

Multi-Objective Optimization Techniques using ANSYS-CFX-DesignXplorer™. Case Study: Optimization of Static Mixer

Lecturer:

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OUTLINE

1. Introduction to Global Optimization
2. Introduction to ANSYS-DesignXplorer™ (ANSYS-DX™)
3. Design of Experiments (DoE)
4. Parameters Correlation to support DoE
5. Response Surface Methods (RSM)
6. Six Sigma Analysis (SSA) and Robust Design
7. Multi-Objective Optimization

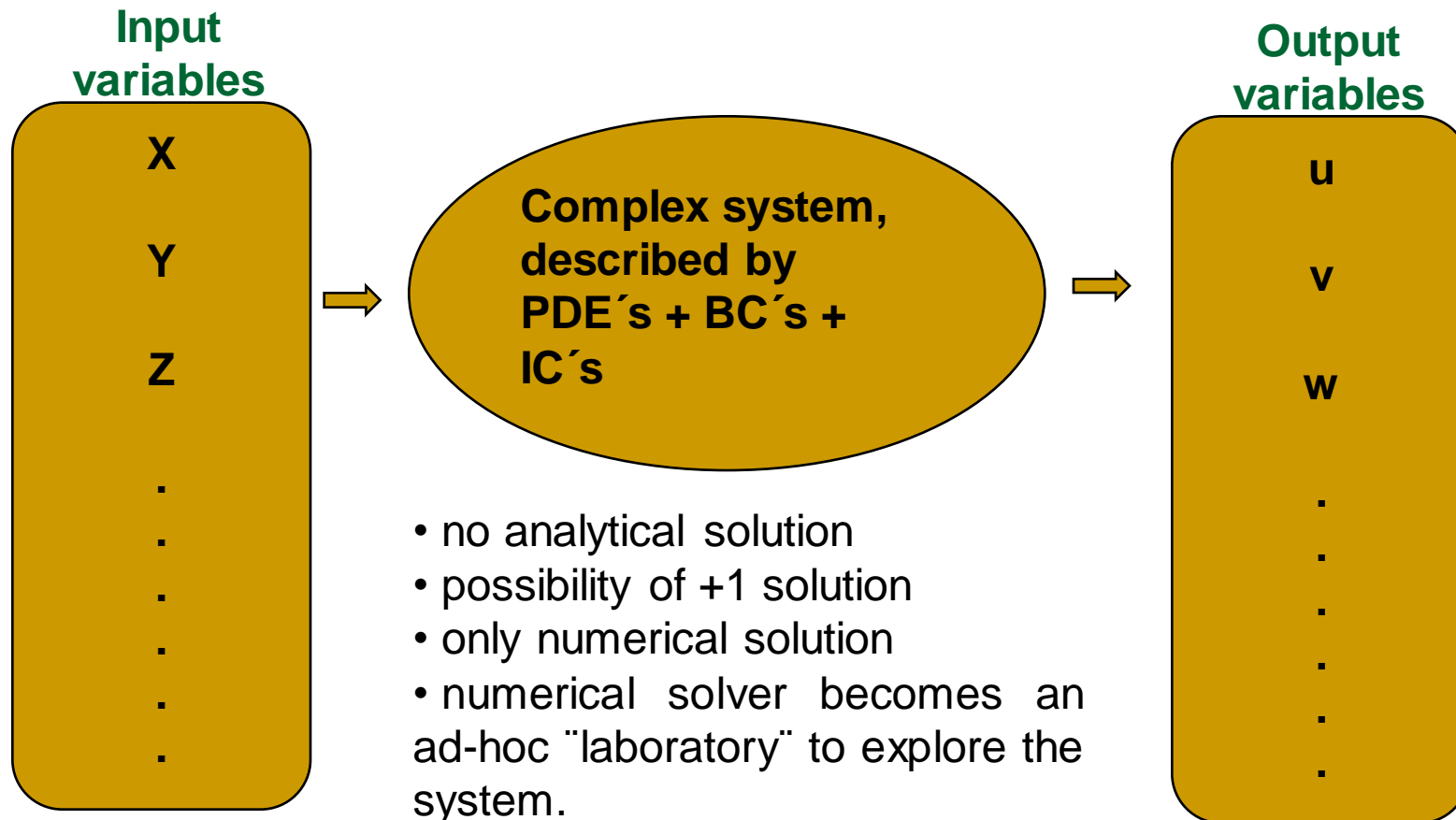
LEARNING OUTCOMES

At the end of this workshop, participants will gain basic knowledge on:

- 1. Optimization Analysis in Computer Aided Engineering applications.**
 - 1.1. Optimization premises**
 - 1.2. Design of Experiment**
 - 1.3. Response Surface**
 - 1.4. Pareto Optimization**
- 2. Creating a complex geometry in ANSYS-DesignModeler (DM).**
- 3. Parametrizing a geometry in DM.**
- 4. Parametrizing Boundary Conditions in CFX-Pre.**
- 5. Defining an Objective Function with Output functions.**
- 6. Setting up and running Optimization algorithm in ANSYS-Workbench.**

1. Introduction to Global Optimization

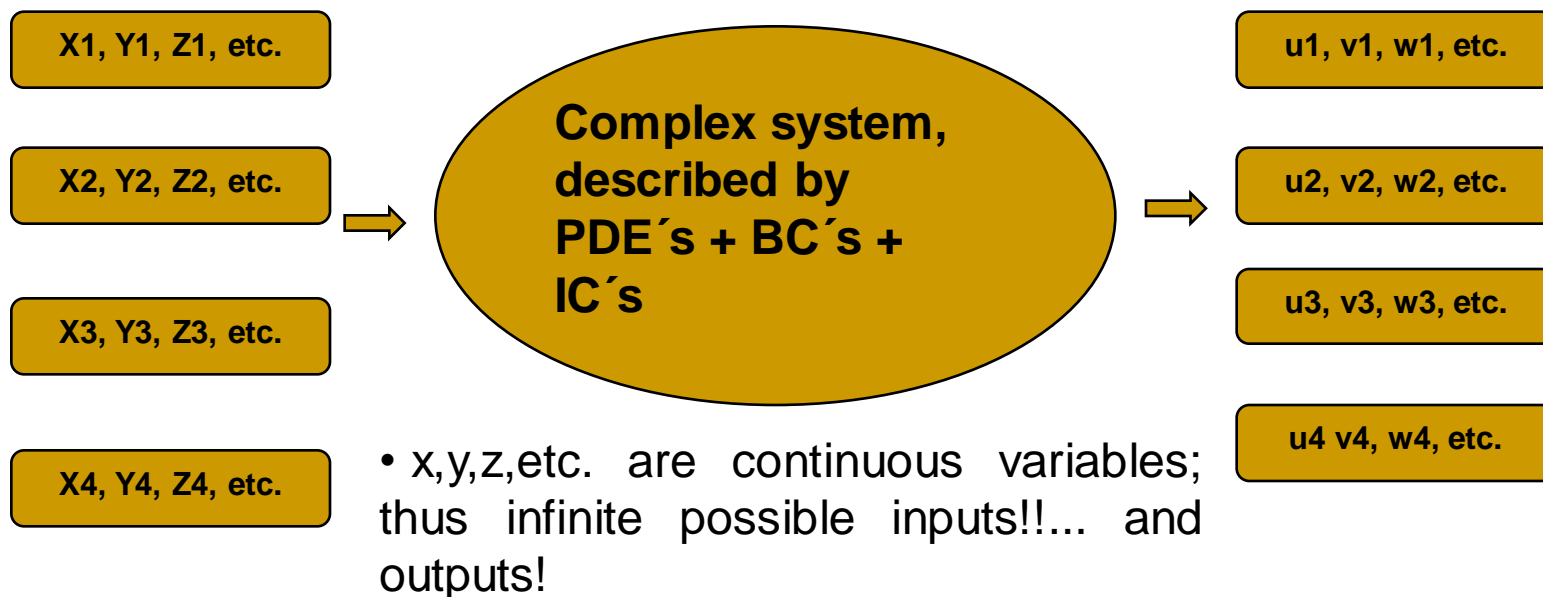
Optimization of Complex Systems



How to optimize the system performance?

