Development of a verification, validation and uncertainty quantification roadmap for multiphase flows with preliminary results for hopper bin discharge problem

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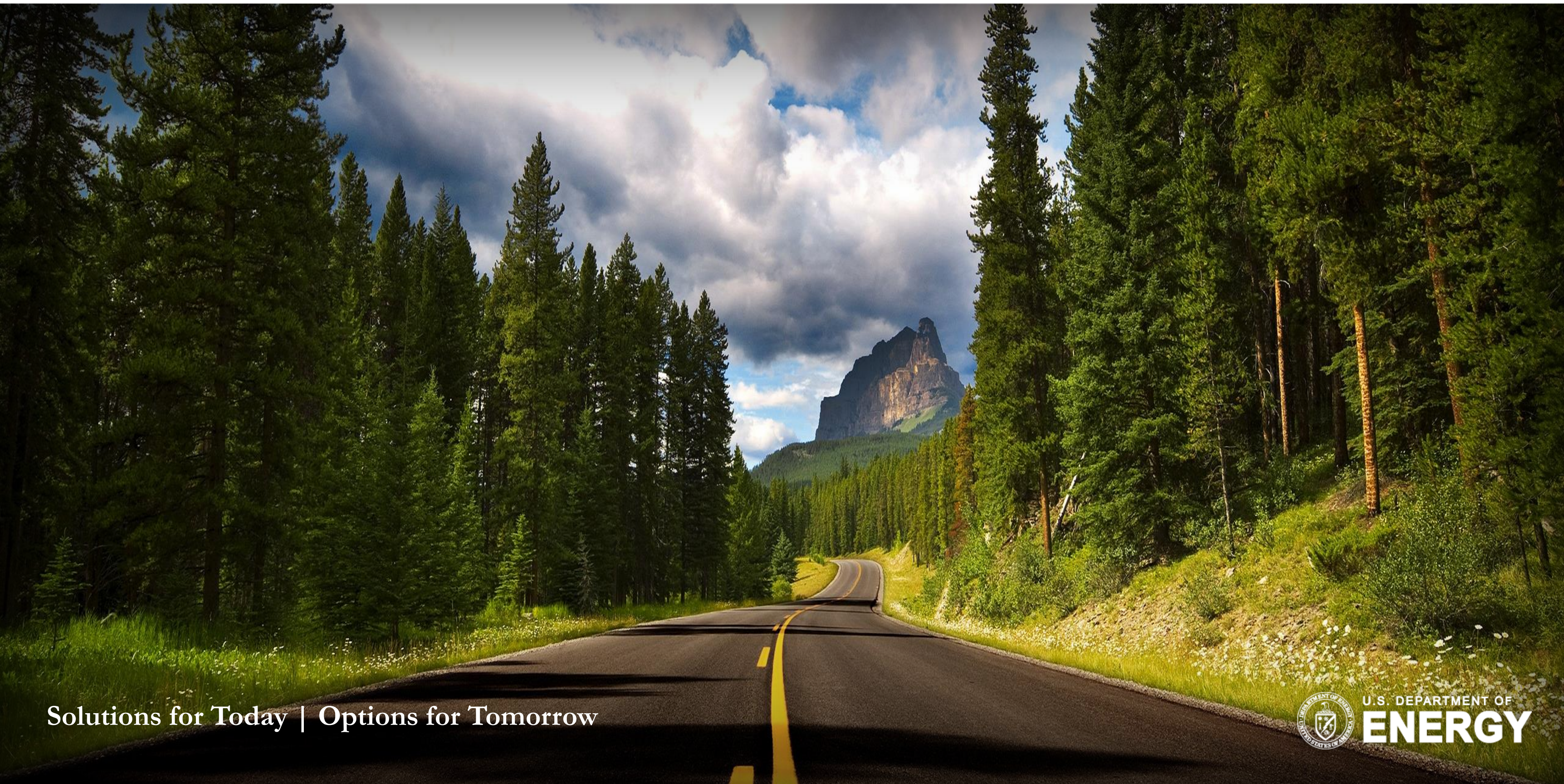

Outline

- **Development and application of a systematic VVUQ approach for multiphase flows**
  - Extension of the existing methodologies
  - Survey of subject matter experts and tollgates for review
  - Systematic simulation campaign and design of experiments
- **Benchmark problem and preliminary experiments: Hopper discharge**
  - Bench-scale experiments to enable a quick turnaround for Discrete Element Modeling (DEM) simulations
  - Design criteria to ensure mass flow operation mode
- **MFIX-DEM simulation campaign**
  - Validation of MFIX-DEM linear spring dashpot (LSD) model
  - Sensitivity analysis of model parameters on the quantities of interest

Motivation

- **VVUQ standards have been established to quantify the degree of accuracy using CFD solution and experimental data for a specified variable at a specified validation point**

- **Application to multiphase flow modeling and simulation has encountered several challenges**
  - Assessing uncertainty due to numerical discretization
  - Lack of readily available objectively-assessed experimental uncertainty

- **Explore the extension of the VVUQ procedures for multiphase flow applications using some demonstrative cases starting with granular discharge through a conical hopper**

