Calibration of a Particle-In-Cell Simulation Model for Gravitational Settling Bed Application

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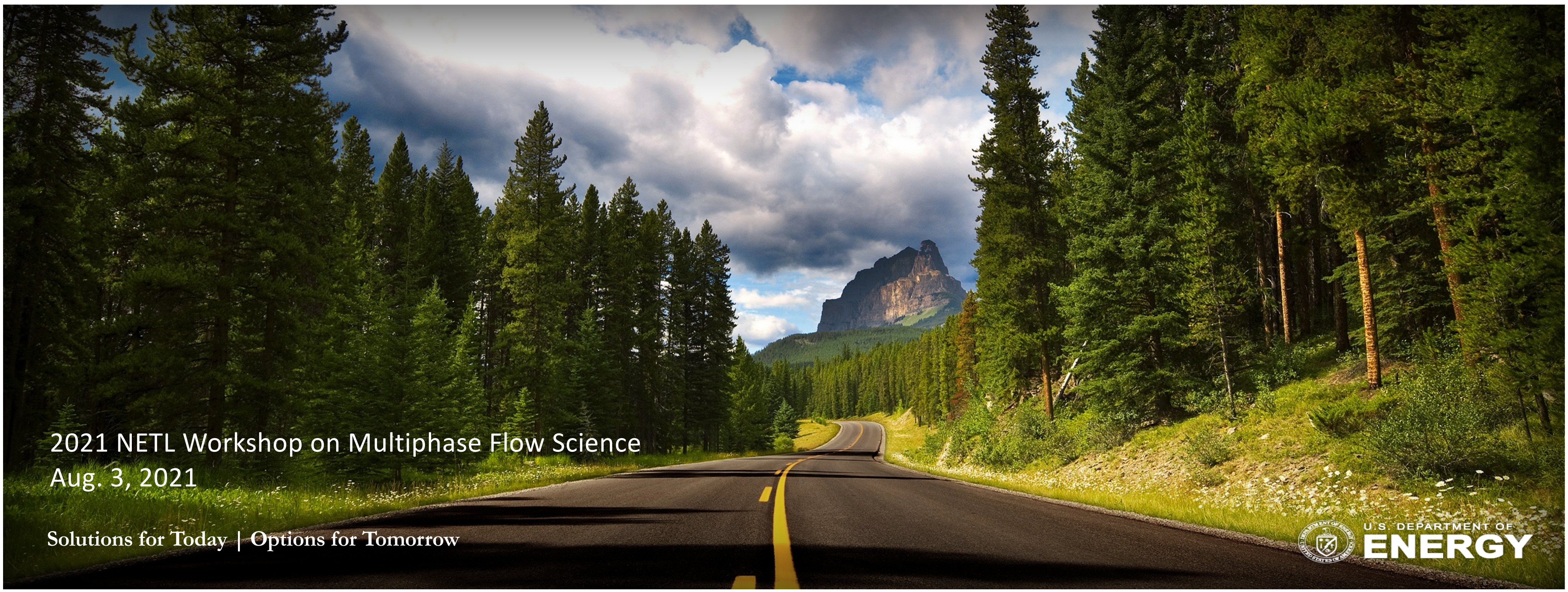

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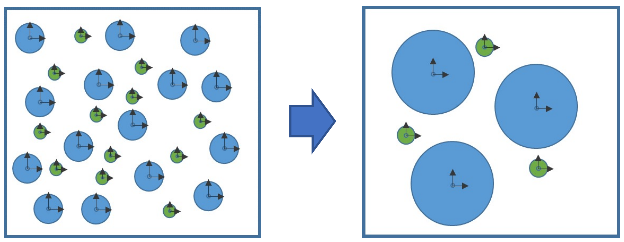
Outline

- Brief Overview of MFiX-PIC
- Representative Problems for the Calibration Study
- Brief Overview of Calibration Methods
- Simulation Campaigns to Construct Surrogate Models
- Assessment of Deterministic Calibration Results
- Concluding Remarks

Brief Overview of MFiX-PIC

Concept: When particles are of equal physical property, they can be grouped together as larger parcels. Multiple particle types can be managed as separate parcel distributions.

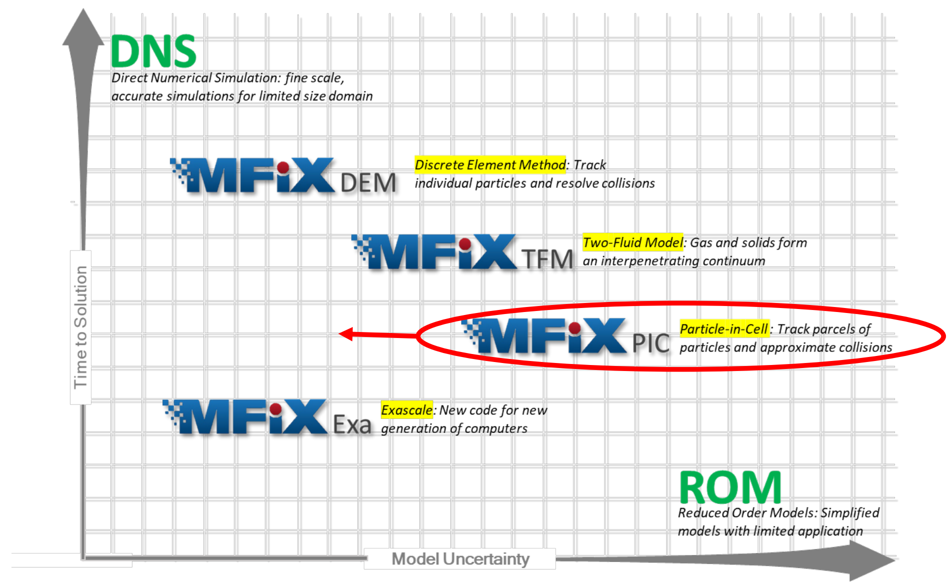


Instead of managing each particle with Newtonian physics, parcel motion is influenced by a collisional stress model.

$$\frac{d\overrightarrow{V_p}}{dt} = \beta\left(\overrightarrow{U_g} - \overrightarrow{V_p}\right) - \frac{1}{\rho_p}\nabla p - \frac{1}{\epsilon_p \rho_p}\nabla \tau_p + \vec{g}$$

$$\tau_p = \frac{P_p \epsilon_p^{\gamma}}{\max\left(\epsilon_{cp} - \epsilon_p, \delta(1 - \epsilon_p)\right)}$$

Solids stress



A reduced computational load allows the simulations to proceed very rapidly. Lagrange tracking of parcels results in excellent visual graphics of statistically weighted particle motion.

Representative Problems for the Calibration Study

- **Cases selected to cover a broad range of flow conditions**
  - Particle Settling: $U/U_{mf} < 1.0$ ($P_0 \sim 1$) (Simulation campaign)
  - Bubbling Fluidized bed: $U/U_{mf} \sim 1$ ($P_0 \sim 10$)
  - Circulating Fluidized bed: $U/U_{mf} >> 1.0$ ($P_0 \sim 100$)

Parcel momentum equation

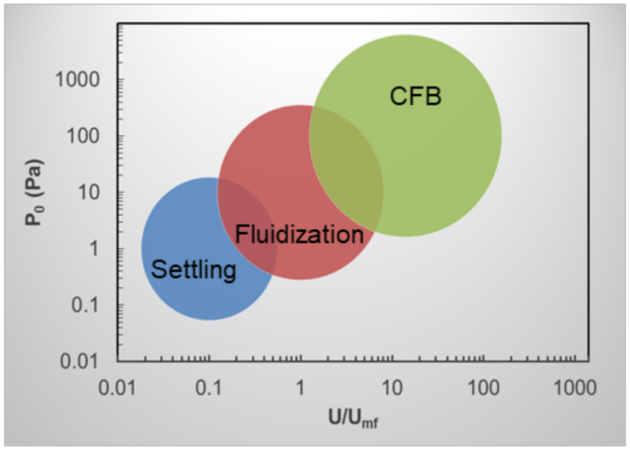
$$\frac{d\vec{V_p}}{dt} = \beta\left(\vec{U_g} - \vec{V_p}\right) - \frac{1}{\rho_p}\nabla p - \frac{1}{\varepsilon_p \rho_p}\nabla \tau_p + \vec{g}$$

$$\tau_p = \frac{P_0 \varepsilon_p^{\beta}}{\max\left(\varepsilon_{cp} - \varepsilon_p, \delta(1 - \varepsilon_p)\right)}$$

- **Summary of model parameters used:**

	t1 Pressure linear scale factor	t2 Volume fraction exponential scale factor	t3 Statistical weight	t4 Volume fraction at maximum packing	t5 Solid slip velocity factor
C1: Particle Settling	[1,20]	[2,5]	[3,20]	[0.35,0.5]	[0.5,1.0]
C2: Fluidization	[1,100]	[2,5]	[10,100]	[0.4,0.5]	[0.85,0.98]
C3: Circulating Fluidized Bed	[1,250]	[2,5]	[4]	[0.4,0.5]	[0.85,0.98]

*Parameters selected based on prior sensitivity study



Hypothetical flow regime map

C1: Particle settling

Problem setup

Control variable: Initial solids concentration
Range: [0.05,0.25]