1. Introduction to Global Optimization

Optimization of Complex Systems

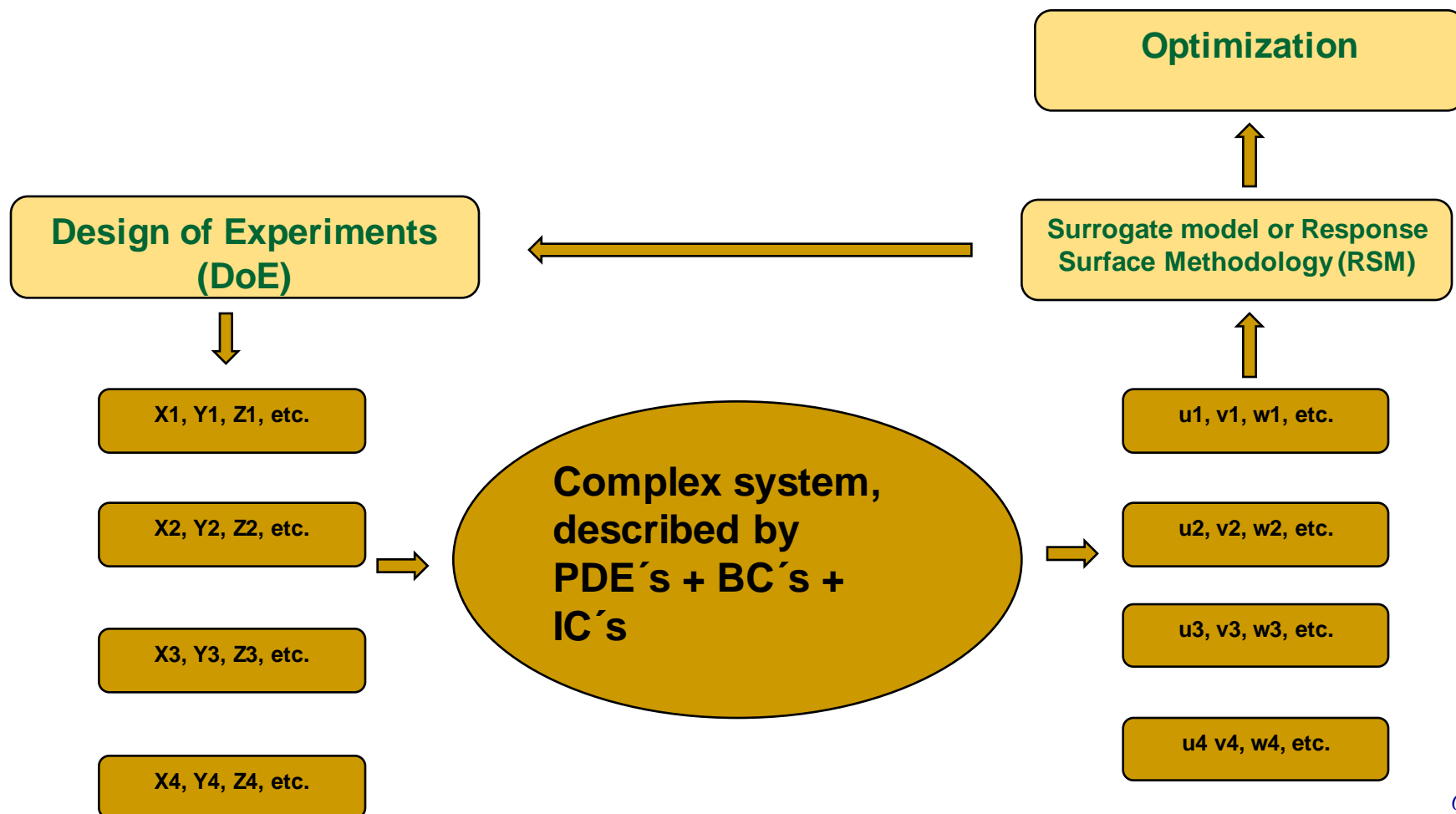


- PDE system of equations requires a large computational effort. It's not viable to run too many case studies to find optimum.

How to reduce the optimization effort?

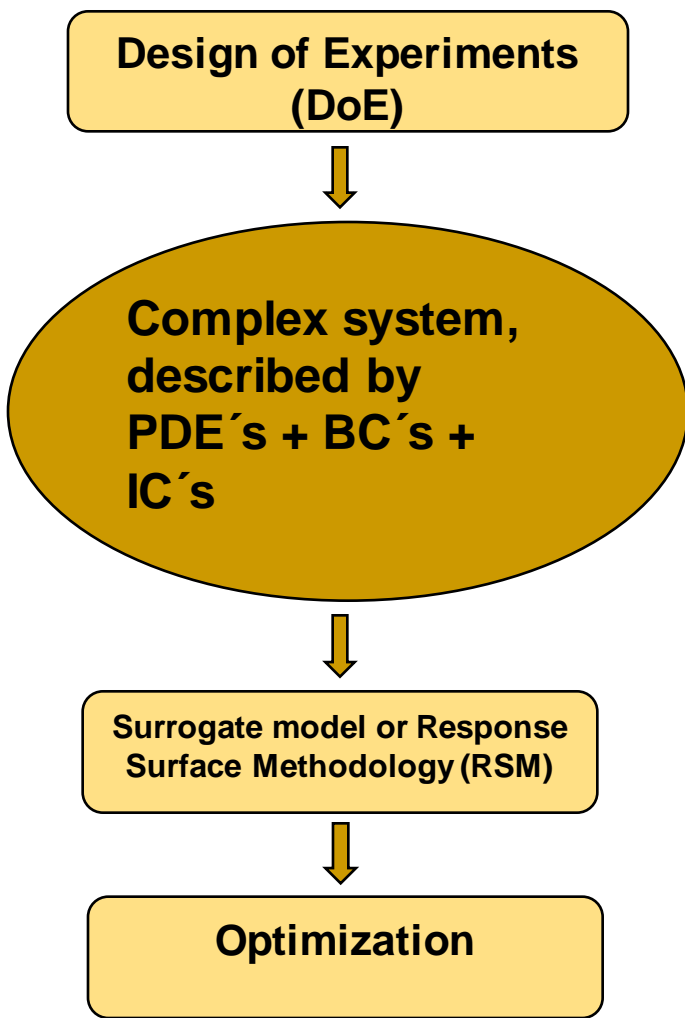
1. Introduction to Global Optimization

Optimization of Complex Systems. Schematics



1. Introduction to Global Optimization

Optimization of Complex Systems. Schematics



Questions to address

- What are the objective functions to max/min? (are there more than 1?)
- What are the constraints?
- What is the min set of Design Points to guarantee enough information to get a satisfactory RSM? How to test it?
- What is the appropriate (accurate/fast) method to max/min the RSM? How to check Local vs. Global max/min?
- What if input variables have low precision?



2. Introduction to ANSYS-DesignXplorer™ (ANSYS instructional slides)



Chapter 1

Introduction

Design Exploration



What is Design Xplorer?



- **DX Provides a tool for designing and understanding response of complex models, including uncertainties in input parameters.**
- **Supports optimization analysis via the use of Response Surface (Surrogate Model).**
- **Uses parameters from DesignModeler (DM) and ANSYS-CFX Pre to explore a wide range of scenarios, based on limited solver executions.**



Parameter Definitions . . .

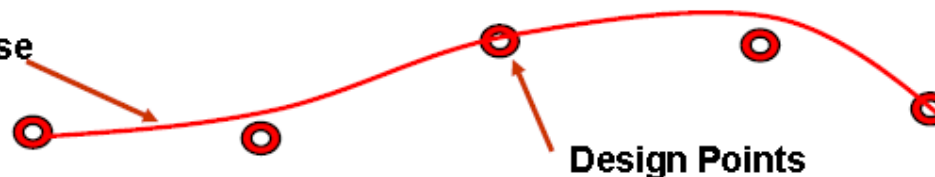
- **DX uses:**
 - **Input parameters. Example:**
 - **Geometry-related (DM)**
 - **BC's**
 - **Physical properties**
 - **Response (Output) parameters. Example:**
 - **Heat flux**
 - **Stress**
 - **Mass flow rate**
 - **Pressure drop**
 - **Derived parameters. Example:**
 - **CEL functions (cannot reference other derived param.)**
 - **Cost function (mass x cost/mass)**
 - **Average or normalized parameters.**

Method Definitions ...



- **Design of Experiments (DOE) method:**
 - **Uses a limited set of input (design) points to build Response Surface.**
- **Default DOE in DX uses Central Composite approach to choose parameter values to be solved.**
- **Once required solutions are completed, Response Surface is created (fitted) to find solutions in conditions not evaluated. See 2D example below.**

Curve fit response



3. Design of Experiments (DoE)

What is the min set of Design Points to guarantee enough information to get a satisfactory System Surrogate or RSM?

Design of Experiments (DoE). Definition.

- **Systematic and rigorous** approach for data collection in engineering problem-solving.
- Uses **statistical principles and techniques** to ensure collected data provide valid and supportable engineering conclusions.
- DoE is carried out under the premise of a **minimal expenditure of engineering runs** (experiments or simulations), time and money.
- For modeling and optimization purposes, DoE aims to provide a **good-fitting (accurate) mathematical surrogate** function (RSM).

3. Design of Experiments (DoE)

What is the min set of Design Points to guarantee enough information to get a satisfactory System Surrogate or RSM?

Design of Experiments (DoE). Steps.

- Define the **problem** and questions to be answered.
- Define the **population** of interest (range of independent variables and discretization).
- Find the appropriate **sampling** (technique and size). A sample is a scientifically drawn group of "**individuals**" that possesses the same characteristics as the population. This is true if the sample is drawn in a **random** manner.

3. Design of Experiments (DoE)

Sequence-sampling

- Latin Square & Hypercube and Monte Carlo sampling
- Full Factorial & Reduced Factorial
- Central Composite Design (CCD) (ANSYS-DX™)
- Optimal Space-Filling Design (ANSYS-DX™)
- Box-Behnken

3. Design of Experiments (DoE)

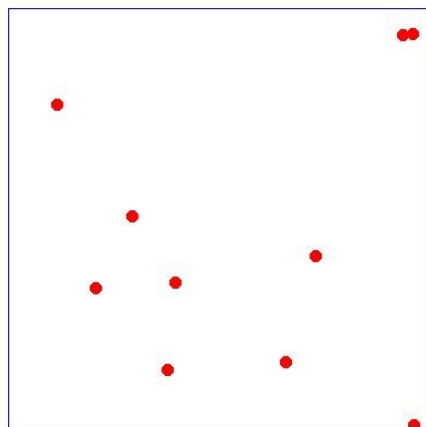
Latin Hypercube y Monte Carlo Sampling

- **Latin Hypercube (LHS)** and **Monte Carlo** algorithms generate “**random**” sampling, according to several statistical distributions (**Normal**, **Cauchy**, **Weibull**, etc.).
- **LHS** is the generalization of **Latin Square** sampling extended to an arbitrary number of dimensions. **Latin Square** is a square grid with sampling positions such that there is only **one sample in each row and each column**.
- **LHS** is a (restricted) **Monte Carlo** sampling. Sometimes, further improved by introduction of **uniformity**.

3. Design of Experiments (DoE)

Uniform Latin Hypercube sampling

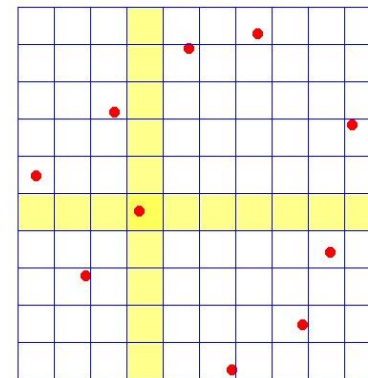
Pseudo-random (Monte Carlo)



$n = 10$

n values are chosen independently, according to the function of **global uniform density**

Uniform Latin Hypercube



The uniform statistical distribution is divided in " n " intervals with same probability. Thus, a **quasi-random** value is chosen in each interval.