Extended VVUQ roadmap for multiphase flows - NETL

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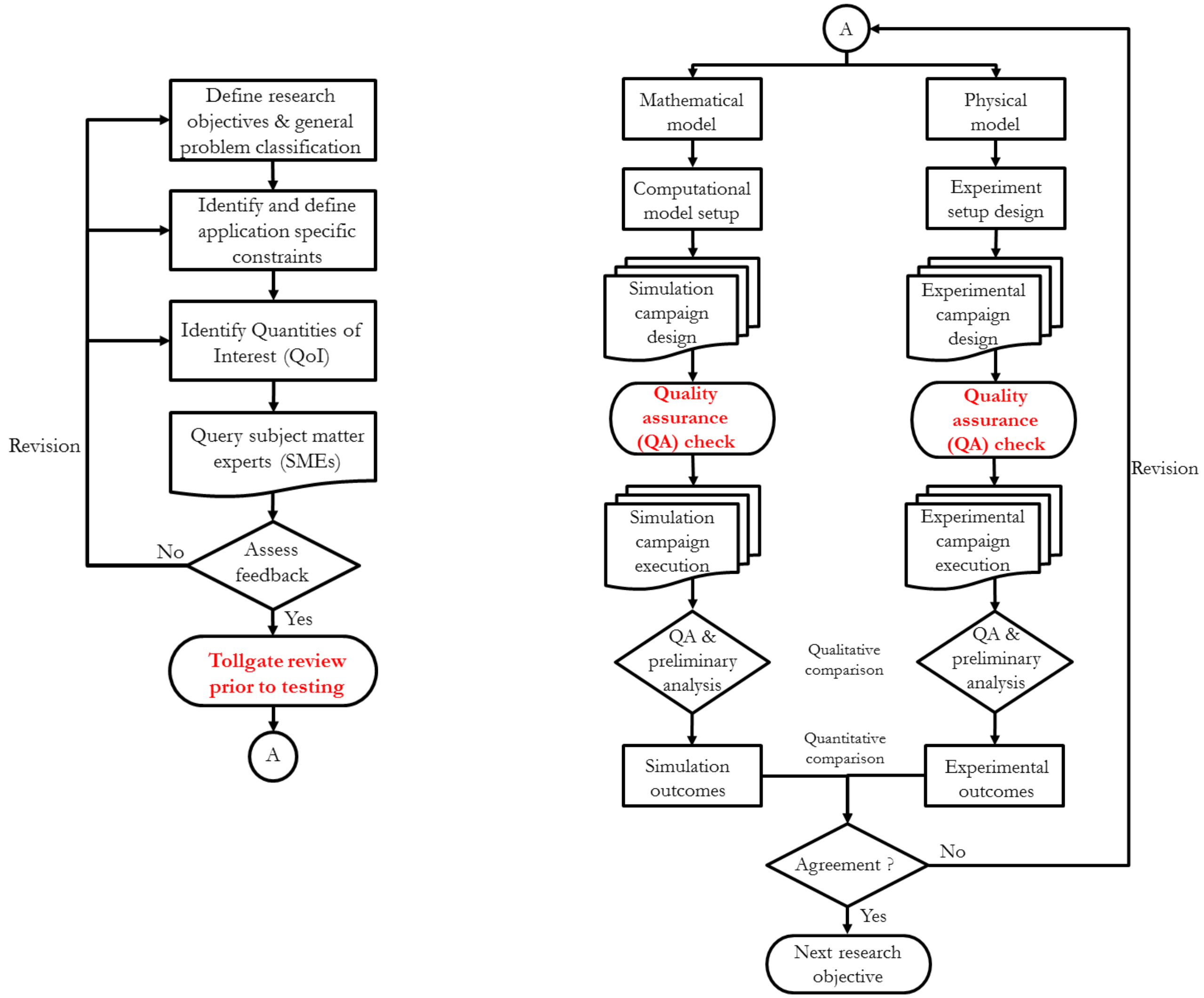
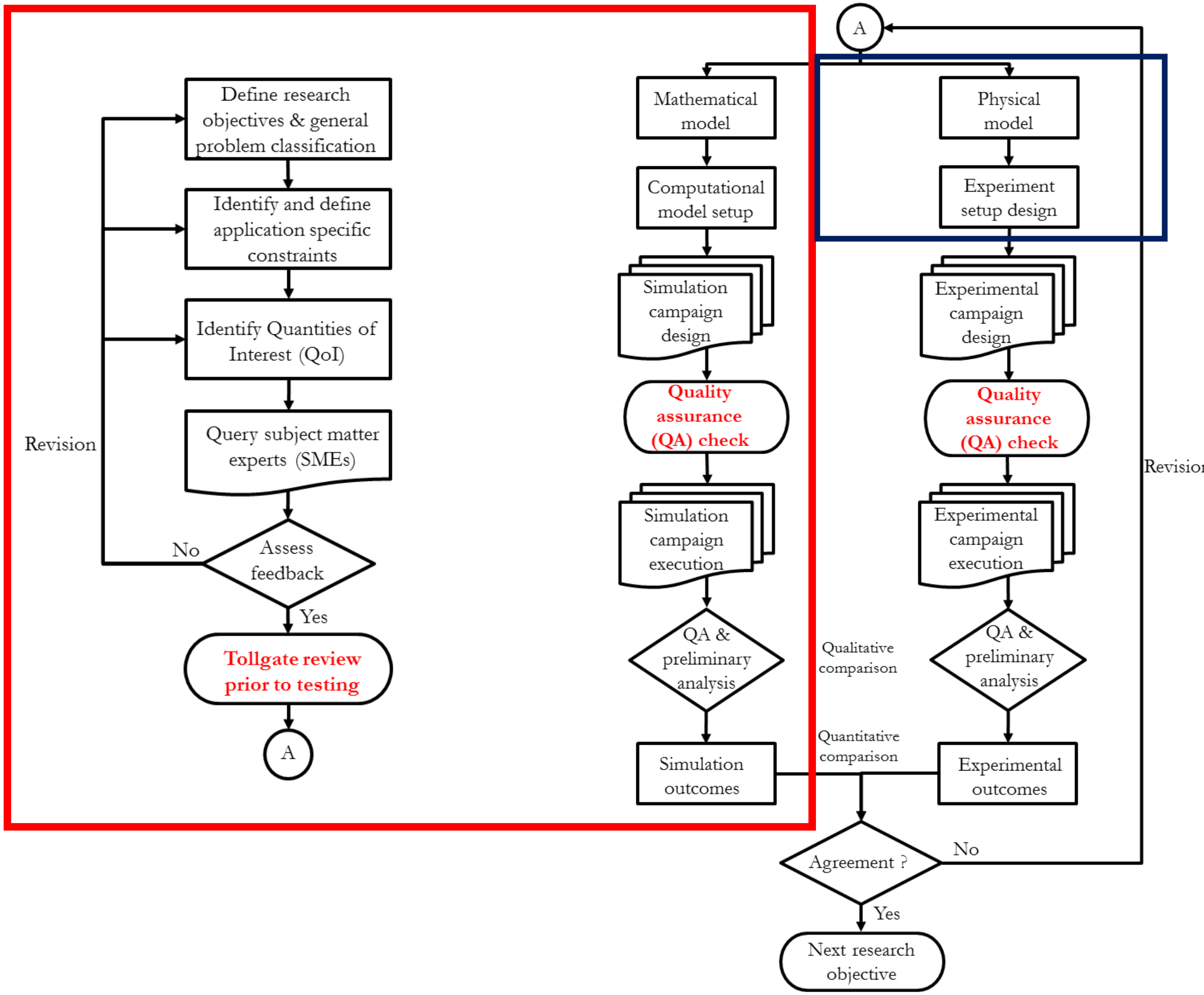
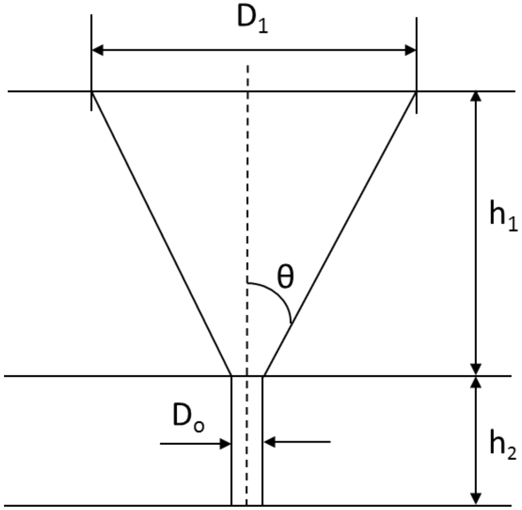