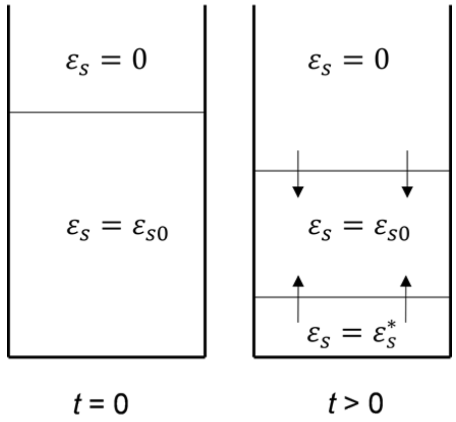
	x1: Initial solids concentration
C1: Particle Settling	[0.05,0.25]

Response variable: Location of filling shock (y2)
CFD results are compared with analytical solutions

Control variables: CFD (PIC parameters)

	t1 or (θ_1): Pressure linear scale factor	t2 or (θ_2): Vol. fraction exponential scale factor	t3 or (θ_3): Statistical weight	t4 or (θ_4): Vol. fraction at maximum packing	t5 or (θ_5): Solid slip velocity factor
C1: Particle Settling	[0.48* , 20]	[2 , 5]	[2.96* , 20]	[0.35* , 0.5]	[0.5 , 1.0]

* Initial targeted lower bound might be slightly different than actual samples generated as part of Latin Hypercube sampling



Analytical Solution:

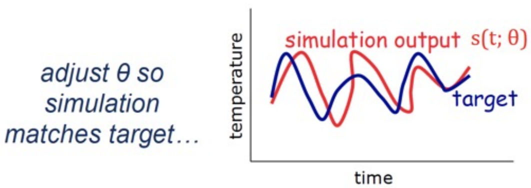
Location of shock $x(t) = -t\left(\frac{\varepsilon_s^* \varepsilon_g^* u_r^* - \varepsilon_{s0}\varepsilon_{g0}u_{r0}}{\varepsilon_s^* - \varepsilon_{s0}}\right)$

Rel. velocity (Stokes' drag) $u_r = \frac{g\Delta\rho d_p^2}{18\mu_g}\varepsilon_g^{3.65}$

Brief Overview of Calibration Methods

Deterministic versus Statistical Calibration

- Maximize agreement between simulation and experiment target by improving the characterization of model parameters, θ_i (e.g., P_0, β) using available data.



- Also known as parameter estimation /identification, inverse problem modeling
- Calibration ≠ validation

Source: DAKOTA Software Training: Model Calibration (SAND2015-6813PE)

Two approaches:

- Deterministic Calibration:
  - Framed as minimization problem that seeks one or more sets of parameter values that reduce the error between simulation ($s_i(\boldsymbol{\theta})$) and data y_i, typically in a norm:

$$\min_{\theta} f(\theta) = SSE(\boldsymbol{\theta}) = \sum_{i=1}^{n}[(s_i(\boldsymbol{\theta}) - y_i]^2 = \sum_{i=1}^{n}[r_i(\boldsymbol{\theta})]^2$$

  - Available in UQ software: DAKOTA (SNL), PSUADE (LLNL), OpenTURNS (Airbus+ONERA), Nodeworks (NETL) with some modifications
- Statistical calibration (Bayesian):
  - Instead of standalone parameter values, it seeks a statistical characterization of parameters most consistent with the data.
  - Available in UQ Software: PSUADE (LLNL), DAKOTA (SNL), OT, GPM/SA & SEPIA (LANL)

Deterministic Calibration Procedure

Calibration Proposed Settings for Model Parameters

- Utilize the constructed surrogate model and the set of analytical solutions (used in lieu of experiments) to perform the deterministic calibration.

- Deterministic calibration problem can be reframed as a minimization problem, i. e.,
- find a set of theta values that minimizes the residuals for all experiment data points

Analytical solution

$$\min_{\theta} f(\theta) = SSE(\boldsymbol{\theta}) = \sum_{i=1}^{n} [(s_i(\boldsymbol{\theta}) - y_i]^2 = \sum_{i=1}^{n} [r_i(\boldsymbol{\theta})]^2$$

Surrogate model evaluation for any given $\theta_{1...}\theta_5$ values

- Utilized PSUADE and DAKOTA UQ toolkits to perform the optimization.
- Recently implemented the workflow in Nodeworks

Deterministic Calibration Procedure

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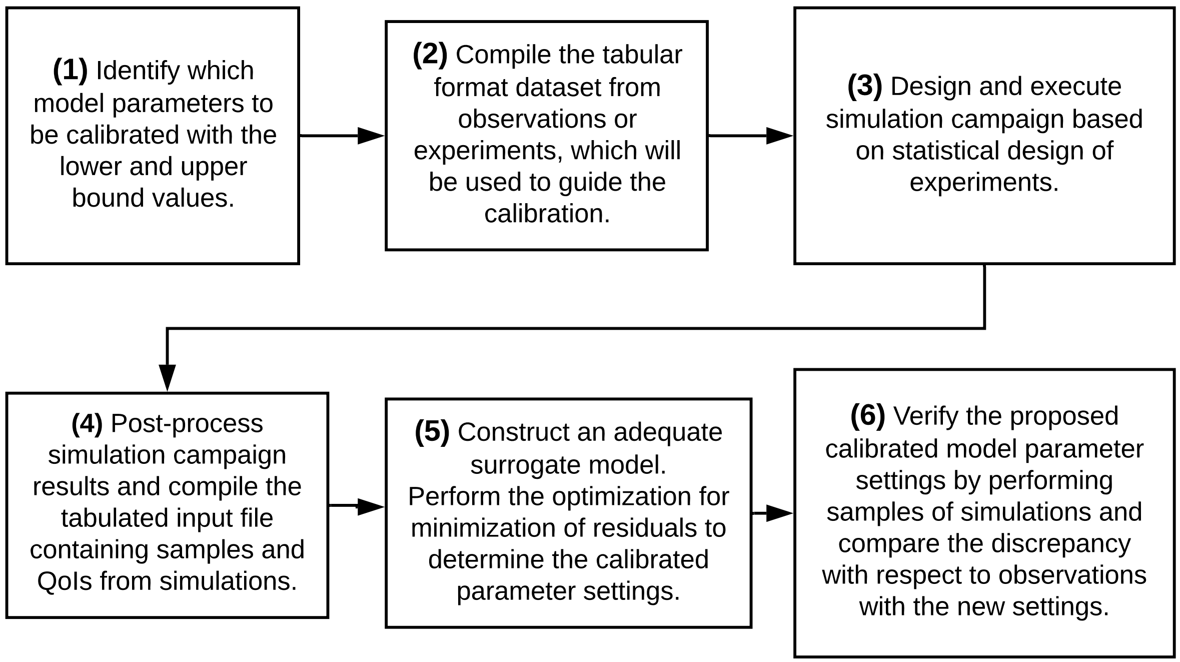
Workflow



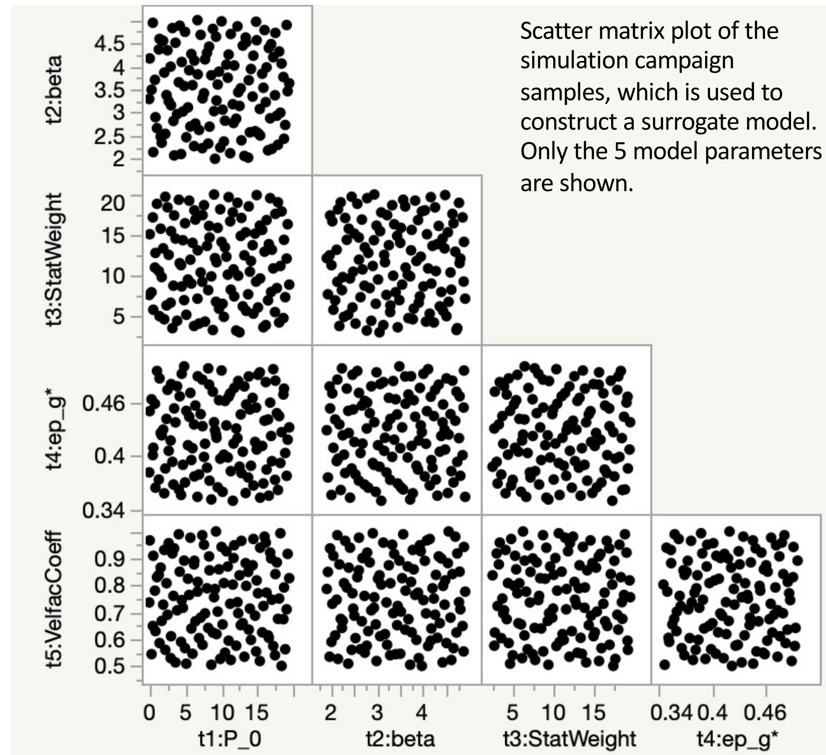
- Multiple step workflow followed for deterministic calibration procedure
- Design of the simulation campaign in Step (3) was carried out with Nodeworks, simulations were performed with MFiX-PIC on Joule 2.0
- Step (5) was performed with PSUADE, DAKOTA and Nodeworks by providing the same tabulated file that contains simulation campaign input and responses.