Uniformity is guaranteed !

3. Design of Experiments (DoE)

Factorial sampling

Full factorial: Number of designs = m^n

m = base of each variable (number of possible values)

n = number of design variables

- It gives all the information related to the **interaction among variables**.
- The number of experiments increases by a **factor of m** per variable added.

3. Design of Experiments (DoE)

Example of Factorial DoE

2-level Full Factorial, n variables or factors

2ⁿ Experiments permit to calculate 1st-order interactions

n. design	x1	x2	x3	fit
1	+	+	+	f1
2	+	+	-	f2
3	+	-	+	f3
4	+	-	-	f4
5	-	+	+	f5
6	-	+	-	f6
7	-	-	+	f7
8	-	-	-	f8

*Function with 3 input
variables (x_1, x_2, x_3) $0 < x_i < 1$*

range $[0, 0.5] \Rightarrow -$

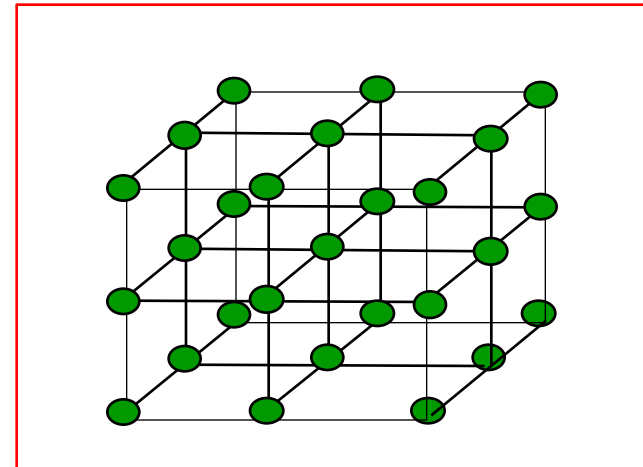
range $[0.5, 1] \Rightarrow +$

3. Design of Experiments (DoE)

Factorial DoE. 3-level, n variables.

3-level Full Factorial

3^n Experiments permit
calculation of 2nd-orden
interactions



3 variables

27 experiments

3. Design of Experiments (DoE)

Factorial DoE. Pros and Cons

Full Factorial Pros:

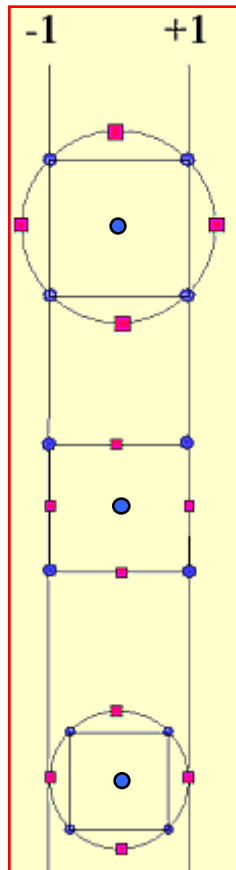
- ❑ For each variable, we have the same number of designs in (+)range and (-)range.
- ❑ Gives knowledge about interaction among all variables.

Full Factorial Cons:

- ❑ For a large number of variables, the number of required designs becomes really huge.

3. Design of Experiments (DoE)

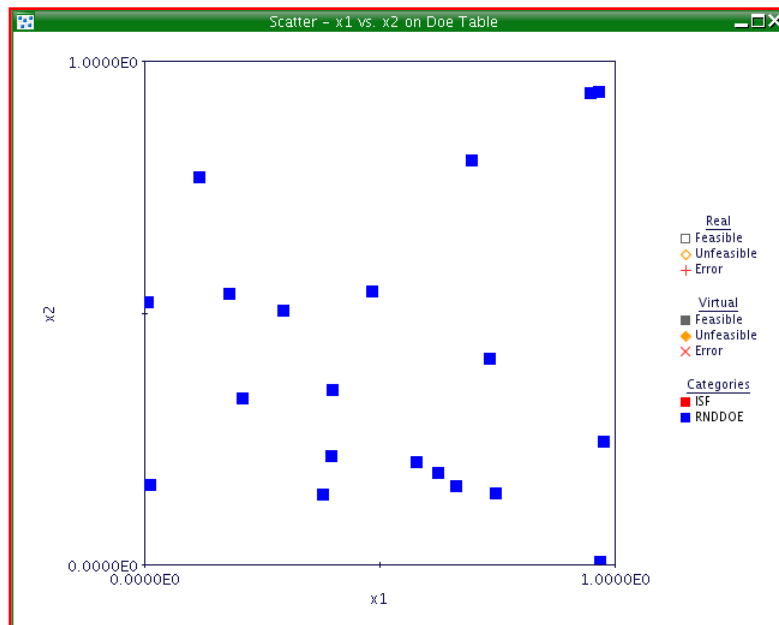
(Box-Wilson) Central Composite Design (CCD) (ANSYS-DX™)



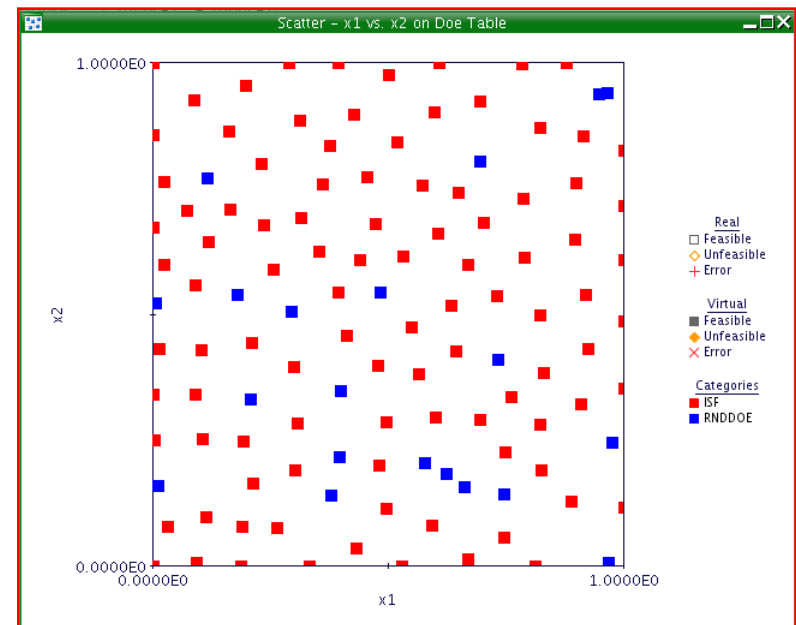
- Original **CCD**. Expands original design limits and requires 5 levels for each variable (factor). Also called **circumscribed** or **rotatable**.
- **Face Centered** with star points at center of each face. Requires only **3 levels**.
- **Inscribed CCD**, used when limits have to be strictly respected. Also requires **5 levels**.

3. Design of Experiments (DoE)

Optimal Space-Filling Design (ANSYS-DX™)



Existing design points
(previously generated)



New points are added to
uniformly fill gaps.

4. Parameters Correlation to support DoE

- Before building a definitive DoE table for RSM and/or Optimization purposes, we may find that our problem has too many input parameters.
- Two many input parameters may turn the problem intractable in terms of sampling points. Then, a previous Parameters Correlation exercise may help us to answer:
 - What are the most important **design variables**?
 - Can we **reduce** the variables space?
 - What is a reasonable number of **objectives and constraints** to be defined?

4. Parameters Correlation to support DoE

Parameters Correlation in ANSYS-DX™

- It is a preliminary DoE exercise. Sampling is based in **Latin Hypercube** sequence, with correlation of input parameters smaller than 5%.
- If Auto Stop is enabled, simulations (DP's) stop when levels of Mean and Standard Deviation error reach the specified level or maximum number of samples is reached.
- An exhaustive examination of DoE (**Pearson**, **Spearman**, etc.) accelerates the optimization process, by reducing de number of variables in the parametric analysis.
- The statistical tools though, need DoE tables that **correctly** represent the design space.

4. Parameters Correlation to support DoE

Dependence and Correlation

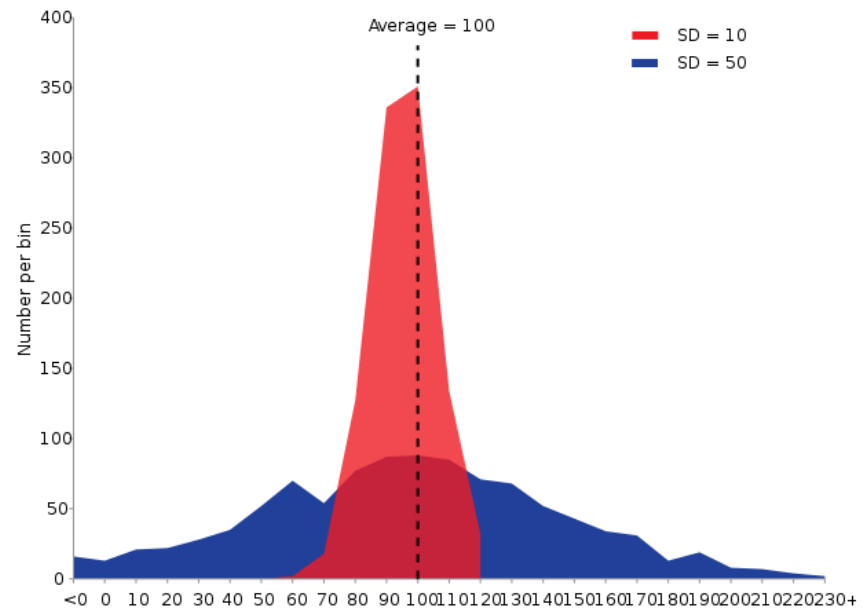
- **Dependence:** refers to any statistical relationship between two variables or sets of data.
- **Correlation:** refers to any of a broad class of statistical relationships involving dependence. Mostly, related to standard deviation, variance and co-variance.
 - **Pearson correlation**
 - **Spearman correlation**

4. Parameters Correlation to support DoE

Pearson and Spearman Correlations

- **Standard deviation** : measures the **variation** or **dispersion** for a given variable, from its **mean value**.

$$\sigma = \sqrt{\frac{\sum x_i^2}{n} - \left(\frac{\sum x_i}{n}\right)^2}$$



4. Parameters Correlation to support DoE

Pearson and Spearman Correlations

- **Covariance σ_{xy} :** measures how two statistical variables change together. Its value depends on the units used for the variables.
- If X grows when Y grows and X decays when Y decays, then covariance is positive and large; and viceversa.
- If there is no *linear* relation between X and Y, then $\sigma_{xy} = 0$.