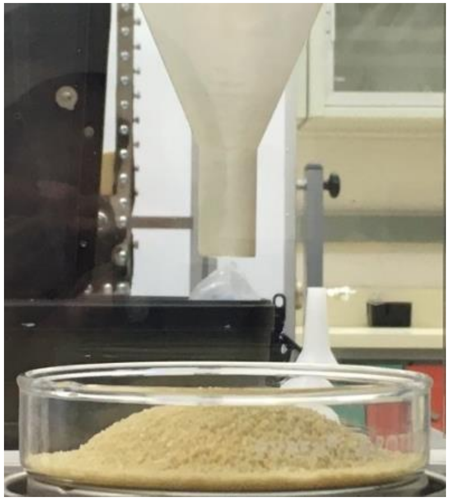
Extended VVUQ roadmap for multiphase flows - NETL



Benchmark problem – Preliminary experiments

- Discharge through conical hopper having pure granular flow commonly seen in industries (chemical, pharmaceutical, food, mining)
- Simplified hydrodynamics to focus on particle-particle and particle-wall interactions. Interfacial gas neglected (High Bagnold number).
- Bench-scale experiments to enable a quick turnaround, 3-D printed geometries to ensure consistency between experiments and simulations





Benchmark problem – Preliminary experiments

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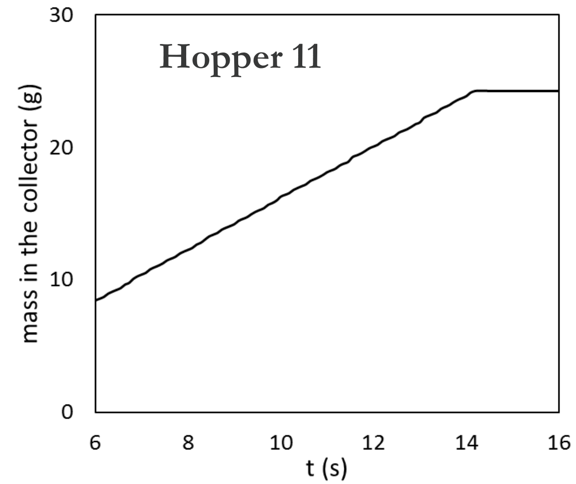
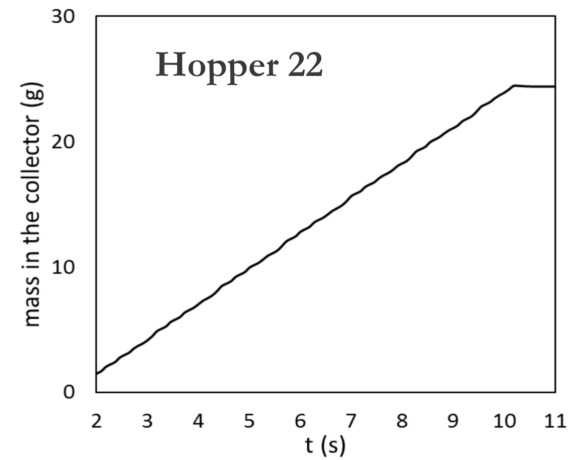
- **Control variables**
  - Orifice diameter
  - Apex angle
- **Quantities of interest (QoI)**
  - Discharge flow rate
  - Angle of repose
- **Material: High density polyethylene (HDPE)**
  - Geldart B classification
  - Mean particle diameter: **848 μm**
  - Density: **884 kg/m^3**

Index	θ (deg)	h_1 (cm)	h_2 (cm)	D_o (mm)	D_1 (cm)
11	13.44	10	2.5	5.8	5.36
12	13.12	10	2.5	7	5.36
21	23.63	10	2.5	5.8	9.33
22	23.34	10	2.5	7	9.33





Benchmark problem – Simulations

- Increasing demand for DEM simulations with improving computational resources
- Focus on particle properties before including the gas phase
- Solution methodology: Alternating use of Force-displacement law and Newton's second law of motion. Time step size based on spring stiffness provided by the user (fixed).
- Isolating uncertainties due to model parameters related to particle-particle and particle-wall interactions from the other sources including spatio-temporal discretization

Survey of Subject Matter Experts

- **Survey pertaining to experiments and DEM simulations was carried out with the subject matter experts to identify:**
  - Quantities of interest (or response variables)
  - Control variables, which are to be varied systematically
  - Held-constant factors for experiments and modeling
  - Known nuisance factors for the experiments

- **Based on the feedback, 10 control variables were identified for DEM simulations as important but without any consistent and objective ranking of importance**

- **Screening study initiated to quantitatively determine the most influential factors on the response variables**

Example illustration of survey:
- Identification and Characterization of Control Variables for CFD Simulations:

8. Subject Matter Expert (SME) Feedback Summary	
Computational model - Response Variables	
Accepted - Ranked by overall score 1. Discharge rate (kg/s) 2. Angle of repose (degree)	**Rejected** • Particle Size Distribution (PSD) of discharged particles • Flow pattern - lowest point in hopper • Flow pattern - Highest point in hopper • particle-wall friction coefficient • Particle-particle restitution coefficient • Young's Modules • Particle-particle dynamic friction coefficient • Particle-particle static friction coefficient
Computational model - Control Variables	
Accepted - Ranked by overall score 1. PP coefficient of friction (sliding) 2. PW coefficient of friction (sliding) 3. PP restitution coefficient 4. PP LSD normal spring stiffness coefficient 5. PW restitution coefficient 6. PW LSD normal spring stiffness coefficient 7. PP LSD tangential spring stiffness coefficient 8. PW LSD tangential spring stiffness coefficient 9. PP LSD tangential damping factor 10. PW LSD tangential damping factor	**Rejected** • Coefficient of friction (rolling) • Initial voidage • Initial bed height • Particle density • Initial particle size distribution (PSD) • Wall asperities • Orifice diameter • Apex angle • Height above collection plate
Computational model - Held Constant Variables	
Accepted - Ranked by overall score 1. Particle density (kg/m^3) 2. Particle diameter (m) 3. Particle sphericity	**Rejected** • Normal spring stiffness • Time step

Computational model - Rejected Response Variables

SME	Rejected response variable	Justification of rejected response variable
1	PSD of discharged particles	Computational simulations will be conducted with mono-disperse particles so there is no PSD will be generated of discharged particles
3	Flow pattern - highest and lowest points in hopper	These are connected to model input parameters, specifically the total number of particles.
4	Particle-wall friction coefficient	This is a model input parameter.
4	Particle-particle restitution coefficient	This is a model input parameter.
4	Particle-particle friction coefficients	This is a model input parameter.