C1: Particle Settling Simulation Campaigns

Construct Surrogate Model from Simulation Campaign (120 samples)

	min	0.488	2.000	2.964	0.350	0.501	0.050
	max	20.000	5.000	20.008	0.500	1.000	0.250
		Uncertain Input Parameters/Factors:					
Phases	MFIX-PIC	θ_1	$\theta 2$	θ_3	θ_4	θ_5	X_1
	Simulation Number	Emp.Pres. Constant	Vol. Fraction Exp. Scale Factor	Stat. Weight	Void Fraction at max packing	Solid slip velocity factor	Initial solids concentration
	1	4.375	2.965	4.388	0.478	0.707	0.243
	2	17.049	2.182	6.917	0.441	0.614	0.246
	3	3.860	2.817	8.729	0.368	0.761	0.128
	4	19.782	3.462	16.329	0.418	0.917	0.079
	5	1.572	2.662	18.853	0.495	0.830	0.098
	6	9.356	4.811	3.246	0.472	0.625	0.106
	7	4.613	3.656	19.361	0.363	0.990	0.173
	8	8.892	2.695	14.690	0.372	0.856	0.136
	9	15.462	4.566	19.936	0.407	0.818	0.075
	10	9.795	4.642	6.737	0.424	1.000	0.130
	11	14.360	3.700	18.536	0.489	0.636	0.089
	12	3.531	3.157	15.467	0.480	0.611	0.074
	13	18.016	3.374	5.465	0.373	0.541	0.157
	14	3.201	3.244	12.546	0.406	0.956	0.107
	15	11.773	2.120	16.688	0.470	0.732	0.132
	16	17.773	4.197	10.865	0.497	0.575	0.061
	17	12.139	3.181	17.799	0.350	0.803	0.154
	18	10.386	2.243	18.177	0.397	0.527	0.179
	19	6.361	4.267	8.992	0.395	0.640	0.137
	20	1.927	4.594	4.961	0.486	0.586	0.167
	21	7.923	3.308	17.454	0.433	0.579	0.095
	22	13.928	4.625	15.328	0.359	0.882	0.244
	23	2.432	4.554	13.349	0.429	0.728	0.239
	24	10.716	3.062	6.490	0.360	0.655	0.084
	25	15.648	2.557	6.035	0.490	0.771	0.110
	26	1.282	3.708	10.969	0.458	0.780	0.198
	27	3.034	4.347	18.420	0.474	0.691	0.183
	28	14.002	4.521	5.618	0.457	0.798	0.053
	29	6.734	2.274	3.743	0.435	0.878	0.102
	30	6.781	4.125	18.047	0.377	0.891	0.111
	31	14.277	2.025	7.665	0.376	0.850	0.190
	32	15.903	3.078	16.156	0.493	0.519	0.219
	33	17.346	2.876	19.556	0.459	0.921	0.126
	34	19.639	4.896	12.084	0.378	0.711	0.170
	35	18.600	4.322	4.181	0.444	0.751	0.152
	36	10.571	4.975	14.150	0.495	0.943	0.157
	37	12.609	2.867	3.183	0.431	0.576	0.174
	38	0.488	3.294	7.583	0.382	0.737	0.212
	39	5.184	3.023	14.355	0.390	0.717	0.058
	40	0.563	4.171	15.091	0.450	0.967	0.144
	41	2.085	2.477	15.783	0.426	0.866	0.205
	42	10.212	3.885	5.890	0.462	0.859	0.249

(a) Design of experiments matrix (first 42 out of 120 samples shown)



(b) Scatter matrix plot of the simulation campaign input dataset

Optimal Latin Hypercube Sampling based Simulation Campaign

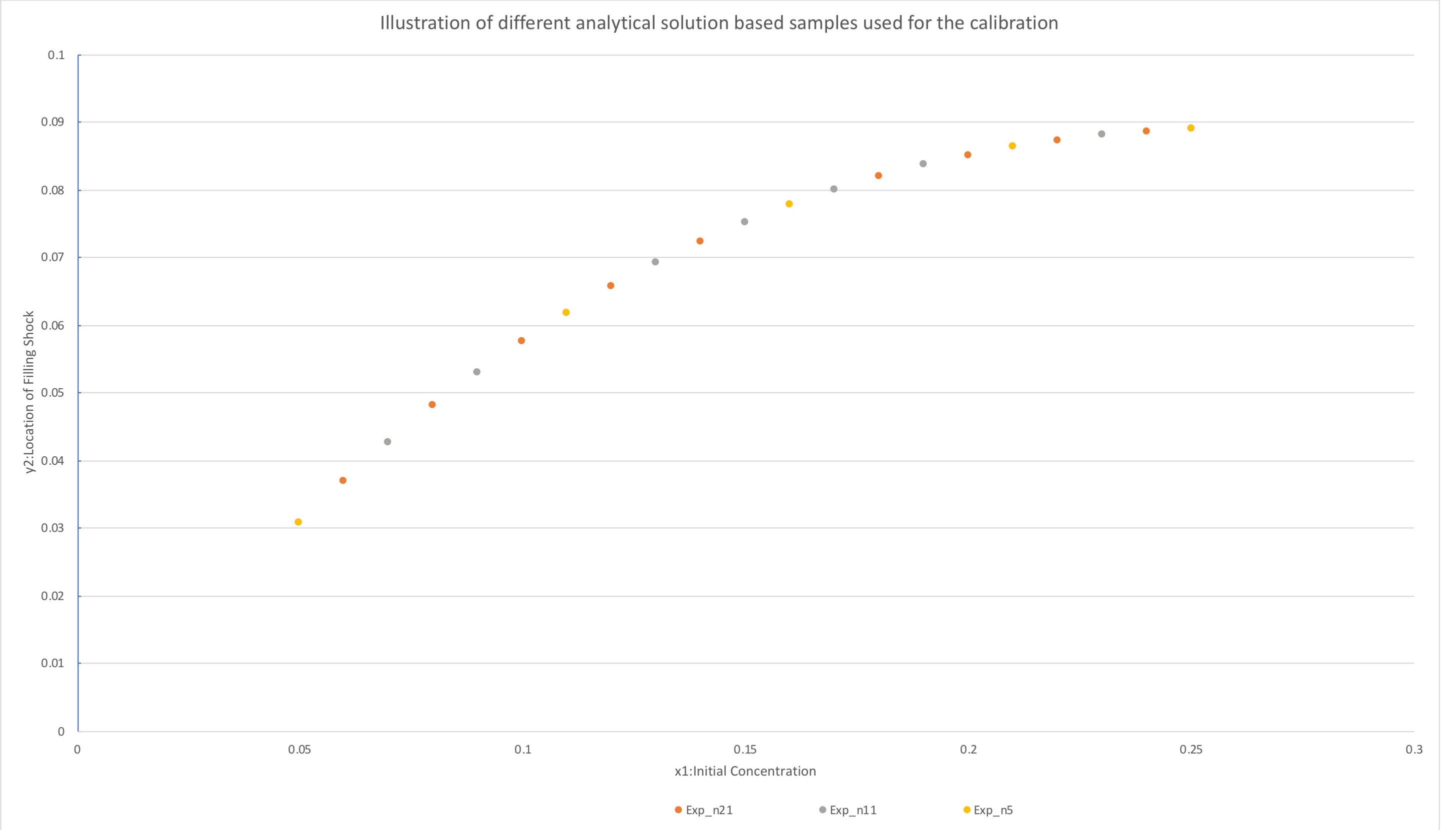
C1: Particle Settling Analytical Solution

Available Analytical Solution Used for Deterministic Calibration

To guide the calibration process, analytical solution was used in lieu of actual experiments.

Three different scenarios are employed by computing the analytical solution for $0.05 \leq x1 \leq 0.25$ range with different number of samples :