4. Parameters Correlation to support DoE

Pearson and Spearman Correlations

- **Pearson correlation ρ_{xy} :** normalizes the covariance and takes values $[-1,1]$. 1 means a perfect linear relationship with positive slope; while, -1 means the opposite. 0 means no linear relationship at all (i.e., no correlation or a nonlinear relation may exist).

$$\rho_{xy} = \frac{\sigma_{xy}}{\sigma_x \sigma_y} = \frac{\sum_{i=1}^n ((x_i - \bar{x})(y_i - \bar{y}))}{\sqrt{\sum_{i=1}^n (x_i - \bar{x})^2 \sum_{i=1}^n (y_i - \bar{y})^2}}$$

4. Parameters Correlation to support DoE

Geometrical interpretation of Pearson Correlation:

Given two variables V and T , for example, measured over a universe of "n" points within the space, treating both variables as vectors in the n-dimensional space: $V (V_1, V_2, \dots, V_n)$ and $T(T_1, T_2, \dots, T_n)$. **Centering** these vectors around the mean:

$$V(V_1 - \bar{V}, V_2 - \bar{V}, \dots, V_n - \bar{V}) \quad \text{and} \quad T(T_1 - \bar{T}, T_2 - \bar{T}, \dots, T_n - \bar{T})$$

$$r = \cos(\alpha) = \frac{\sum_{i=1}^N (x_i - \bar{x})(y_i - \bar{y})}{\sqrt{\sum_{i=1}^N (x_i - \bar{x})^2} \sqrt{\sum_{i=1}^N (y_i - \bar{y})^2}}$$

If $r = 1$, $\alpha = 0^\circ$

If $r = 0$, $\alpha = 90^\circ$

If $r = -1$, $\alpha = 180^\circ$

4. Parameters Correlation to support DoE

Pearson and Spearman Correlations

- **Spearman correlation:**

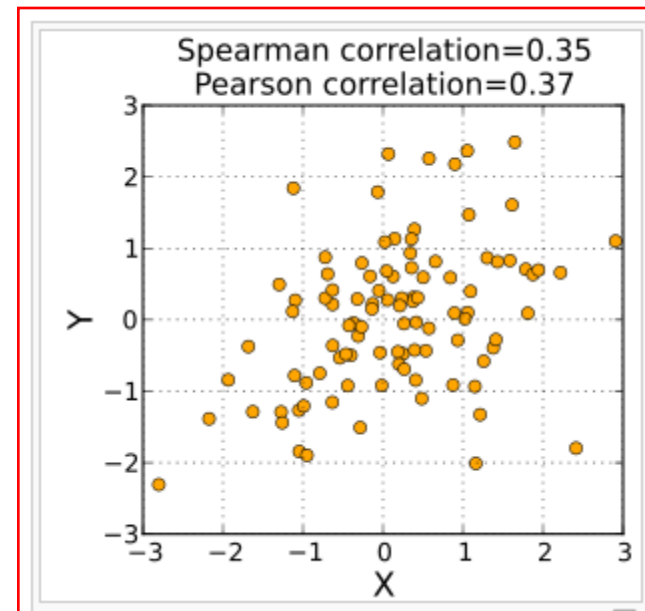
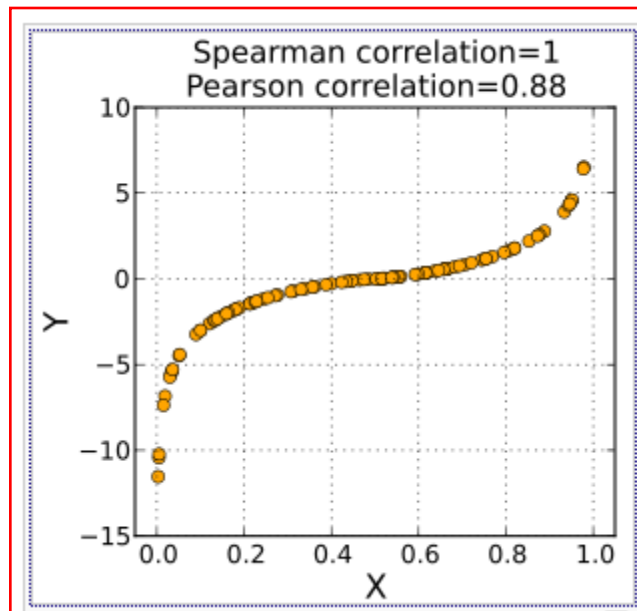
$$\rho_{xy} = 1 - \frac{6 \sum d^2}{n(n^2 - 1)}$$

- Once the first variable is ordered from small to large (rank), then the rank to the second variable is established. Then, $d = \text{abs}(\text{Rank}_x - \text{Rank}_y)$.
- For samples larger than 20, it can be approximated with the **t-Student parameter**.

4. Parameters Correlation to support DoE

Pearson and Spearman Correlations

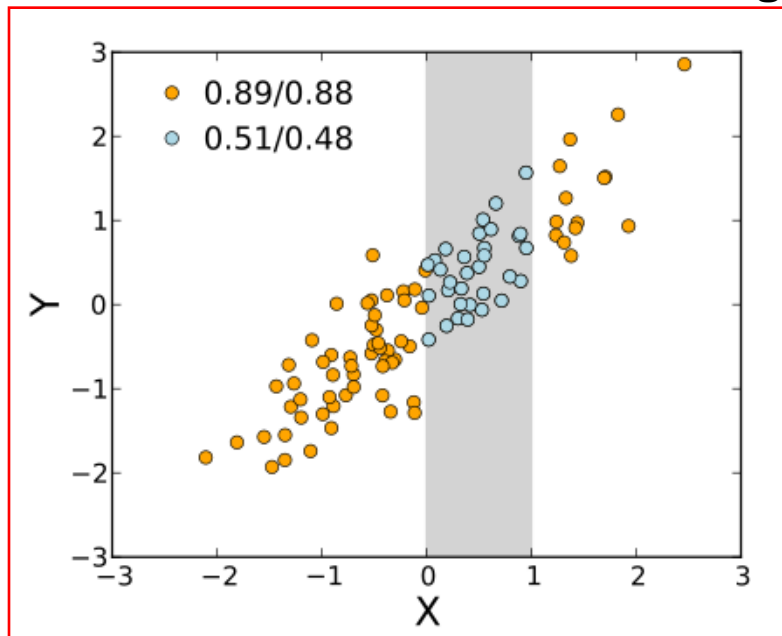
- **Spearman correlation ρ_{xy} :** measures the statistical dependence between two variables. If the dependence is perfectly *monotonic* with positive slope, then $\rho_{xy}=1$, -1 means the opposite.



4. Parameters Correlation to support DoE

Pearson and Spearman Correlations

■ Spearman and Pearson correlations vs. range dependence

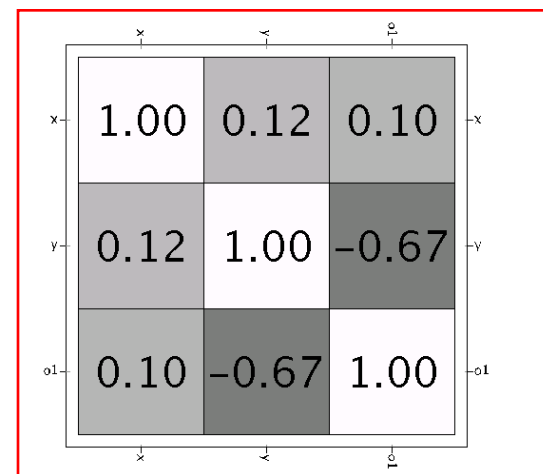
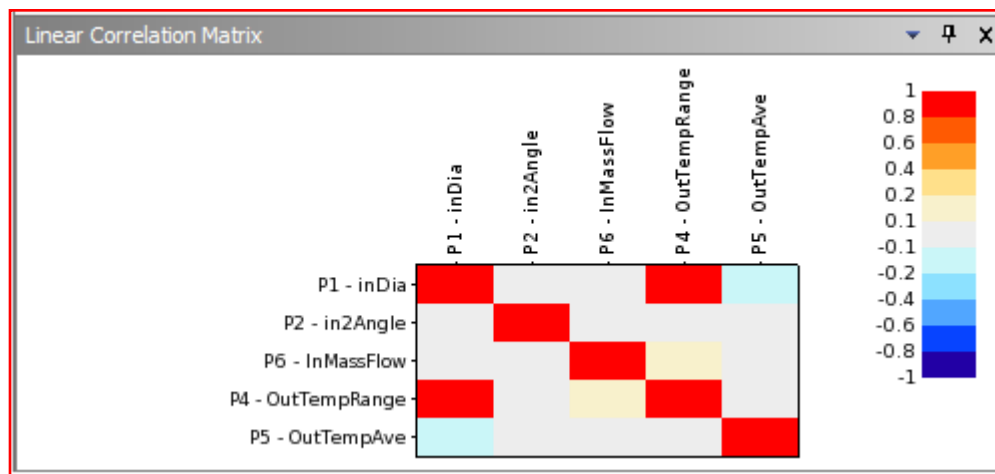


Pearson/Spearman correlation coefficients between X and Y for unrestricted ranges and when the range of X is restricted to (0,1).

4. Parameters Correlation to support DoE

(Linear) Correlation Matrix in ANSYS-DX™

- Shows correlation (between -1 y 1) among all variables.
- If Pearson, it measures linear relation; if Spearman, it measures monotonic dependence.