Computational model - Accepted Control Variables

Particle-particle coefficient of friction (sliding) — **Rank: 1 of 10**

SME	Proposed control variable value range: Rank	Normal	Low	High	Justification
1	1	0.5	0.0	1.0	I have seen the friction coefficient can be very sensitive to things like humidity. It would be best to measure the friction coefficient in house if possible.
2	2	0.3	0.0	1.0	[It is] unclear whether distinction should be made between dynamic/static value but MFIX doesn't have this fine control.
3	7	0.5	N/R	N/R	N/R
4	4	N/R	N/R	N/R	*JM: Rank assumed from list order and inputs of dynamic and static friction.*
5	1	N/R	N/R	N/R	N/R
6	TBD (5)	0.35	0.31	0.39	*JM: Not specific on pp or pw*

Particle-wall coefficient of friction (sliding) — **Rank: 2 of 10**

SME	Proposed control variable value range: Rank	Normal	Low	High	Justification
1	2	0.68	0.45	0.90	I have seen the friction coefficient can be very sensitive to things like humidity. It would be best to measure the friction coefficient in house if possible.
2	4	N/R	N/R	N/R	N/R
3	8	0.5	N/R	N/R	N/R
4	1	N/R	N/R	N/R	*JM: Rank assumed from list order.*
5	2	N/R	N/R	N/R	N/R
6	TBD (5)	0.35	0.31	0.39	*JM: Not specific on pp or pw*

Screening study

- **Morris One-at-a-time (MOAT): Computationally efficient for screening study involving a large parameter space**

- **Elementary effect:** $d_{ij} = \frac{c_i(k_1,k_2,\ldots,k_{j-1},k_j+\Delta,k_{j+1},\ldots,k_m) - c_i(k_1,k_2,\ldots,k_{j-1},k_j,k_{j+1},\ldots,k_m)}{\Delta}$

- **Global effect:** $\mu_{ij} = \frac{\sum|d_{ij}|}{r}$, $\sigma_{ij}^2 = \frac{r\sum(d_{ij})^2 - (\sum d_{ij})^2}{r(r-1)}$

- **Larger mean (μ_{ij})→ more sensitive; larger variance, (σ_{ij}^2)→ more non-linearity/interactive effects**

- **Computational model – Parameters considered based on Subject matter expert (SME) feedback**
  - Particle-Particle coefficient of friction
  - Particle-Wall coefficient of friction
  - Particle-Particle coefficient of restitution
  - Particle-Wall coefficient of restitution
  - Particle-Particle LSD normal spring stiffness
  - Particle-Wall LSD normal spring stiffness
  - Particle-Particle LSD tangential spring stiffness coefficient
  - Particle-Wall LSD tangential spring stiffness coefficient
  - Particle-Particle LSD tangential spring stiffness damping coefficient
  - Particle-Wall LSD tangential spring stiffness damping coefficient

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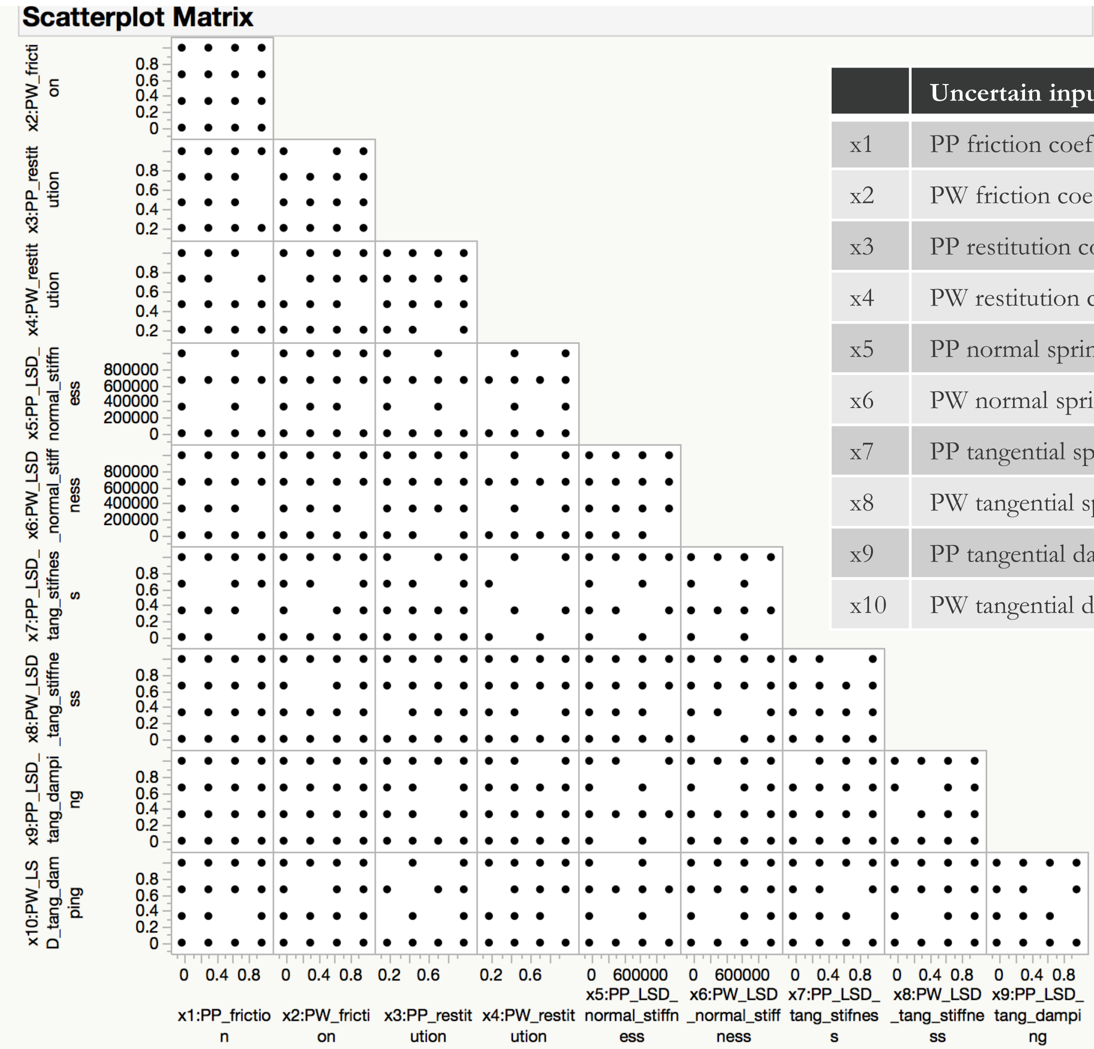
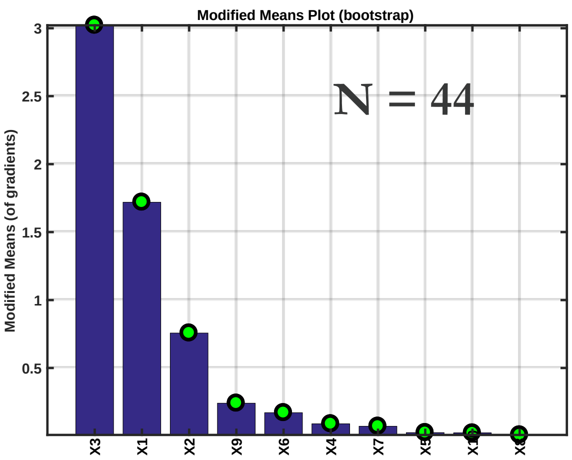
Screening study – Sampling