- 21 samples
- 11 samples
- 5 samples



C1: Particle Settling Simulation Campaigns

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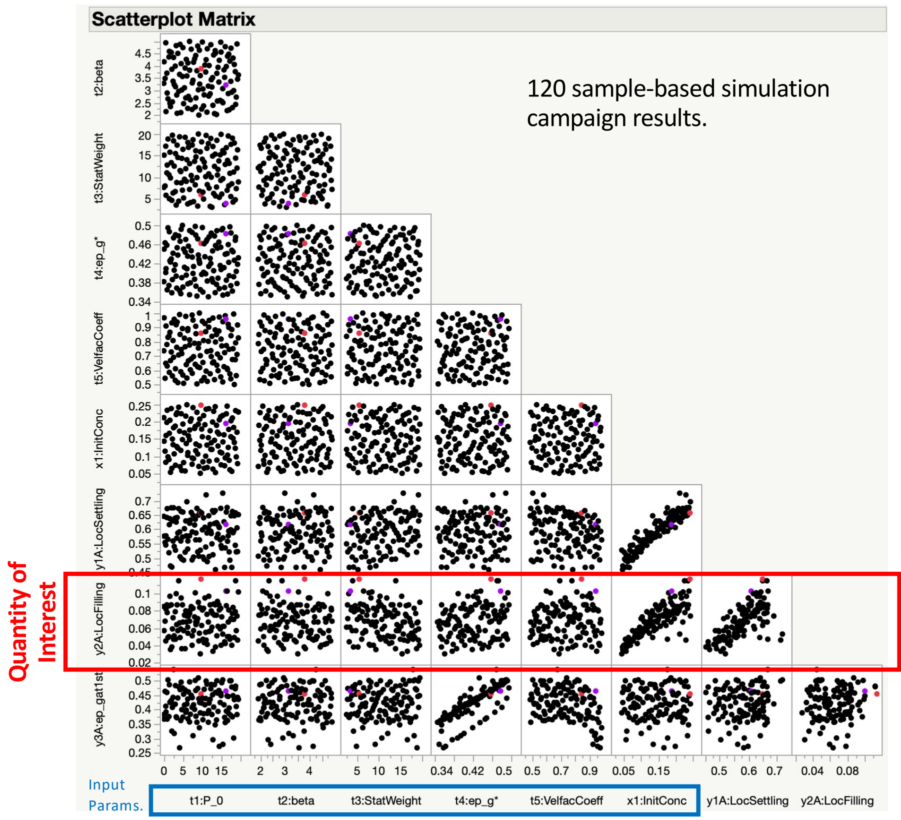
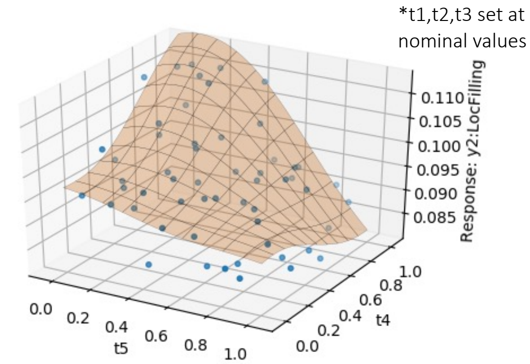
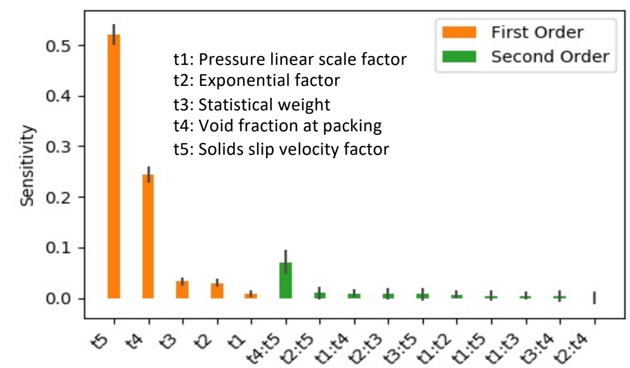
Construct Surrogate Model from Simulation Campaign (120 samples)



3D plot of the data-fitted surrogate model



Sensitivity Analysis using Sobol' Indices



Deterministic Calibration Procedure

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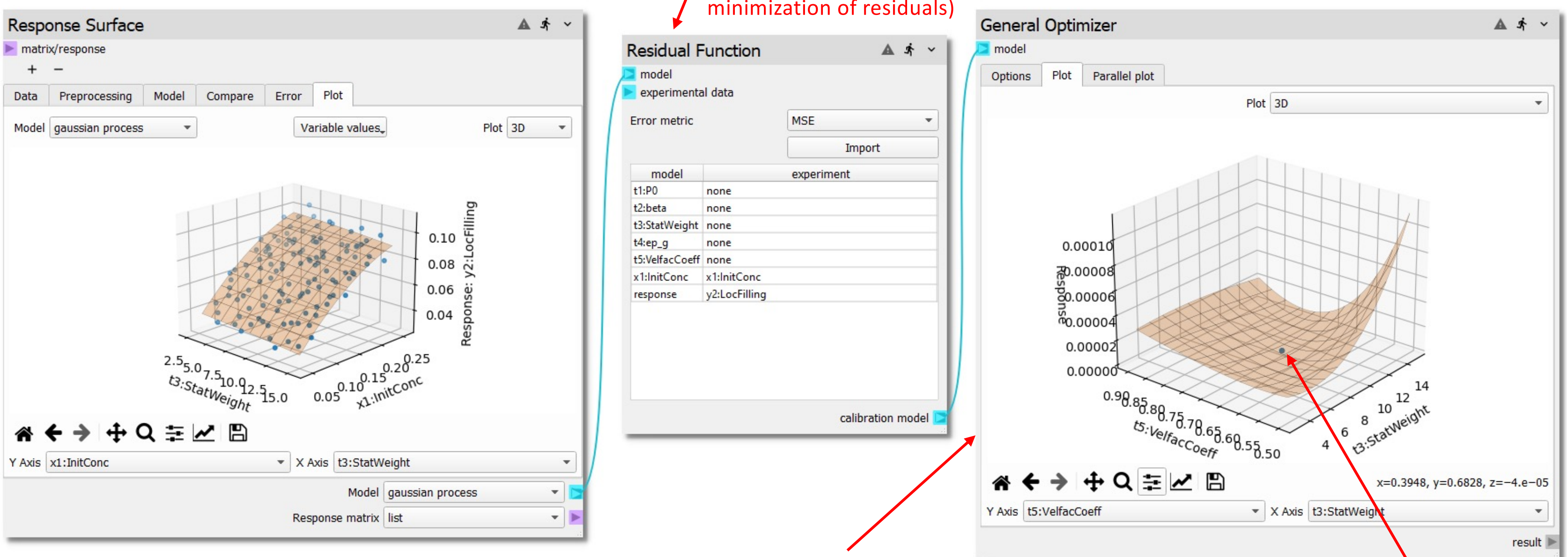
Illustration of Nodeworks Implementation Workflow

New node used to import experimental dataset and perform residual calculations required as part of the optimization (i.e., minimization of residuals)



For more information on Nodeworks please visit: https://mfix.netl.doe.gov/products/nodeworks/ or please scan the QR code :

Minimization performed by the General Optimizer node for: $\min_{\theta} f(\theta) = SSE(\boldsymbol{\theta}) = \sum_{i=1}^{n}[(s_i(\boldsymbol{\theta}) - y_i]^2 = \sum_{i=1}^{n}[r_i(\boldsymbol{\theta})]^2$

Optimal set of parameters identified that minimize the residual [9.55, 3.44, 9.41, 0.4, 0.69]

C1: Verification Simulation Campaigns (n=119)

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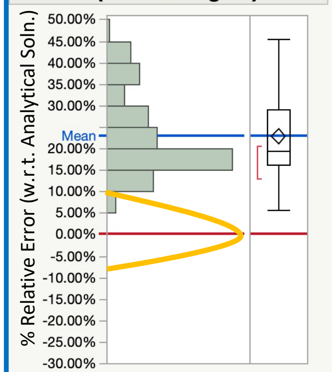
Comparison of Histograms for % Rel. Error Before & After Bug Fix

MFIX-PIC model Parameter	Default Settings	V&V Manual Settings
(θ_1): Pressure linear scale factor	100	10
(θ_2): Vol. fraction exponential scale factor	3.0	3.0
Theta3 (θ_3): Statistical weight	5.0	5.0
Theta4 (θ_4): Vol. fraction at maxi-mum packing	0.42	0.4
Theta5 (θ_5): Solid slip velocity factor	1.0	0.5

Default (before BugFix)



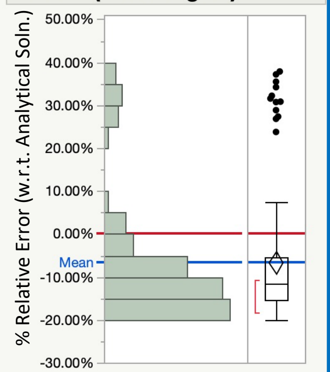
Quantiles

100.0%	maximum	45.45%
99.5%		45.45%
97.5%		44.45%
90.0%		38.59%
75.0%	quartile	29.09%
50.0%	median	19.39%
25.0%	quartile	16.34%
10.0%		13.19%
2.5%		9.08%
0.5%		5.62%
0.0%	minimum	5.62%

Summary Statistics

Mean	0.2299454
Std Dev	0.0950501
Std Err Mean	0.0087132
Upper 95% Mean	0.2471999
Lower 95% Mean	0.2126908
N	119

Default (after BugFix)



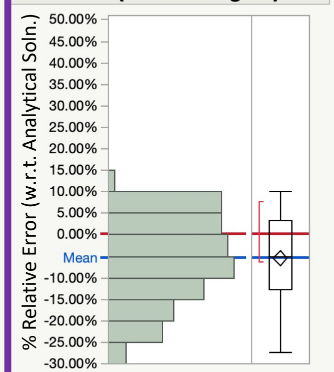
Quantiles

100.0%	maximum	37.82%
99.5%		37.82%
97.5%		35.44%
90.0%		26.80%
75.0%	quartile	-5.42%
50.0%	median	-11.46%
25.0%	quartile	-15.47%
10.0%		-17.50%
2.5%		-18.88%
0.5%		-19.95%
0.0%	minimum	-19.95%

Summary Statistics

Mean	-0.066134
Std Dev	0.1449514
Std Err Mean	0.0132877
Upper 95% Mean	-0.03982
Lower 95% Mean	-0.092447
N	119

V&V Man (before BugFix)



