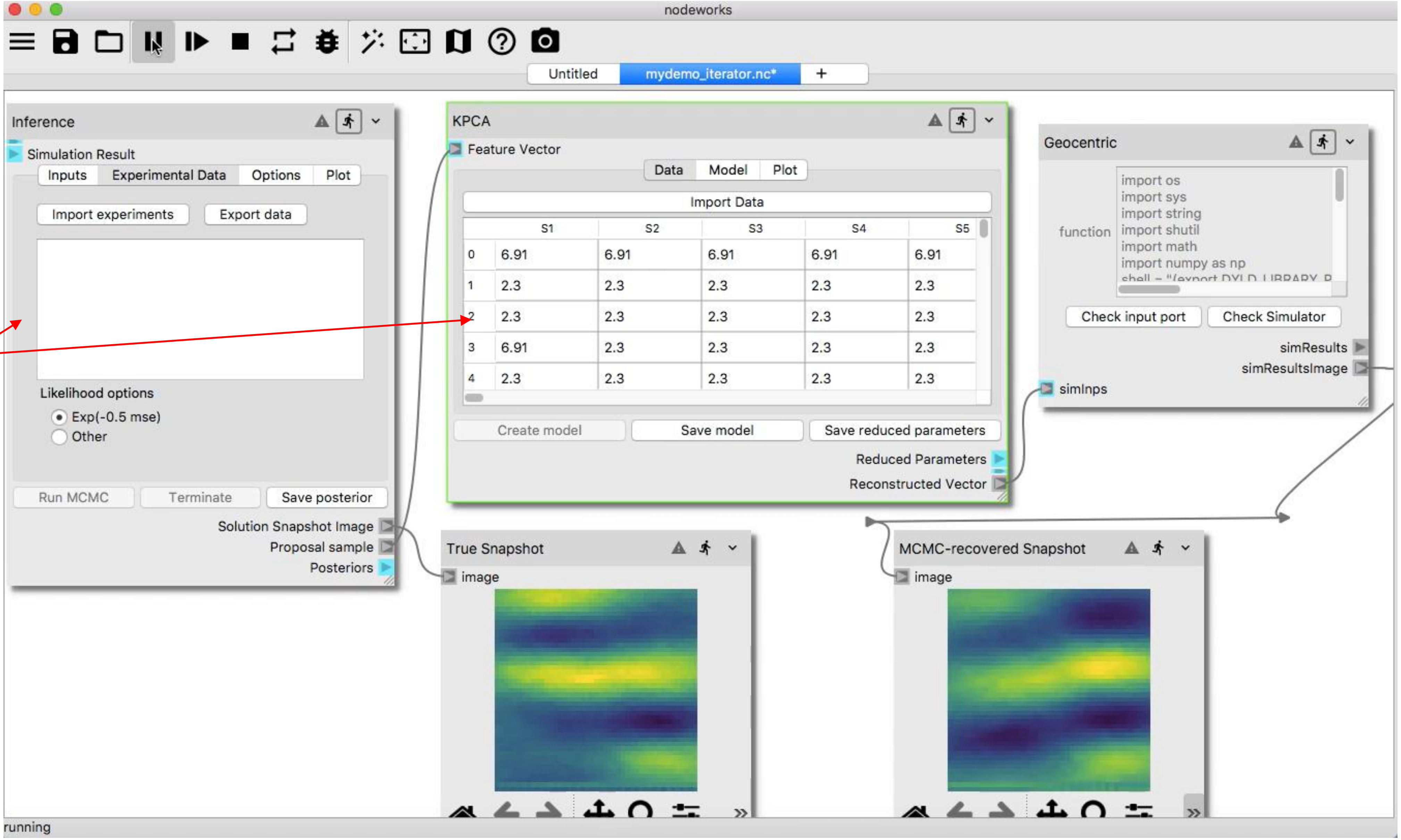
Example 4 | Stochastic Source Inversion (use case @LLNL)



- Simulation: linear elasticity in 2D
- Uncertain inputs: shear and Young's modulus (location-dependent: dimension=4050)
- Scenario: Given an observation strain tensor, recover the shear and Young's modulus
- Method: KPCA for dimension reduction + MCMC for inference