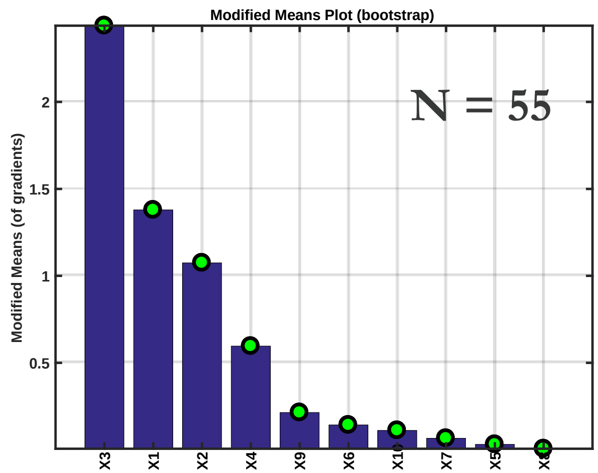


	Uncertain input parameter	Lower bound	Upper bound
x1	PP friction coefficient [−]	0	1
x2	PW friction coefficient [−]	0	1
x3	PP restitution coefficient [−]	0.2	0.99
x4	PW restitution coefficient [−]	0.2	0.99
x5	PP normal spring stiffness [N/m]	1.0E+02	1.0E+06
x6	PW normal spring stiffness [N/m]	1.0E+02	1.0E+06
x7	PP tangential spring stiffness coefficient [−]	0.1	0.9
x8	PW tangential spring stiffness coefficient [−]	0.1	0.9
x9	PP tangential damping factor [−]	0.1	0.9
x10	PW tangential damping factor [−]	0.1	0.9

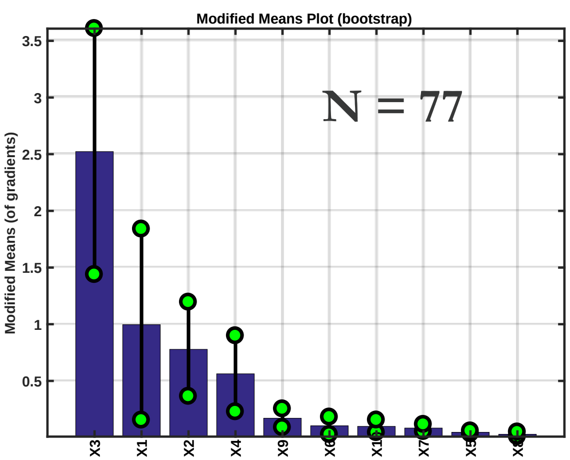
Morris method (MOAT)
No. of input parameters : 10
Preferred sample size: 110
Most conservative sample size : 44

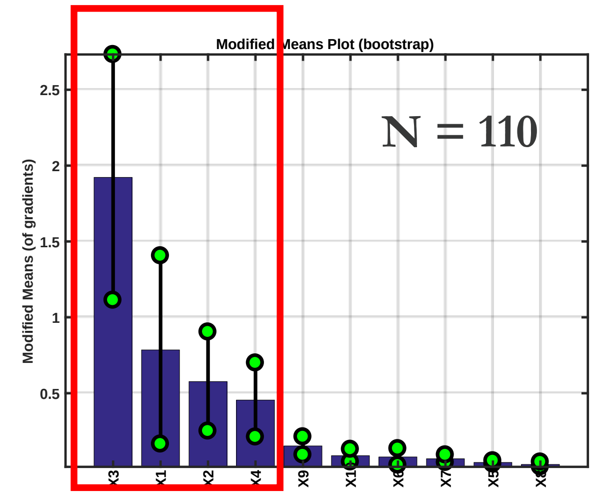
Screening study – Results





Rank	N=44	N=55	N=77	N=110
1	x3	x3	x3	x3
2	x1	x1	x1	x1
3	x2	x2	x2	x2
4	x9	x4	x4	x4
5	x6	x9	x9	x9
6	x4	x6	x6	x10





- Ranking order:
  1. $e_{p\text{-}p}$, 2. $\mu_{p\text{-}p}$, 3. $\mu_{p\text{-}w}$, 4. $e_{p\text{-}w}$
- Time for completion – 2 days to 2 months depending on k_n which determines Δt
- k_n=100 N/m for global sensitivity analysis based on screening study

Global Sensitivity Analysis (GSA)

- **Question:** What is the extent to which the input parameters or their interactions influence the quantities of interest?