4. Parameters Correlation to support DoE

(Non-linear/Quadratic) Correlation in ANSYS-DX™

- Sometimes, we'd like to evaluate the non-linear dependence between two parameters.
- ANSYS-DX™ performs a quadratic least-square fitting ($Y_f = a + b.X + c.X^2$) and calculates the Regression Coefficient R and the Coefficient of Determination R^2 :

Sum of Squared Errors:

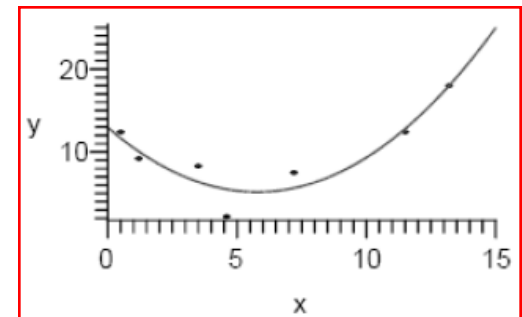
$$SSE = \sum_{i=1}^n (Y_i - Y_{fi})^2$$

Sum of Squared (Value-Mean):

$$SST = \sum_{i=1}^n (Y_i - \bar{Y})^2$$

Correlation Coefficient and Coefficient of Determination:
(the closer to 1 the larger quadratic dependence)

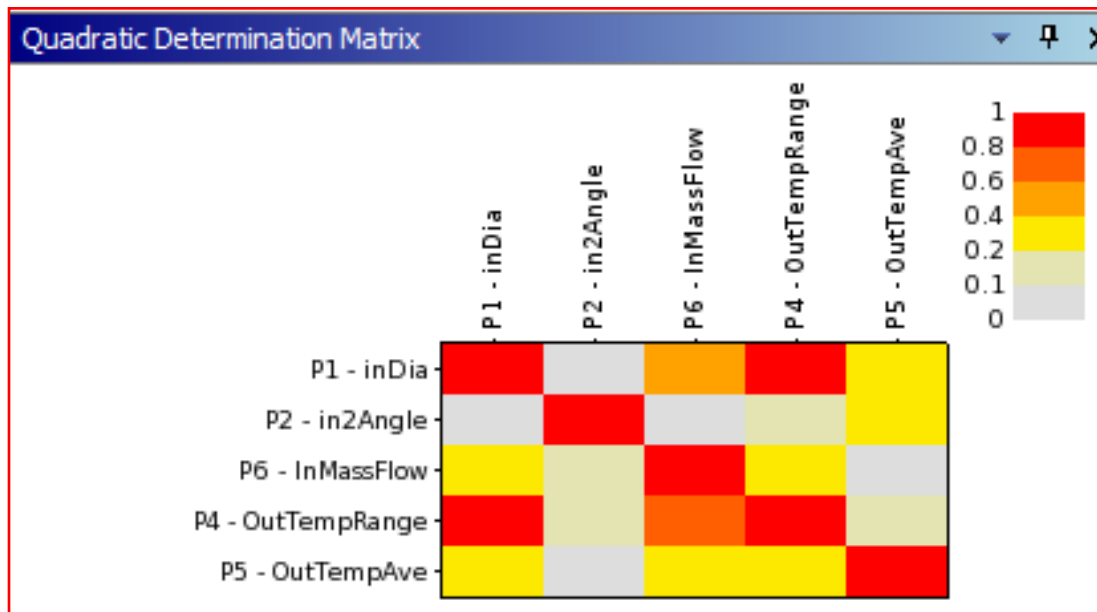
$$R = \sqrt{1 - \frac{SSE}{SST}} \Rightarrow R^2 = 1 - \frac{SSE}{SST}$$



4. Parameters Correlation to support DoE

(Quadratic) Determination Matrix in ANSYS-DX™

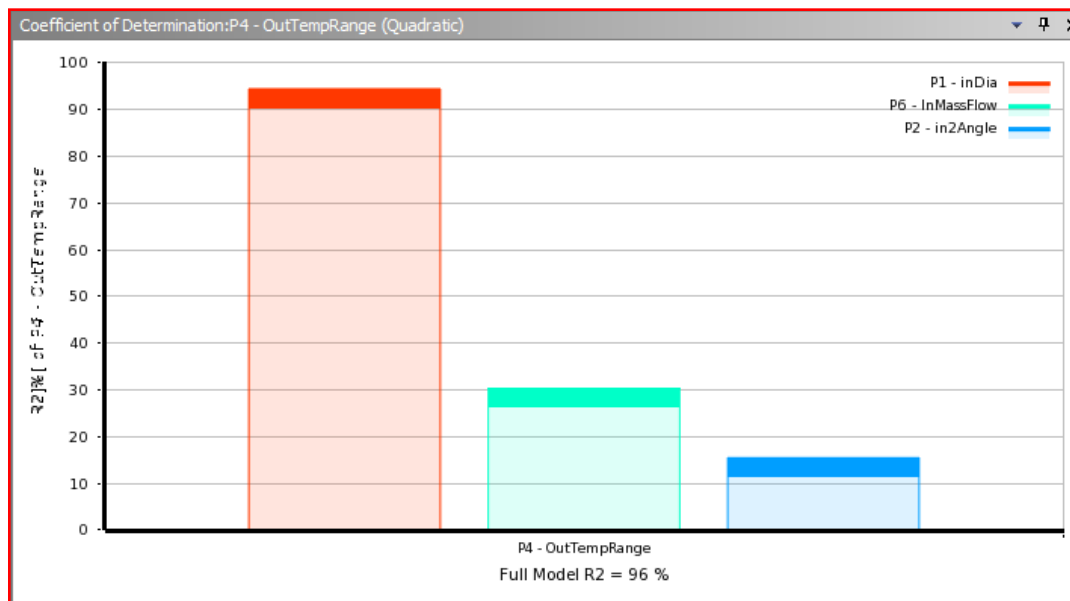
- The Coefficient of Determination R^2 is displayed for every pair of parameters. The closer to 1, the better the quadratic regression is.
- The Determination Matrix (R^2) is not symmetric:



4. Parameters Correlation to support DoE

Determination Histogram in ANSYS-DX™

- Might be based on linear or quadratic Determination Coefficient R^2 of the full model for a given output parameter vs. input parameters.
- User sets the linear/quadratic, threshold to show influence and output parameter.



Problem Overview

ANSYS-DX Tutorial: Optimizing Flow in a Static Mixer

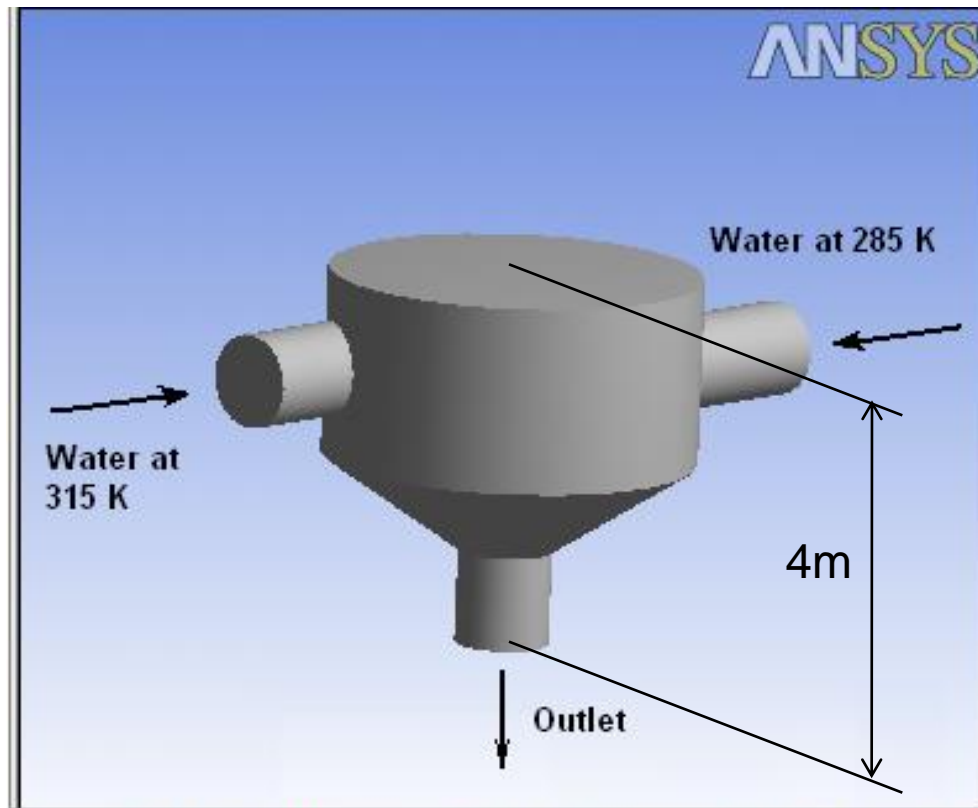
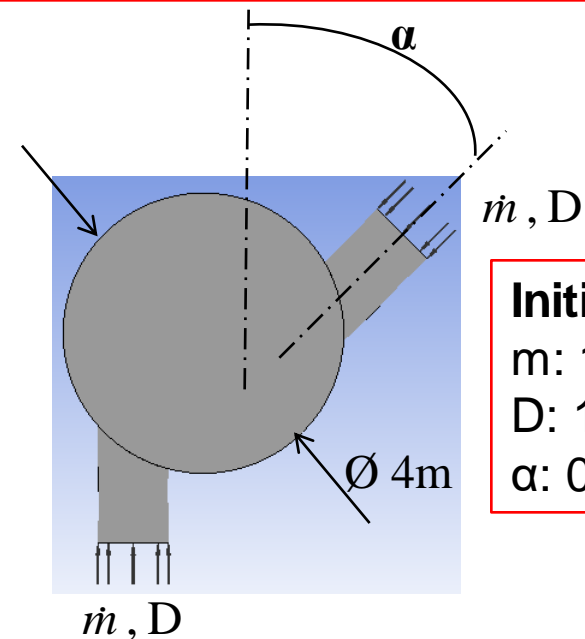


Figure 1. Static Mixer with 2 Inlet Pipes and 1 Outlet Pipe

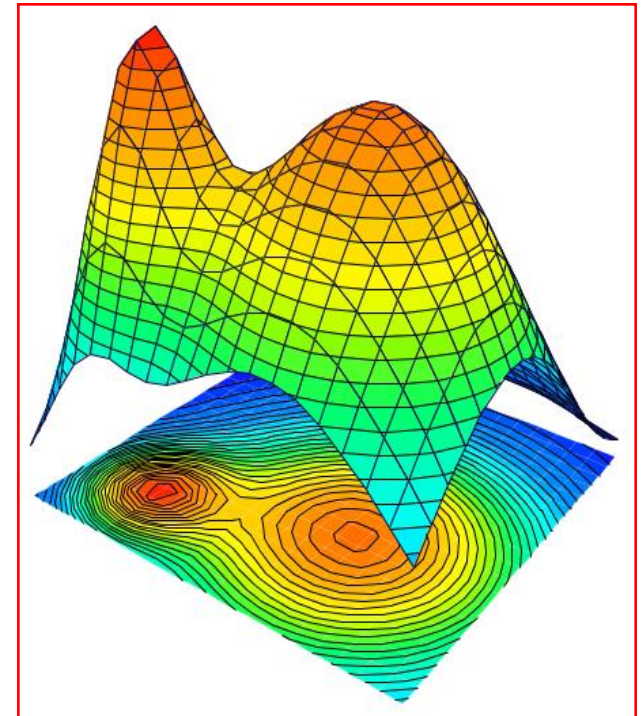
What are the combination of m , D and α to obtain an optimum stream mixing?