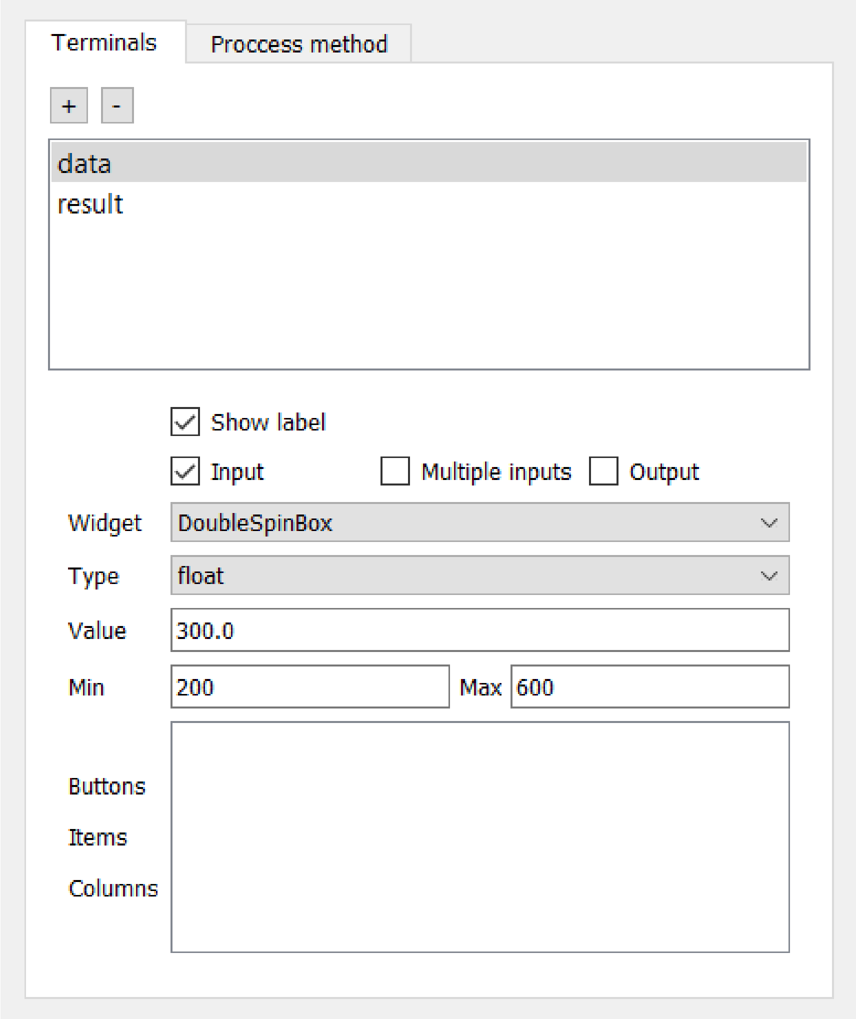
Example 4 | Stochastic Source Inversion

New customized nodes have been developed to encoding, inference, and decoding. Some of these tasks are performed by PSUADE behind the scenes though the interface.



What is in the future?

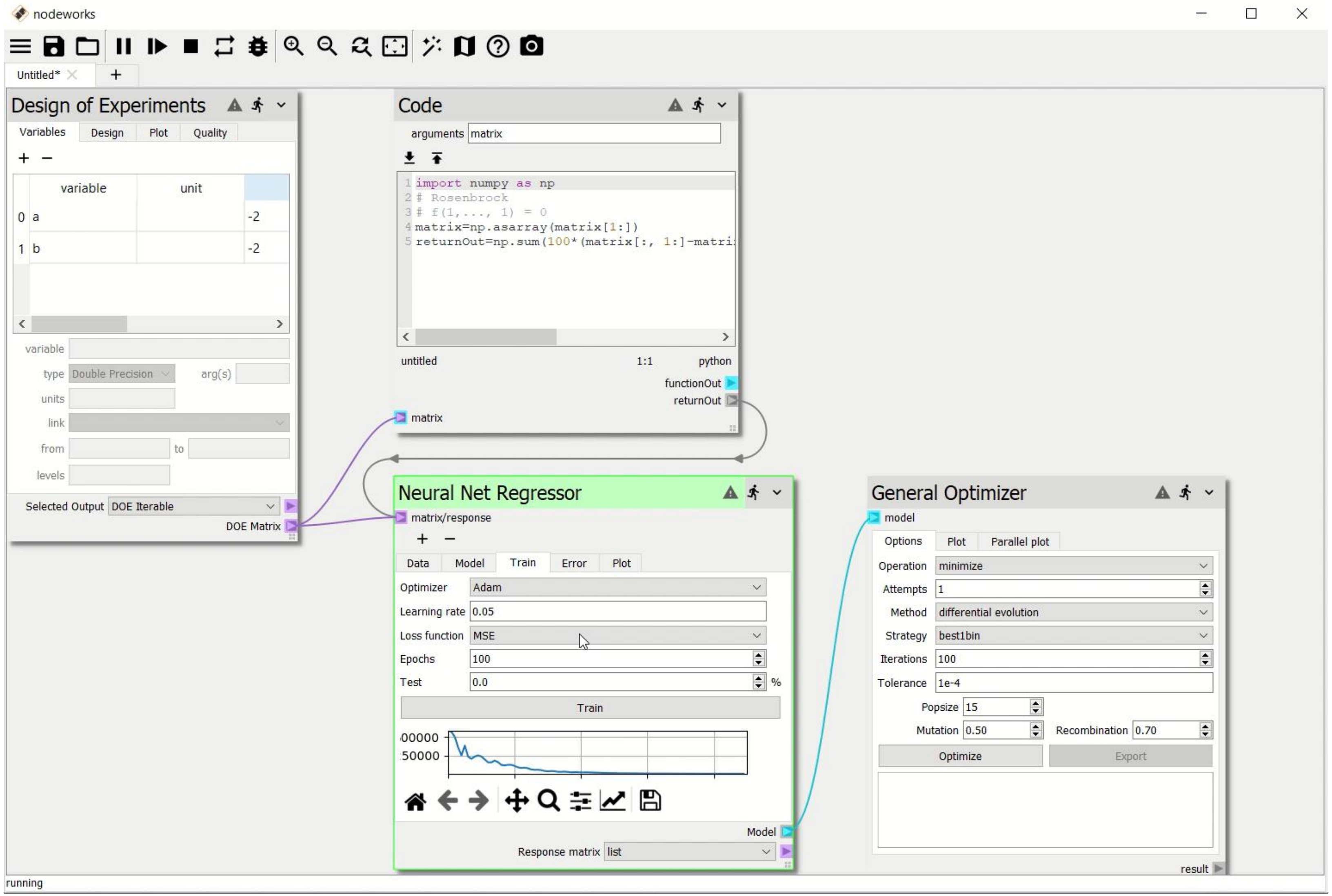
- Better support for feedback loops
- Add more nodes for machine learning workflows
- Build a node creator
- Look into better dispatch tools
    - Cloud/local/HPC
- Better integration with other UQ tools
- Export workflows
- Automatic report generation



Thanks!

Website
mfix.netl.doe.gov/nodeworks/

Questions?



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