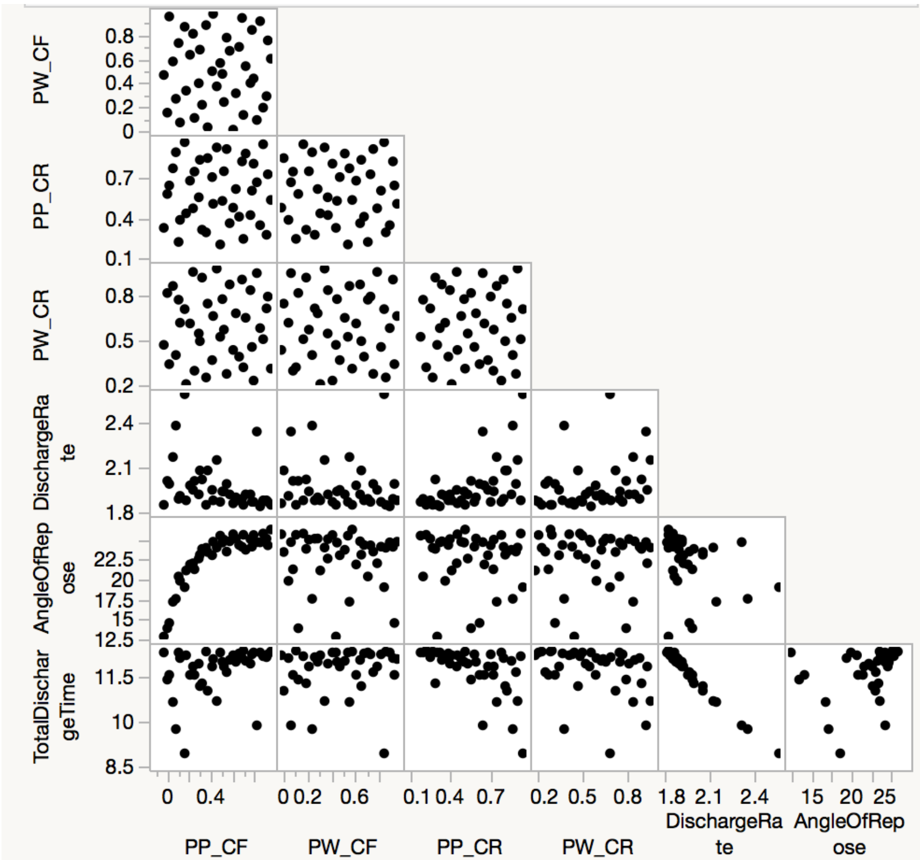
- Top four parameters determined by the screening study were selected for Global Sensitivity Analysis

- A new set of design of experiments was generated
  - 40 samples having 4 parameters varied systematically

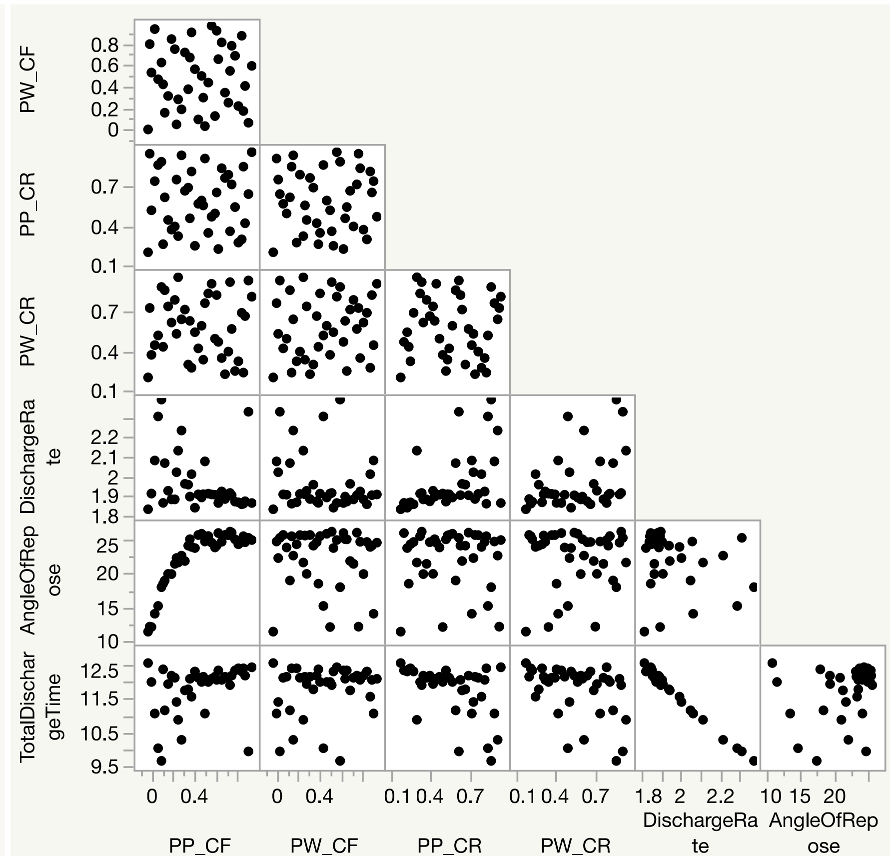
- The effect of sampling methodology was also investigated
  - Space-filling design based Optimized Latin Hypercube (OLH) sampling (R library)
  - Quasi Monte-Carlo sampling (LPTAU sampling in PSUADE UQ toolkit from LLNL)