Initial values
 m : 1500 kg/s
 D : 1m
 α : 0 degrees

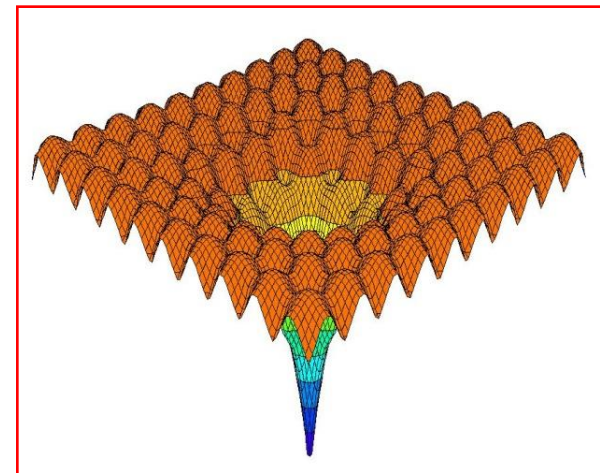
5. Response Surface Methods (RSM)

Response Surface Methodologies (RSM), with special attention to ANSYS-DX™



5. Response Surface Methods (RSM)

- RSM is typically an **empirical relationship** between a variable y and a set of independent variables X_1 , X_2 , etc.).
- Typically used in engineering to build approximate **surrogates of higher-order** analytical tools (e.g., FEA, CFD, ect.).
- Predictions within the space design are called interpolation, while those outside it are called extrapolations and require caution from user.



5. Response Surface Methods (RSM)

RSM in ANSYS-DX™

- Standard Response Surface or **Full 2nd Order Polynomial** (default)
- **Kriging** (accurate interpolation method).
- **Non-parametric Regression**: provides improved RS and requires **initial seed** from a previous DoE.
- **Neural Network**: non-linear statistical approximation inspired from biological neural network operation. Number of Cells controls the quality of the RSM. Typically, it should range from 1 to 10; 3 is the default.
- **User Response Surface** (analytical expression).

5. Response Surface Methods (RSM)

Standard Response Surface or Full 2nd Order Polynomial

- It should be always the first to try due to its low cost and simplicity.
- This method finds coefficients that minimize the sum of **standard deviations squared** between DP's and fitted curve.
- It requires at least **6** DP's. **As a reference**, min number of DP's: Linear metamodels (3); Quadratic (6); Cubic (10).

5. Response Surface Methods (RSM)

Kriging*

- **Very accurate** methodology, belonging to **linear** least squares fitting methodologies.
- Not very computational expensive.
- Can **interpolate** a given field with limited DP's but keeping the theoretical spatial correlation.
- Originally developed for geosciences, but currently widely used in hydrology and other earth sciences.

(*) Named after Daniel Krige's Master Thesis, under the advisorship of Professor Georges Matheron (France)

5. Response Surface Methods (RSM)

Non-Parametric Regression (NPR)

- It is recommended for predicted high **non-linearity** between input and output variables.
- Assumes a **quadratic relationship** between output and minimum number of inputs given at chosen hyperplanes, assuming that such DP's represent the output properly.
- Once this reduced set of DP's is chosen, a **Quadratic training function** is used to fit the RS.

5. Response Surface Methods (RSM)

Neural Network

- **Neural Network (NN)** is inspired in the human brain neural system operation. **NN's** are widely used to solve **complex problems**.
- The behavior of a **NN** is defined by the way its **neurons** are connected.
- A **NN** may **learn**, but also may be **trained** to perform a specific task.
- **NN's** are not limited by normality or linearity.

5. Response Surface Methods (RSM)

Goodness to Fit Analysis (1/4)

Once a RSM has been performed, clicking on any Output Parameter will give the Goodness-to-fit option to its RSM, based on current DP's, but also, we can create Verification Points (VP's) to test the fitness. Fitness can be assessed by:

- **Coefficient of Determination R^2 (CD):**

where,

y_i = value of the output parameter at the i -th sampling point

\hat{y}_i = value of the regression model at the i -th sampling point

\bar{y} is the arithmetic mean of the values y_i

σ_y is the standard deviation of the values y_i

N = number of sampling points

P = number of polynomial terms for a quadratic response surface (not counting the constant term)

$$1 - \frac{\sum_{i=1}^N (y_i - \hat{y}_i)^2}{\sum_{i=1}^N (y_i - \bar{y})^2}$$

5. Response Surface Methods (RSM)

Goodness to Fit Analysis (2/4)

- Adjusted Coefficient of Determination (ACD):

$$1 - \frac{N-1}{N-P-1} \frac{\sum_{i=1}^N (y_i - \hat{y}_i)^2}{\sum_{i=1}^N (y_i - \bar{y})^2}$$

- Maximum Relative Residual (MRR):

$$\max_{i=1:N} \left(\text{Abs} \left(\frac{y_i - \hat{y}_i}{\bar{y}} \right) \right)$$

- Root Mean Square Error:

$$\sqrt{\frac{1}{N} \sum_{i=1}^N (y_i - \hat{y}_i)^2}$$

- Relative Maximum Absolute Error:

$$\frac{1}{\sigma_y} \max_{i=1:N} (\text{Abs}(y_i - \hat{y}_i))$$

5. Response Surface Methods (RSM)

Goodness to Fit Analysis (3/4)

Physical meaning or application:

- **Coefficient of Determination (CD).** Determines if the Response Surface were to pass through the DP's. In such a case, **CD =1 (Kriging)**.
- **Adjusted Coefficient of Determination (ACD).** Appropriate if there are **less than 30 DP's**.
- **Maximum Relative Residual.** Maximum distance from all DP's from calculated DP's out of the Response Surface.
- **Root Mean Square Error.** Square root of average square of residuals at DoE points for regressions. For **Kriging**, it is 0.
- **Relative Maximum Absolute Error.** Absolute max. **normalized with σ** .
- **Relative Average Absolute Error.** Similar as before, but uses average.

5. Response Surface Methods (RSM)

Goodness to Fit Analysis (4/4)

Graphical Rating of Results:

- Rating is divided in 6 scales: "****", "***", "**", "+", "++", "+++".
- While "****" is the best possible result, "+++" is the worst.
- The rating is used only for bounded features. For example, the root mean square error is not rated graphically because it is not bounded.
- Between the "*" and "+" scale ratings there is a "-" (neutral) rating.
- Calculation is as follows:

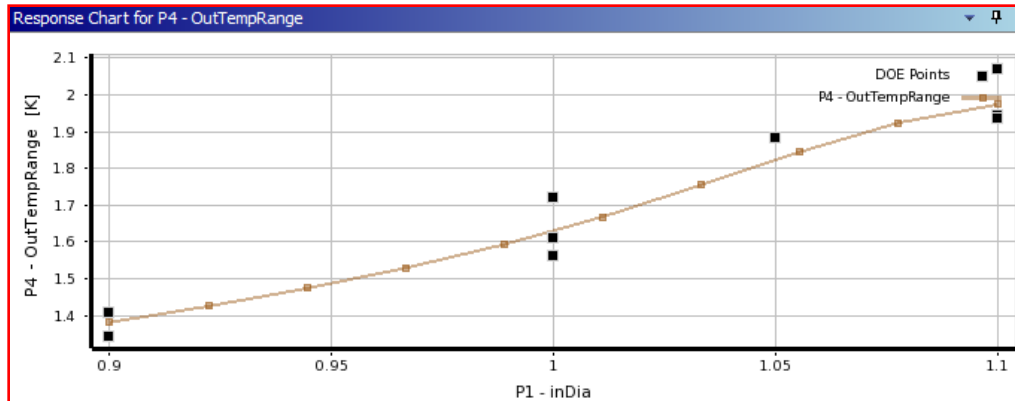
Given a feature that goes from 0 to 100, being 100 the best, if we have the actual value of it equal to 70, then:

$((\text{Abs}(70-100))/(100-0))*6 - (6/2) = -1.2 \approx -1 (\equiv "**")$. Negative means better!