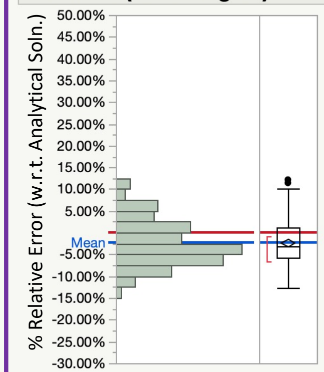
Quantiles

100.0%	maximum	10.06%
99.5%		10.06%
97.5%		8.51%
90.0%		6.98%
75.0%	quartile	3.26%
50.0%	median	-5.10%
25.0%	quartile	-12.86%
10.0%		-20.05%
2.5%		-26.41%
0.5%		-27.44%
0.0%	minimum	-27.44%

Summary Statistics

Mean	-0.055093
Std Dev	0.0954646
Std Err Mean	0.0087512
Upper 95% Mean	-0.037763
Lower 95% Mean	-0.072423
N	119

V&V Man (after BugFix)



Quantiles

100.0%	maximum	12.16%
99.5%		12.16%
97.5%		10.06%
90.0%		5.55%
75.0%	quartile	1.09%
50.0%	median	-3.25%
25.0%	quartile	-5.72%
10.0%		-8.38%
2.5%		-11.75%
0.5%		-12.53%
0.0%	minimum	-12.53%

Summary Statistics

Mean	-0.022515
Std Dev	0.0522297
Std Err Mean	0.0047879
Upper 95% Mean	-0.013034
Lower 95% Mean	-0.031996
N	119

C1: Proposed Calibrated Settings

Deterministic calibration with additional simulation campaigns (using 120 samples with different bounds)

Bounds of the parameter space for Model Parameters

Control variables: CFD (PIC parameters)

C1: Particle Settling	t1 or (θ_1): Pressure linear scale factor	t2 or (θ_2): Vol. fraction exponential scale factor	t3 or (θ_3): Statistical weight	t4 or (θ_4): Vol. fraction at maximum packing	t5 or (θ_5): Solid slip velocity factor
Original Bounds **[OB]**	[0.48 , 20]	[2 , 5]	[2.96 , 20]	[0.35 , 0.5]	[0.5 , 1.0]
New Bounds **[NB]**	[0.48 , 20]	[2 , 5]	[2.94 , 15]	[0.38 , 0.43]	[0.5 , 0.9]

Simulation campaign with New Bounds [NB] (120 samples)

Phases	MFIX-PIC Simulation Number	θ_1 Emp.Pres. Constant	θ_2 Vol. Fraction Exp. Scale Factor	θ_3 Stat. Weight	θ_4 Void Fraction at max packing	θ_5 Solid slip velocity factor	X_1 Initial solids concentration
		Uncertain Input Parameters/Factors:					
	1	4.375	2.965	3.954	0.423	0.666	0.243
	2	17.049	2.182	5.744	0.410	0.591	0.246
	3	3.860	2.817	7.026	0.386	0.709	0.128
	4	19.782	3.462	12.407	0.403	0.833	0.079
	5	1.572	2.662	14.195	0.428	0.764	0.098
	6	9.356	4.811	3.145	0.421	0.600	0.106
	7	4.613	3.656	14.554	0.384	0.892	0.173
	8	8.892	2.695	11.247	0.387	0.785	0.136
	9	15.462	4.566	14.961	0.399	0.755	0.075
	10	9.795	4.642	5.616	0.405	0.900	0.130
	11	14.360	3.700	13.970	0.426	0.609	0.089
	12	3.531	3.157	11.797	0.423	0.589	0.074
	13	18.016	3.374	4.716	0.388	0.532	0.157
	14	3.201	3.244	9.729	0.399	0.865	0.107
	15	11.773	2.120	12.662	0.420	0.685	0.132
	16	17.773	4.197	8.539	0.429	0.560	0.061
	17	12.139	3.181	13.448	0.380	0.742	0.154
	18	10.386	2.243	13.716	0.396	0.522	0.179
	19	6.361	4.267	7.213	0.395	0.612	0.137
	20	1.927	4.594	4.359	0.425	0.569	0.167
	21	7.923	3.308	13.204	0.408	0.563	0.095
	22	13.928	4.625	11.699	0.383	0.806	0.244
	23	2.432	4.554	10.297	0.406	0.683	0.239
	24	10.716	3.062	5.442	0.383	0.624	0.084
	25	15.648	2.557	5.120	0.427	0.716	0.110
	26	1.282	3.708	8.613	0.416	0.724	0.198
	27	3.034	4.347	13.888	0.421	0.653	0.183
	28	14.002	4.521	4.824	0.416	0.738	0.053
	29	6.734	2.274	3.497	0.408	0.802	0.102
	30	6.781	4.125	13.624	0.389	0.813	0.111
	31	14.277	2.025	6.274	0.389	0.780	0.190
	32	15.903	3.078	12.285	0.428	0.515	0.219
	33	17.346	2.876	14.692	0.416	0.837	0.126
	34	19.639	4.896	9.402	0.389	0.669	0.170
	35	18.600	4.322	3.807	0.411	0.701	0.152
	36	10.571	4.975	10.865	0.428	0.854	0.157
	37	12.609	2.867	3.100	0.407	0.561	0.174
	38	0.488	3.294	6.216	0.391	0.689	0.212
	39	5.184	3.023	11.010	0.393	0.673	0.058
	40	0.563	4.171	11.531	0.413	0.873	0.144
	41	2.085	2.477	12.020	0.405	0.793	0.205
	42	10.212	3.885	5.017	0.417	0.787	0.249
	43	13.528	4.449	5.217	0.398	0.628	0.231
	44	7.214	5.000	5.892	0.381	0.721	0.148
	45	0.994	4.944	13.008	0.397	0.619	0.082
	46	11.440	3.754	7.994	0.396	0.796	0.100

C1: Proposed Calibrated Settings

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MFIX-PIC model Parameters	Default Settings	V&V Manual Settings	PS Exp_n11 [NB]	DK Exp_n21 [NB]	PS Exp_n21 [NB]	DK Exp_n21 [OB]
Theta1 (θ_1): Pressure linear scale factor	**100**	**10**	2.71	**16.1**	**3.08**	**4.2**
Theta2 (θ_2): Vol. fraction exponential scale factor	**3.0**	**3.0**	3.74	**2.04**	**3.71**	**2.1**
Theta3 (θ_3): Statistical weight	**5.0**	**5.0**	8.86	**10.51**	**8.93**	**8.49**
Theta4 (θ_4): Vol. fraction at maxi-mum packing	**0.42**	**0.4**	0.4	**0.4**	**0.4**	**0.38**
Theta5 (θ_5): Solid slip velocity factor	**1.0**	**0.5**	0.7	**0.53**	**0.69**	**0.66**
Avg. % Rel. Err.	-6.61%	-2.25%	-5.9%	-2.63%	-6.17%	-2.53%
Min % Rel. Err.	-19.95%	-12.53%	-21.7%	-12.63%	-18.66%	-8.81%
Max % Rel. Err.	37.82%	12.16%	8.28%	7.09%	9.66%	5.23%

Note: % Rel. Err. Is the % Relative Error calculated by (Surrogate model evaluation – Analytical Soln.)/ Analytical Soln.

Column Legend:

Default Settings: Settings in MFiX-PIC

V&V Manual Settings: Settings determined by trial-error.

PS Exp_n11 [NB]: Proposed calibrated model parameter settings obtained with **PSUADE** using a surrogate model constructed from the simulation campaign with **new** bounds and **11** samples of analytical solution to guide calibration

PS Exp_n21 [NB]: Same as above except 21 samples of analytical solution employed.

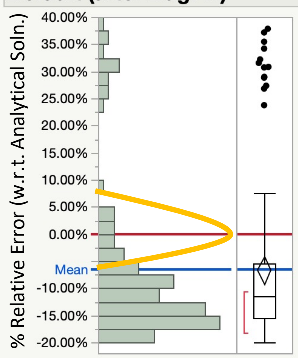
DK Exp_n21 [NB]: Proposed calibrated model parameter settings obtained with **DAKOTA** using a surrogate model constructed from the simulation campaign with **new** bounds and **11** samples of analytical solution to guide calibration

DK Exp_n21 [OB]: Same as above except surrogate model constructed from the simulation campaign with original bounds used.