Effect of sampling methods on GSA

OLH

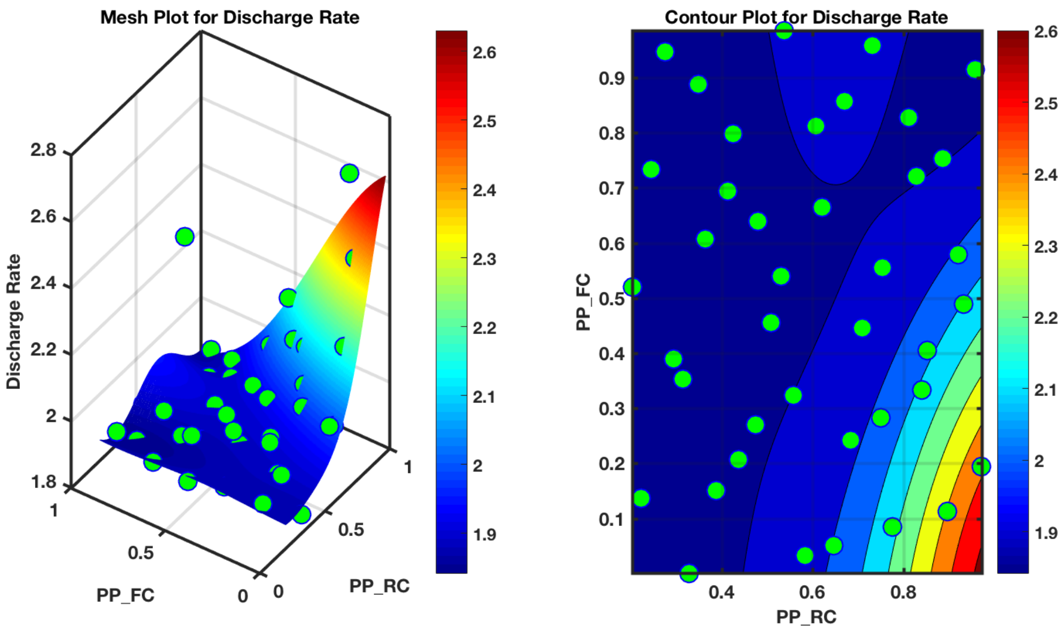


LPTAU



Surrogate model for GSA

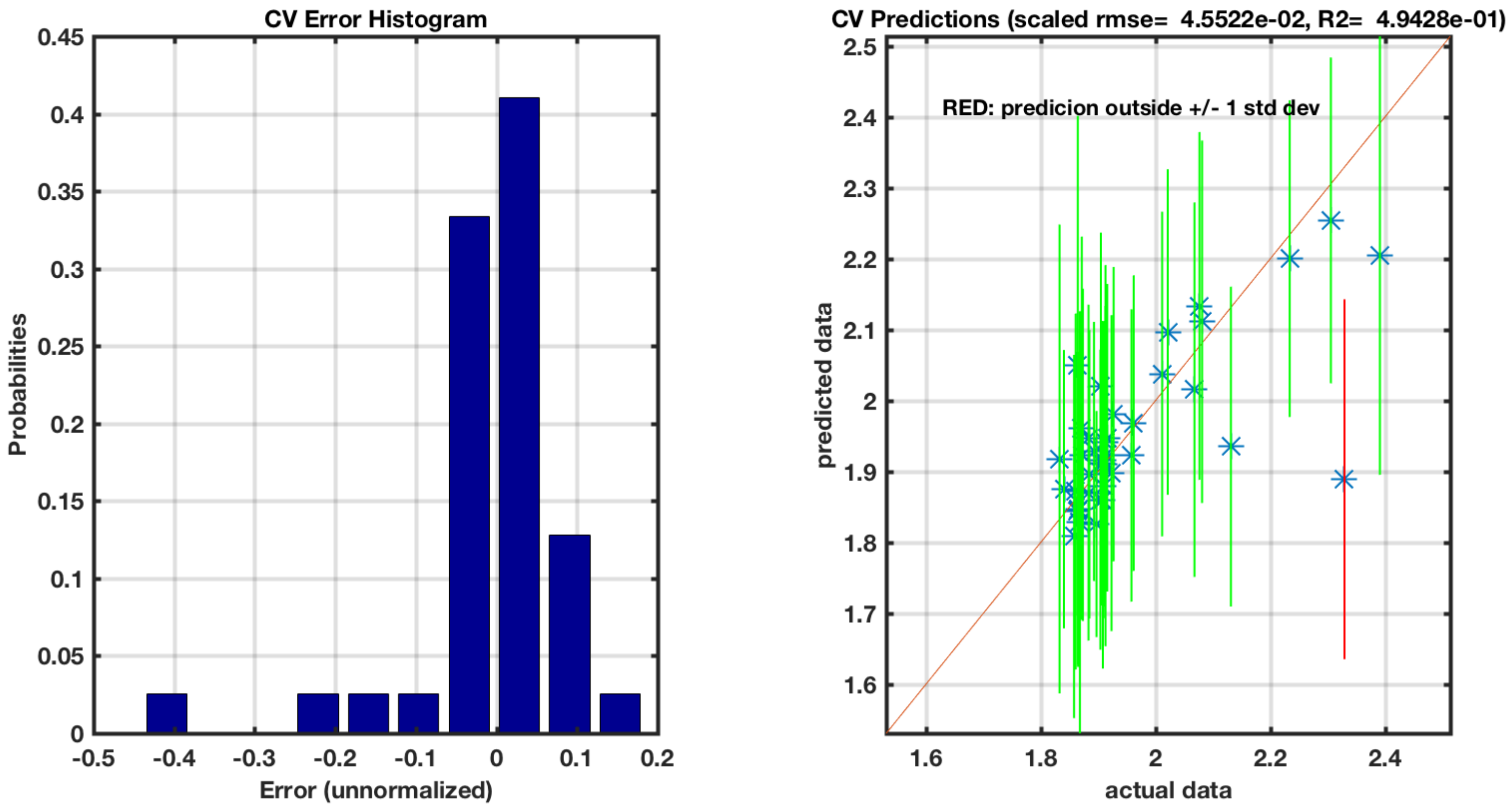
- Monte Carlo sampling based methods are computationally prohibitive for uncertainty quantification analysis of multiphase flows
- Gaussian process based surrogate model built using the OLH sampling simulation results (40 samples)



Note that other two parameters are kept at mid point settings for the construction of surrogate contour plots