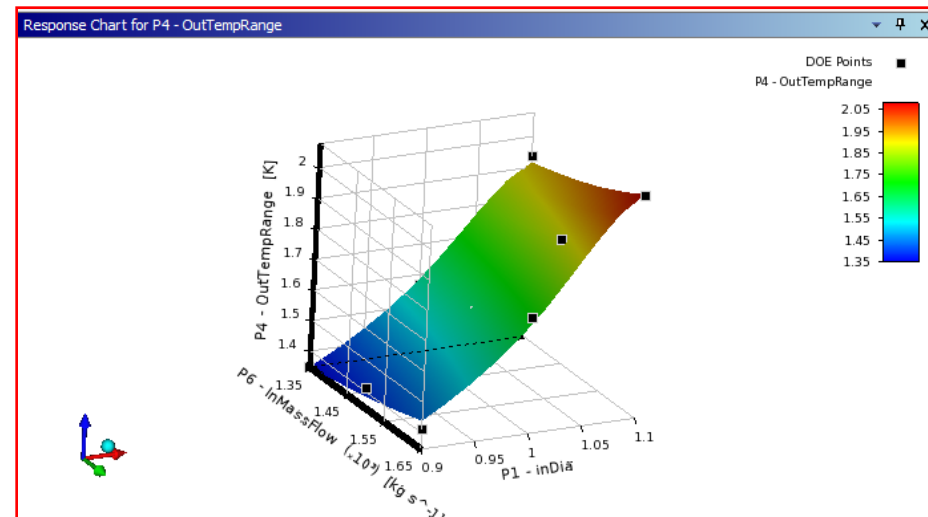
If "0" is the best, then the equation changes to: "...Abs(70-0)..."

5. Response Surface Methods (RSM)

Plots (1/3)



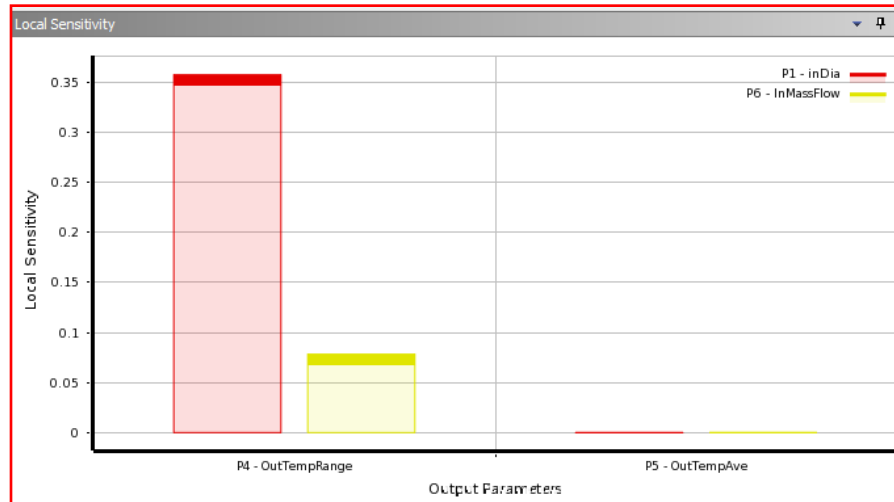
2D RSM fitting



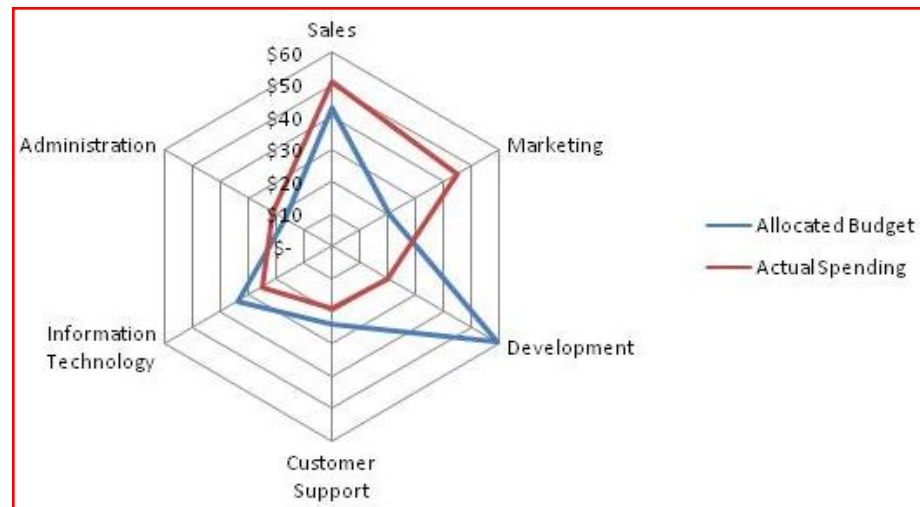
3D RSM fitting

5. Response Surface Methods (RSM)

Plots (2/3)



Local Sensitivity (around a given Response Point)



Spider Plot (multivariate data)

Properties of Schematic B3: Response Surface

	A	B
1	Property	Value
2	General	
3	Component ID	Response Surface
4	Directory Name	GDO
5	Design Points	
6	Preserve Design Points After DX Run	<input checked="" type="checkbox"/>
7	Retain Files for Preserved Design Points	<input checked="" type="checkbox"/>
8	Meta Model	
9	Response Surface Type	Standard Res...
10	Refinement	
11	Refinement Type	Manual
12	Verification Points	
13	Generate Verification Points	<input checked="" type="checkbox"/>
14	Number of Verification Points	1

Preserve DP's

Standard 2nd-order
polynomial RSM
(Default)

Optional Verification
Points, set to 1

Let's first start with 2nd order polynomial **RSM** and 1 **Verification Point (VP)**. VP's are located by the algorithm as far as possible from DP's, but not used to build the RSM. After the RSM is generated, the VP's are run and compared to RSM predictions to check the **Goodness of Fit**.

Goodness of Fit results

Table of Outline A13: Goodness Of Fit				
	A	B	C	
1	Name	P4 - OutTempRange	P5 - OutTempAve	
2	Goodness Of Fit			
3	Coefficient of Determination (Best Value = 1)	★★★ 0.99284	✖✖	0.33904
4	Adjusted Coeff of Determination (Best Value = 1)	★★★ 0.99045	✖✖	0.24462
5	Maximum Relative Residual (Best Value = 0%)	★ 2.3038	★★★	0.01322
6	Root Mean Square Error (Best Value = 0)	0.021202	0.016364	
7	Relative Root Mean Square Error (Best Value = 0%)	★★ 1.3425	★★★	0
8	Relative Maximum Absolute Error (Best Value = 0%)	✖ 12.239	✖✖	185.81
9	Relative Average Absolute Error (Best Value = 0%)	— 7.056	✖✖	48.575

Goodness of Fit
for DP's

Goodness of Fit
for VP's (only 1
in this case)

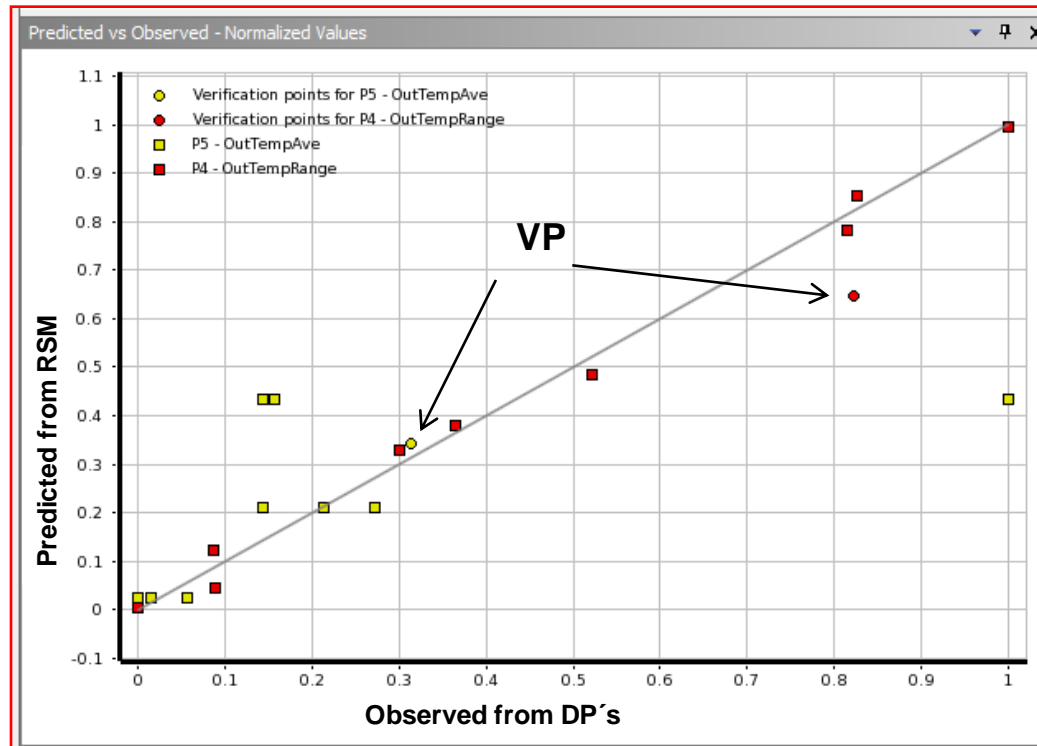
10	Goodness Of Fit for Verification Points		
11	Maximum Relative Residual (Best Value = 0%)	— 6.55	★★ 0
12	Root Mean Square Error (Best Value = 0)	0.12726	0.0020325
13	Relative Root Mean Square Error (Best Value = 0%)	— 6.55	★★ 0
14	Relative Maximum Absolute Error (Best Value = 0%)	✖✖ 48.016	✖ 10.047
15	Relative Average Absolute Error (Best Value = 0%)	✖✖ 48.016	✖ 10.047

6	Verification Points			
7	1	1.0502	1574.8	1.9429
*	New Verification Point			

CFX results

Verification Point automatically generated and calculated (via ANSYS-CFX)