C1: Error Assessment of the Proposed Calibrated Settings

Comparison of PSUADE and DAKOTA (119 unseen samples for x1)

Default (after BugFix)



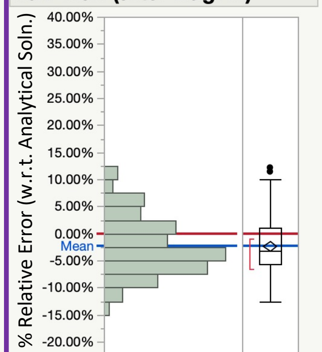
Quantiles

100.0%	maximum	37.82%
99.5%		37.82%
97.5%		35.44%
90.0%		26.80%
75.0%	quartile	-5.42%
50.0%	median	-11.46%
25.0%	quartile	-15.47%
10.0%		-17.50%
2.5%		-18.88%
0.5%		-19.95%
0.0%	minimum	-19.95%

Summary Statistics

Mean	-0.066134
Std Dev	0.1449514
Std Err Mean	0.0132877
Upper 95% Mean	-0.03982
Lower 95% Mean	-0.092447
N	119

V&V Man (after BugFix)



Quantiles

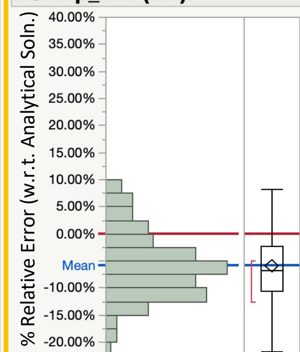
100.0%	maximum	12.16%
99.5%		12.16%
97.5%		10.06%
90.0%		5.55%
75.0%	quartile	1.09%
50.0%	median	-3.25%
25.0%	quartile	-5.72%
10.0%		-8.38%
2.5%		-11.75%
0.5%		-12.53%
0.0%	minimum	-12.53%

Summary Statistics

Mean	-0.022515
Std Dev	0.0522297
Std Err Mean	0.0047879
Upper 95% Mean	-0.013034
Lower 95% Mean	-0.031996
N	119

PSUADE with 11 analytical samples

PS Exp_n11 (NB)



Quantiles

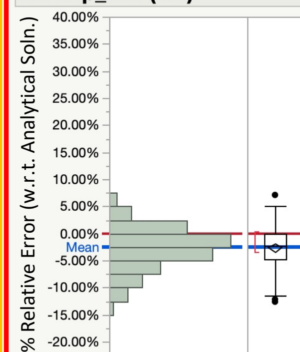
100.0%	maximum	8.28%
99.5%		8.28%
97.5%		7.50%
90.0%		3.24%
75.0%	quartile	-2.28%
50.0%	median	-6.86%
25.0%	quartile	-10.57%
10.0%		-13.15%
2.5%		-18.16%
0.5%		-21.71%
0.0%	minimum	-21.71%

Summary Statistics

Mean	-0.058976
Std Dev	0.0618634
Std Err Mean	0.005671
Upper 95% Mean	-0.047746
Lower 95% Mean	-0.070207
N	119

DAKOTA with 21 analytical samples

DK Exp_n21 (NB)



Quantiles

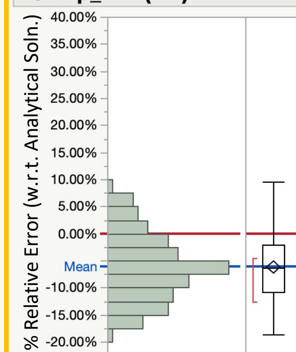
100.0%	maximum	7.09%
99.5%		7.09%
97.5%		4.19%
90.0%		1.70%
75.0%	quartile	-0.05%
50.0%	median	-2.41%
25.0%	quartile	-4.76%
10.0%		-8.56%
2.5%		-11.38%
0.5%		-12.63%
0.0%	minimum	-12.63%

Summary Statistics

Mean	-0.026251
Std Dev	0.038388
Std Err Mean	0.003519
Upper 95% Mean	-0.019283
Lower 95% Mean	-0.03322
N	119

PSUADE with 21 analytical samples

PS Exp_n21 (NB)



Quantiles

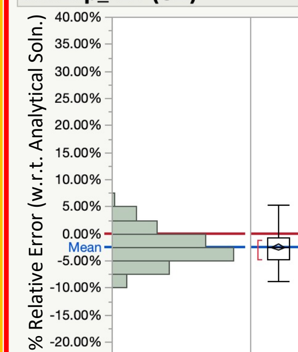
100.0%	maximum	9.66%
99.5%		9.66%
97.5%		7.01%
90.0%		2.71%
75.0%	quartile	-1.99%
50.0%	median	-6.44%
25.0%	quartile	-10.86%
10.0%		-14.15%
2.5%		-16.99%
0.5%		-18.66%
0.0%	minimum	-18.66%

Summary Statistics

Mean	-0.061695
Std Dev	0.0613988
Std Err Mean	0.0056284
Upper 95% Mean	-0.050549
Lower 95% Mean	-0.072841
N	119

DAKOTA with 21 analytical samples

DK Exp_n21 (OB)



Quantiles

100.0%	maximum	5.23%
99.5%		5.23%
97.5%		4.25%
90.0%		1.79%
75.0%	quartile	-0.64%
50.0%	median	-2.62%
25.0%	quartile	-4.71%
10.0%		-6.00%
2.5%		-8.33%
0.5%		-8.81%
0.0%	minimum	-8.81%

Summary Statistics

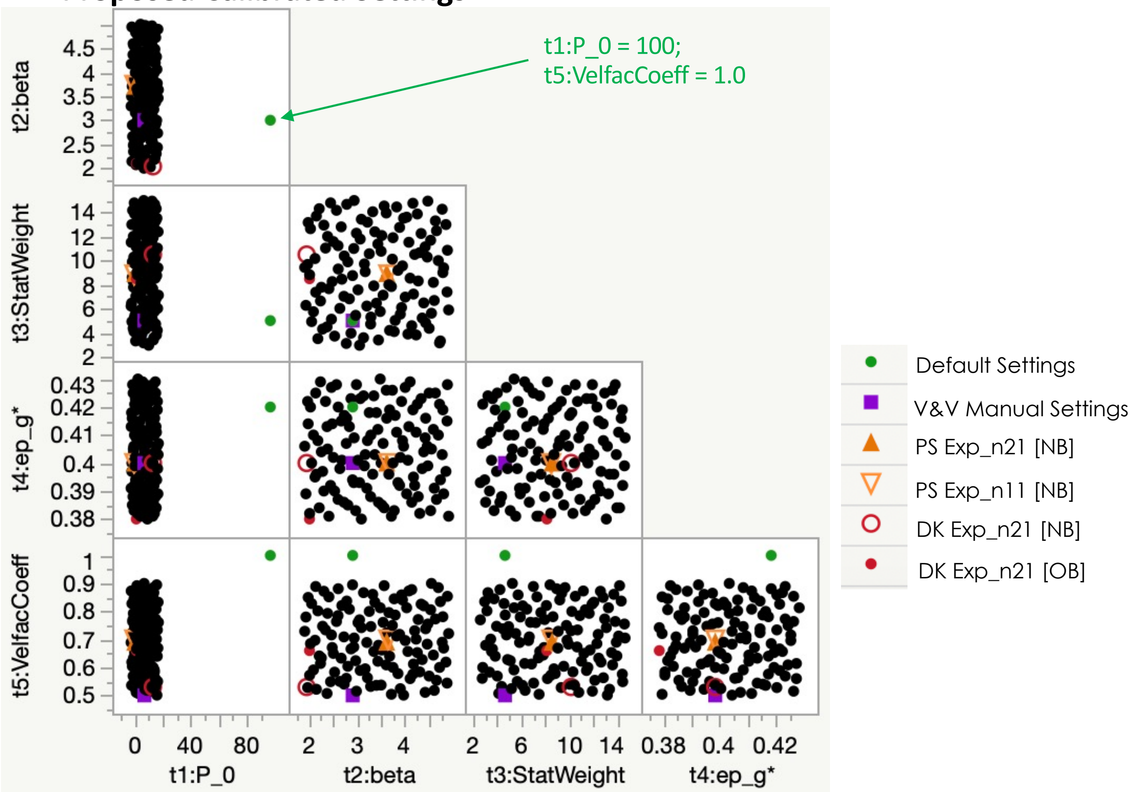
Mean	-0.02525
Std Dev	0.030798
Std Err Mean	0.0028233
Upper 95% Mean	-0.01966
Lower 95% Mean	-0.030841
N	119

Note: NB: surrogate model constructed from a simulation campaign with new bounds for some of the parameters, OB: simulation campaign with original bounds

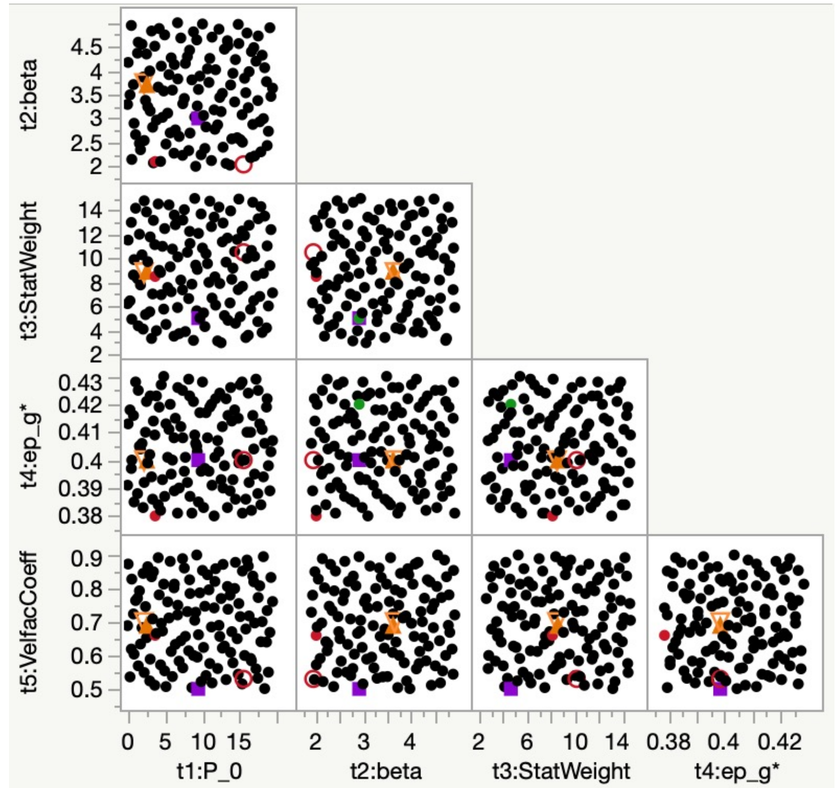
C1: Proposed Calibration Settings

Visualization of Proposed Settings and Simulation Campaign

Proposed Calibrated Settings



Proposed Calibrated Settings (excl. t1=100, t5=1 for Default Settings)