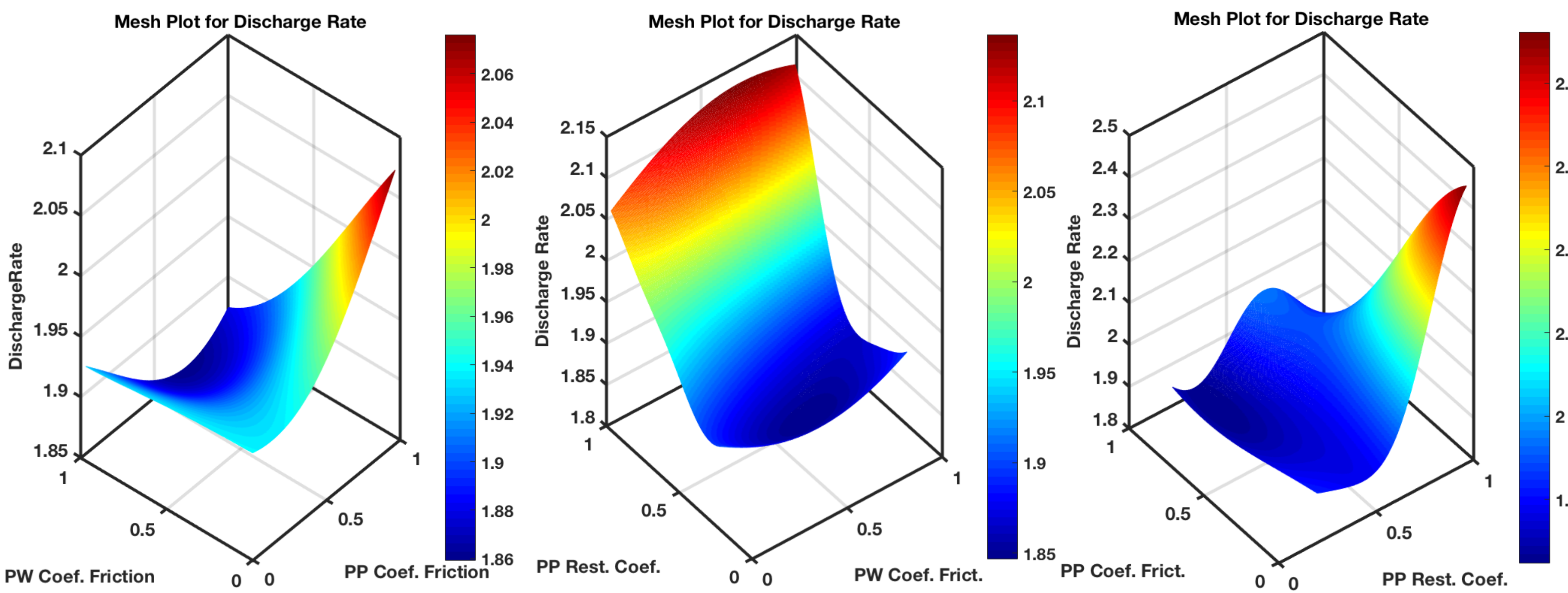
Surrogate model quality

- To assess the quality of the surrogate model perform cross validation
- One sample point outside 1σ



Surrogate model for GSA

- Similar Gaussian process based surrogate model constructed for simulation results obtained through LPTAU sampling



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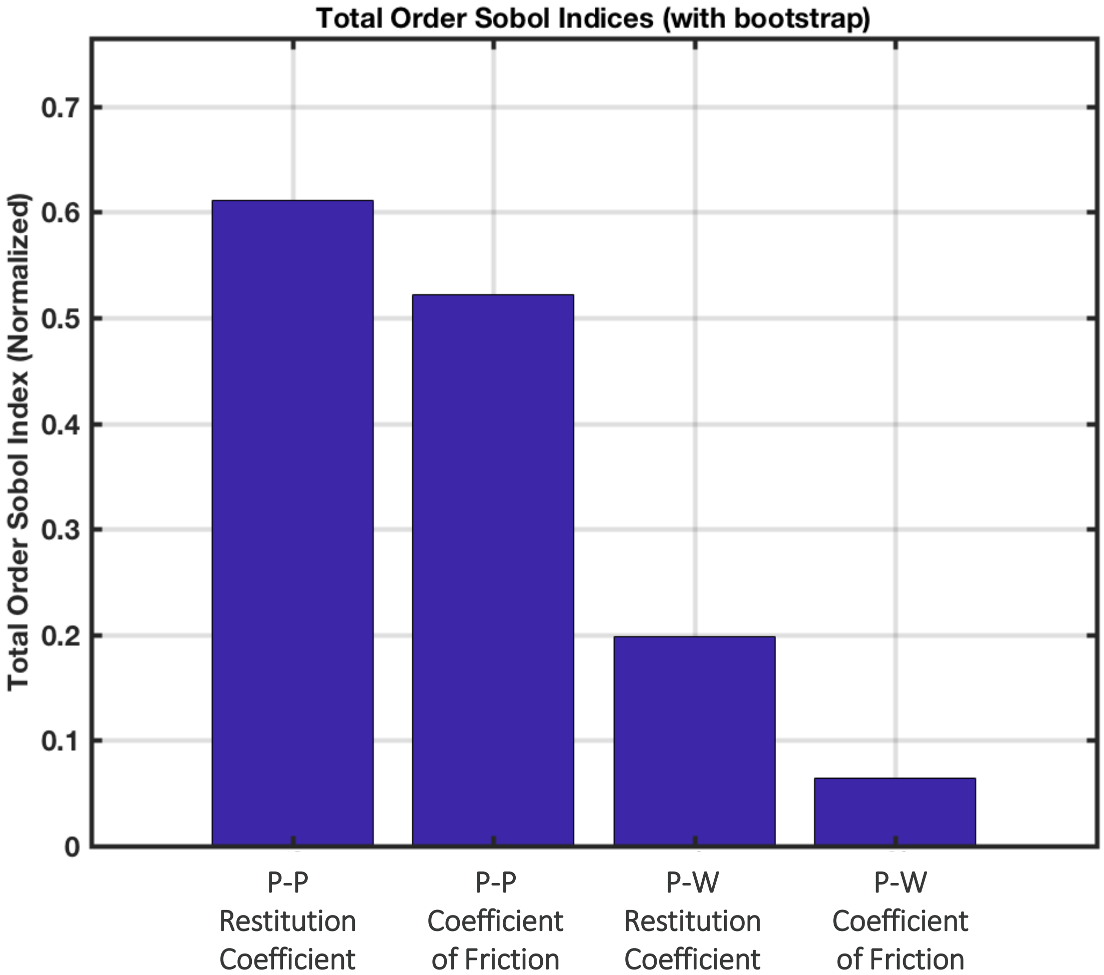
Preliminary GSA results



- Preliminary variance based sensitivity analysis: Sobols' Total Indices Method implemented in PSUADE UQ Toolkit using OLH (40 samples)
- Particle-particle coefficient of restitution is the most influential model parameter
- Analysis of interaction effects in progress

Summary

- Extension of VVUQ methodology with systematic design of experiments and simulations (work in progress)
- Bench-scale experiments to ensure quick turnaround
- 3-D printed geometries to ensure consistency with the simulations
- Survey of subject matter experts for VVUQ methodology input
- Global sensitivity analysis (GSA) shows sampling invariance, possible interaction between model parameters
- Ranking of model parameters for hopper discharge process:
    1. Particle-particle coefficient of restitution
    2. Particle-particle coefficient of friction
    3. Particle-wall coefficient of restitution
    4. Particle-wall coefficient of friction

Thank you for your attention. Questions???