Concluding Remarks

- MFiX-PIC offers substantial savings in time-to-solution, but the trade-off is accuracy.
- Objective was to employ various calibration techniques to assess the most uncertain model parameters specific to Parcel-in-Cell methodology and observe how they vary across different flow regimes.
- Adopted a systematic calibration procedure to identify optimal model parameter settings to minimize the discrepancy between MFiX-PIC and available experimental/analytical dataset. Started with Deterministic calibration as it is cheaper than Bayesian Calibration.
- Test the performance of calibrated model parameters rigorously. Also assessed the effect of varying sample size in the experiments (analytical solution).
- Explored different UQ toolkits such as PSUADE and DAKOTA and implemented the deterministic calibration capability within Nodeworks.
- When compared with the default settings, demonstrated significant accuracy improvement for Particle Settling case with deterministic calibration

Future Work

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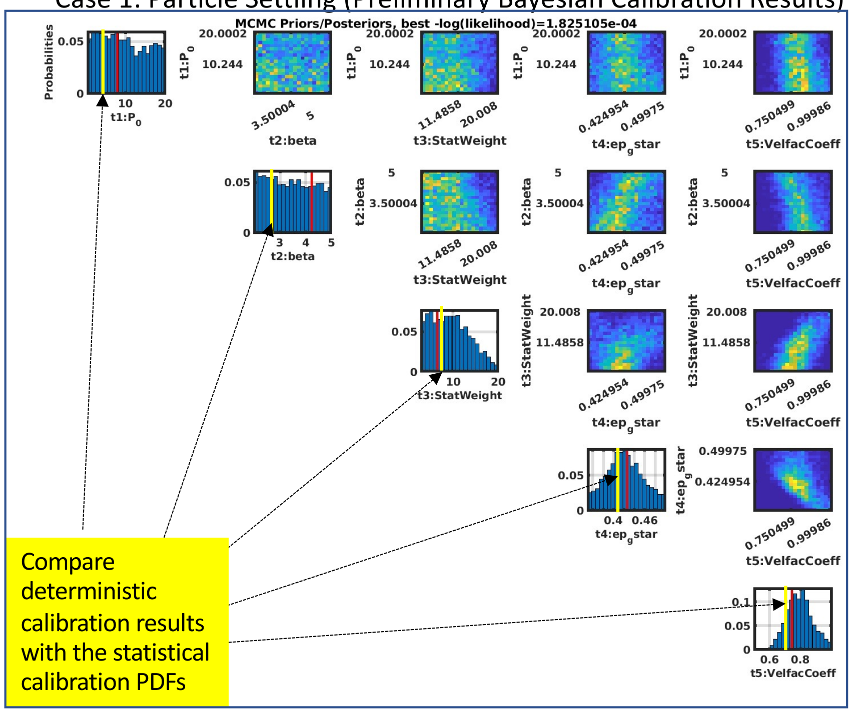
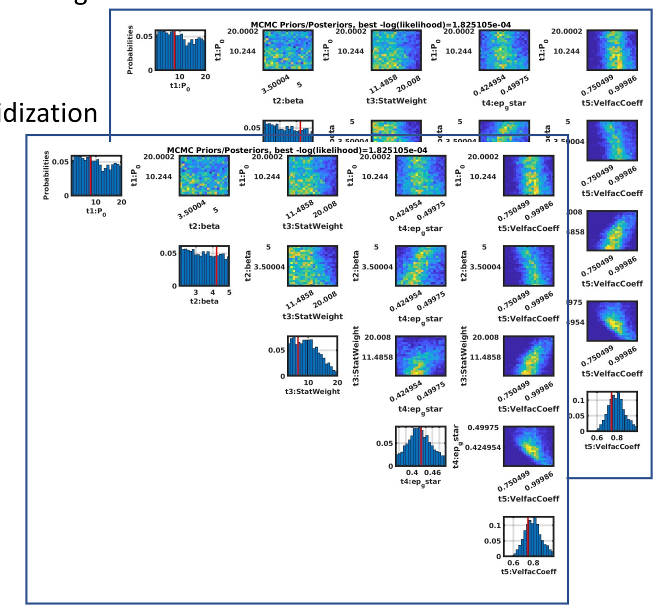
- Perform deterministic calibration and statistical calibration for all selected cases and compare the outcomes from both calibration approaches

Case 1: Particle Settling (Preliminary Bayesian Calibration Results)



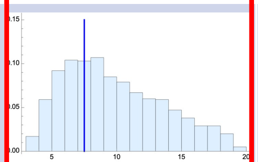
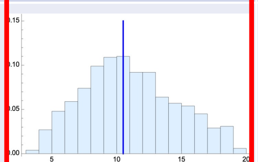
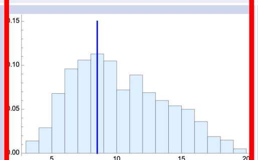
Case 3: Circulating Fluidized Bed

Case 2: Fluidization



Future Work

- Compare proposed calibrated model parameter settings for different flow regimes and provide best practices guidance to MFiX-PIC users on how to set PIC specific parameters based targeted application. For example, for θ_3 :

Cases / Flow Regimes	t1 or (θ_1): Pressure linear scale factor	t2 or (θ_2): Vol. fraction exponential scale factor	t3 or (θ_3): Statistical weight	t4 or (θ_4): Vol. fraction at maximum packing	t5 or (θ_5): Solid slip velocity factor
C1: Particle Settling	….	….		….	….
C2: Fluidization	….	….		….	….
C3: Circulating Fluidized Bed	….	….		….	….

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Note: QR codes for the URL of the references have been included to facilitate easy access via mobile devices.

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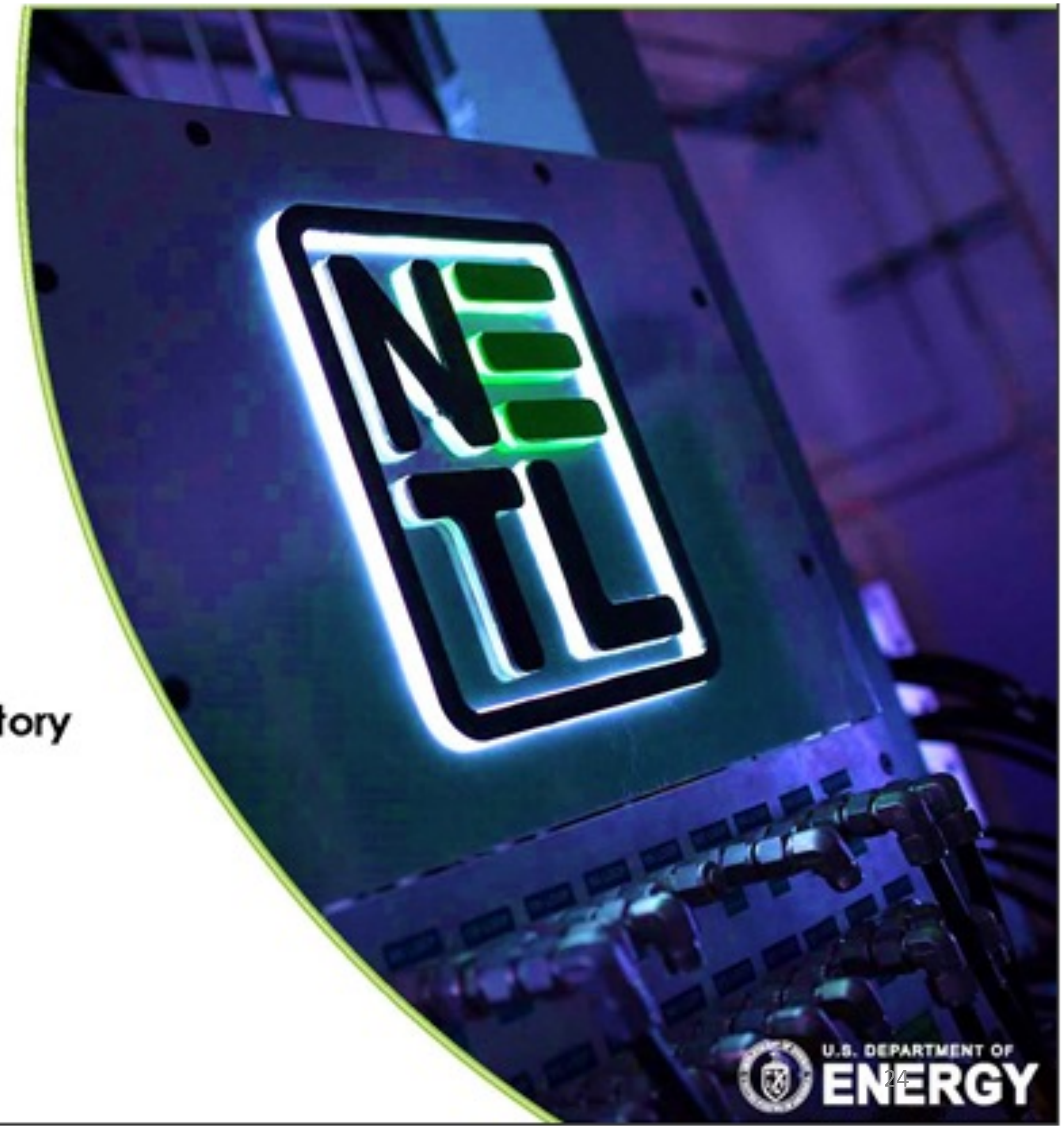
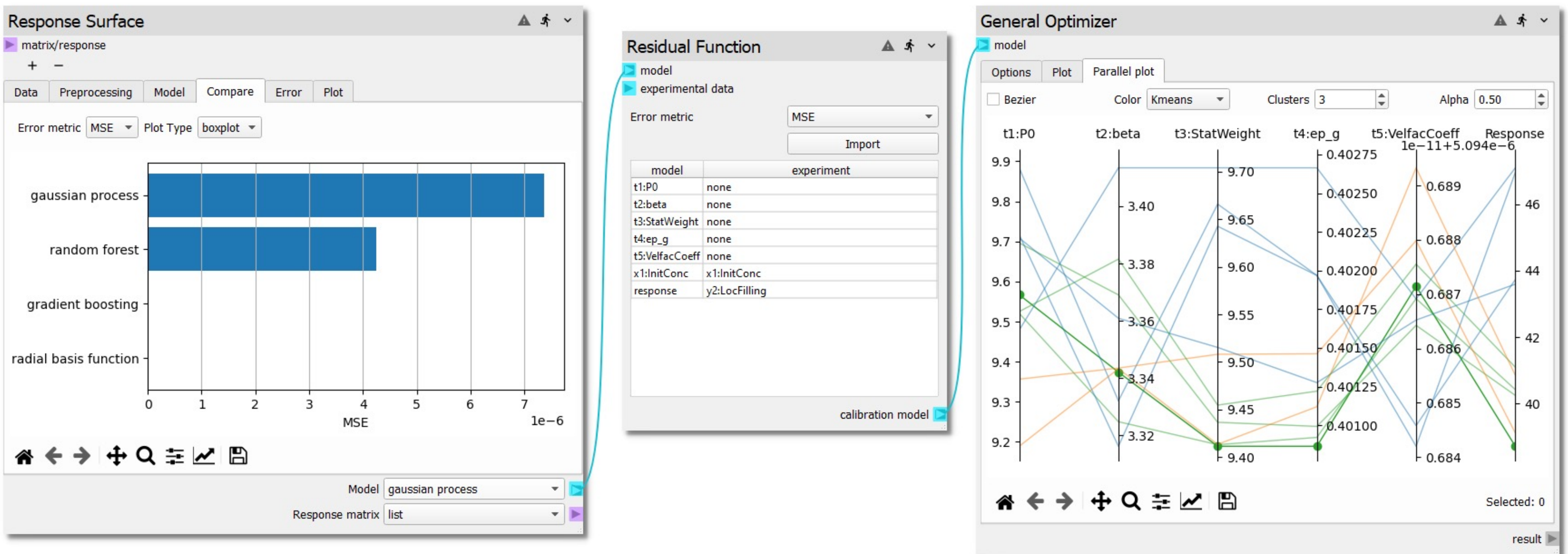


Additional Slides

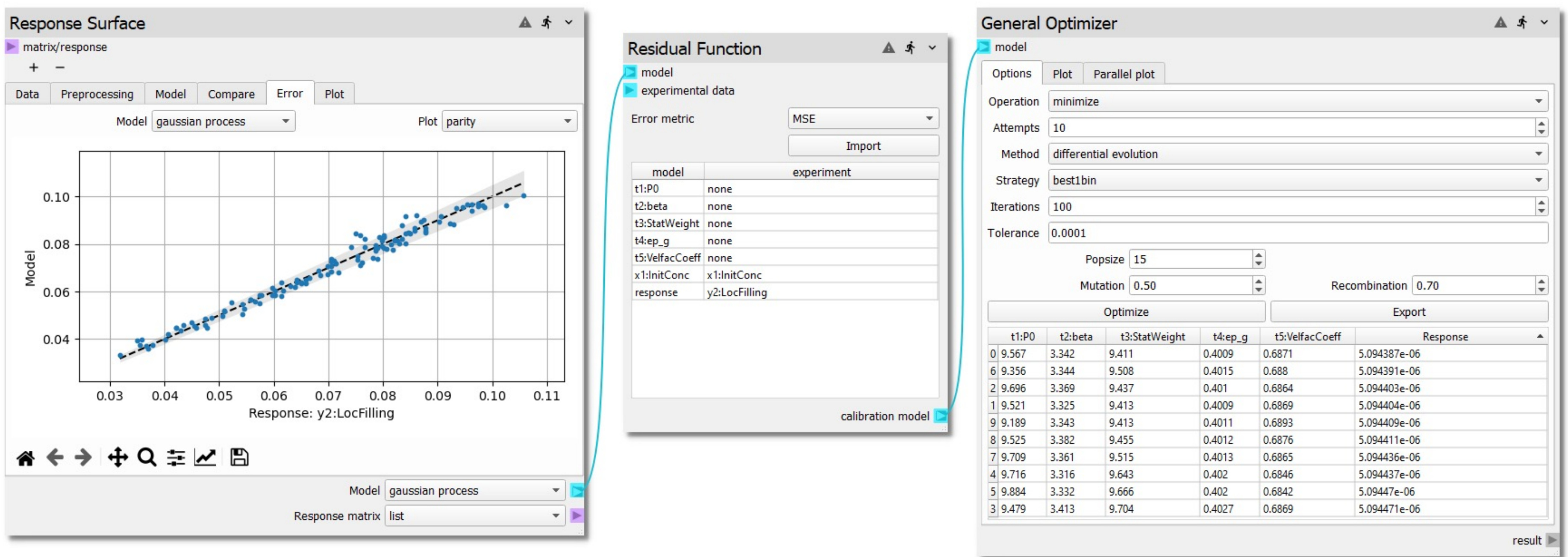
Deterministic Calibration Procedure

Illustration of Nodeworks Implementation Workflow



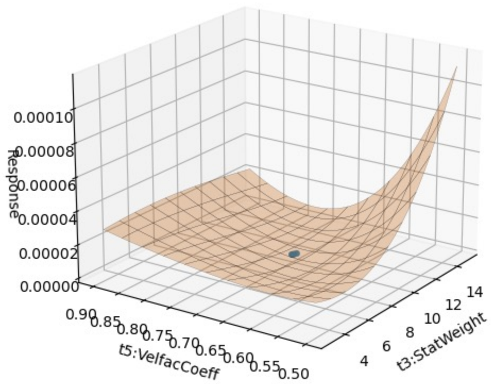
Deterministic Calibration Procedure

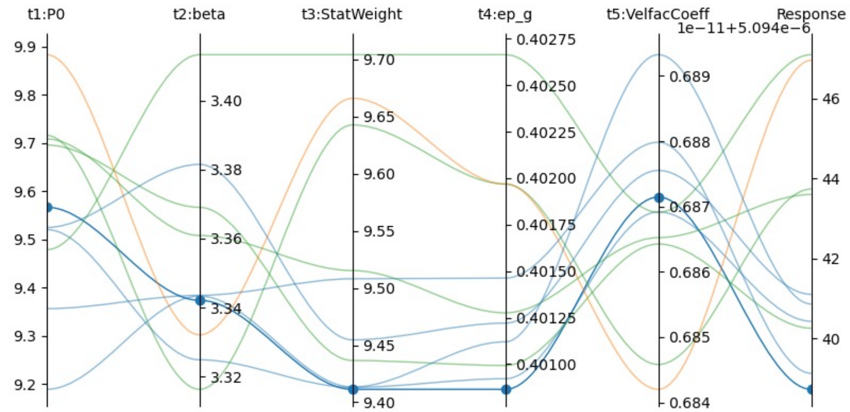
Illustration of Nodeworks Implementation Workflow

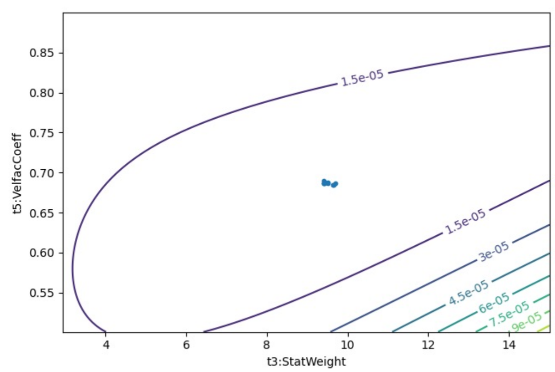


Deterministic Calibration Procedure

Illustration of Nodeworks Implementation Workflow







Deterministic Calibration Procedure

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Illustration of Nodeworks Implementation Workflow