Goodness of Fit results

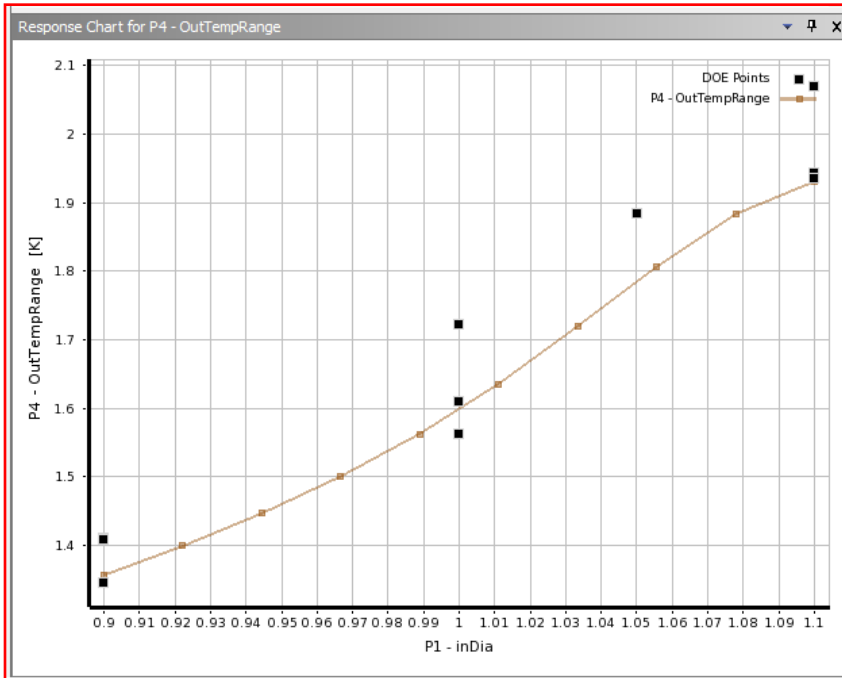


VP introduced into the RSM to obtain predicted output

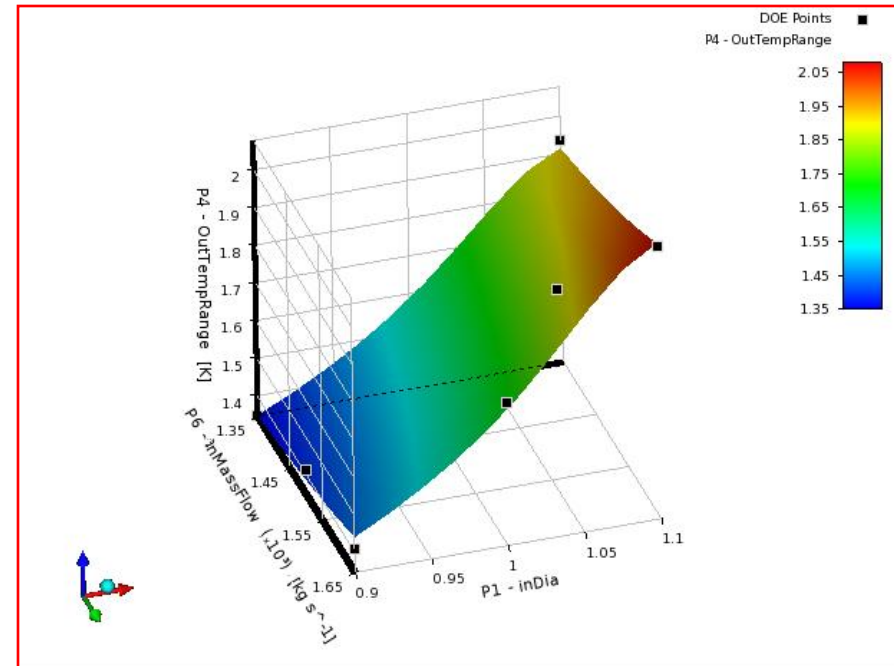
4	Response Points				
5	Response Point	1	1500	1.6232	300.02
6	Response Point 1	1.0502	1574.8	1.8157	300.01
*	New Response Point				
8	Verification Points				
9	1	1.0502	1574.8	1.9429	300.01
*	New Verification Point				

Results may suggest to include further Refinement Points close to the location of the VP, until all errors are within 1%.

Plots of RSM



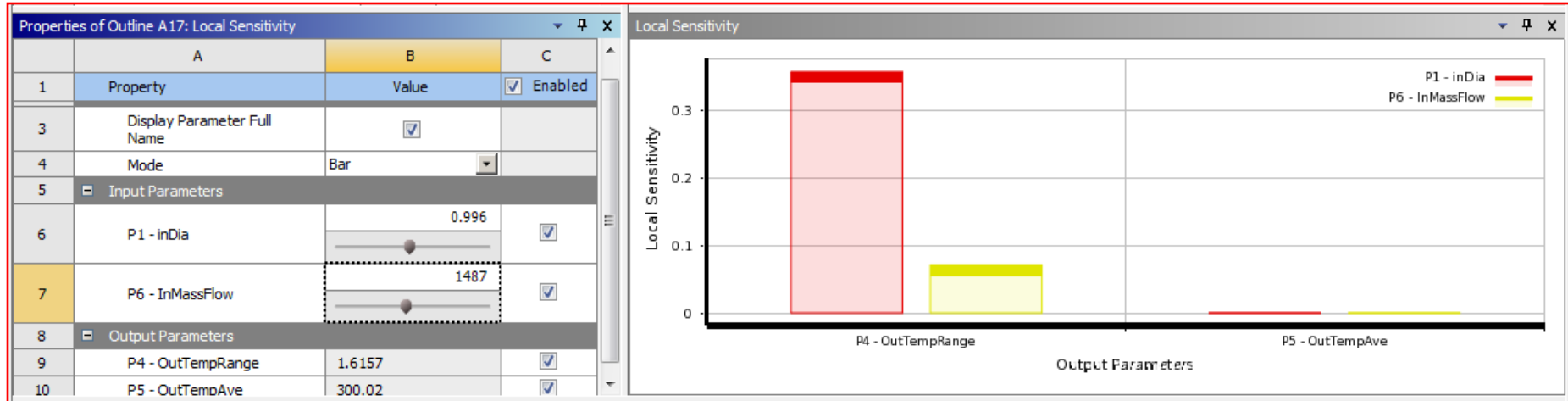
2D (OutTempRange vs. Inlet Diameter)



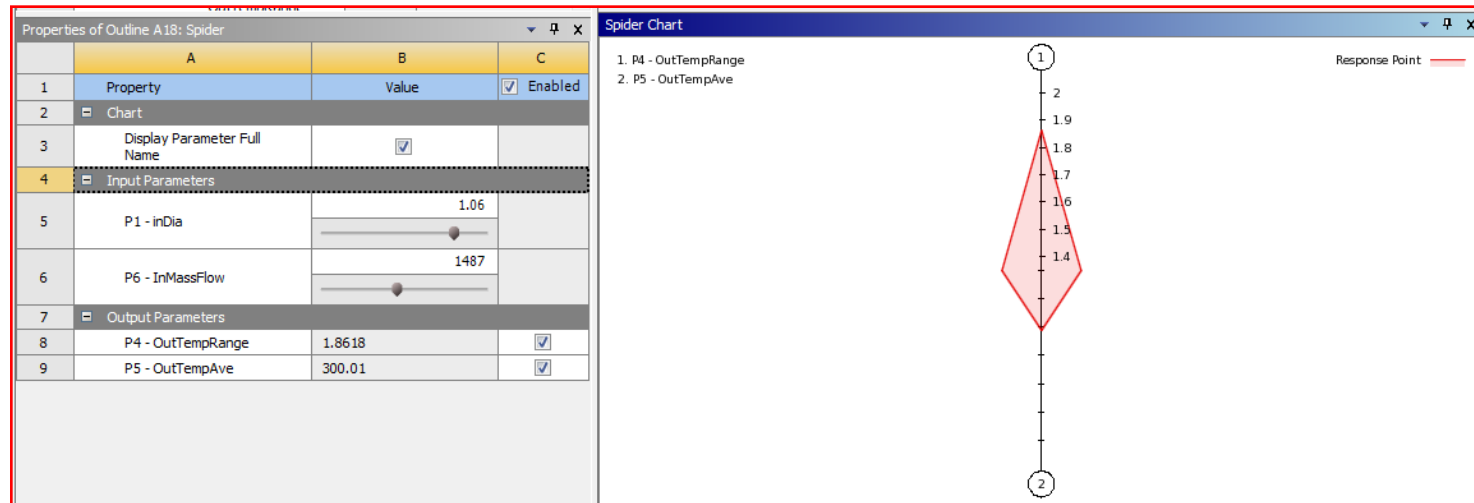
3D (OutTempRange vs. Inlet Diameter, Mass Flow)

2D results suggest that a Kriging fitting might improve the RSM, since apparently, there are significant non-linearities (non-fitted DP's).

Plots of RSM



Local Sensitivity Plot. It shows the relevance of the Inlet Diameter

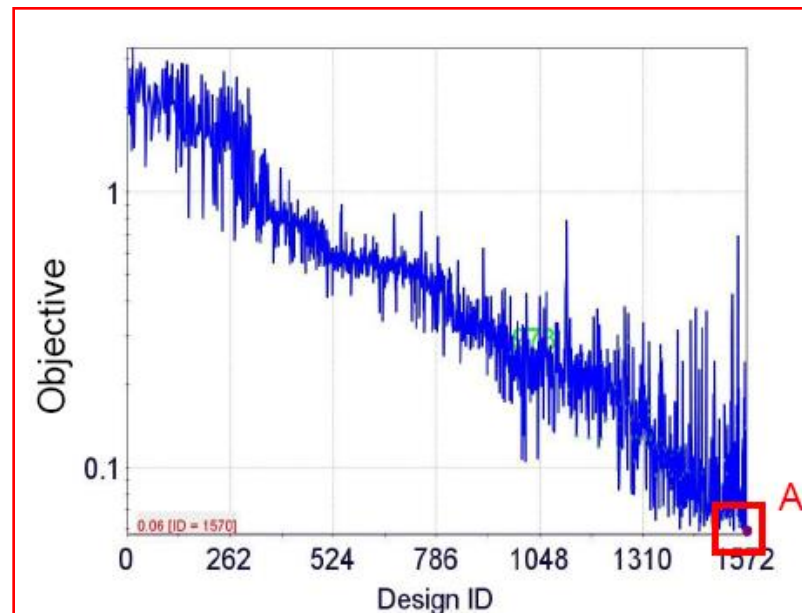


Spider Plot at RP, shows highest influence on OutTempRange

6. Multi-Objective Optimization

Single vs. Multi-Objective Optimization

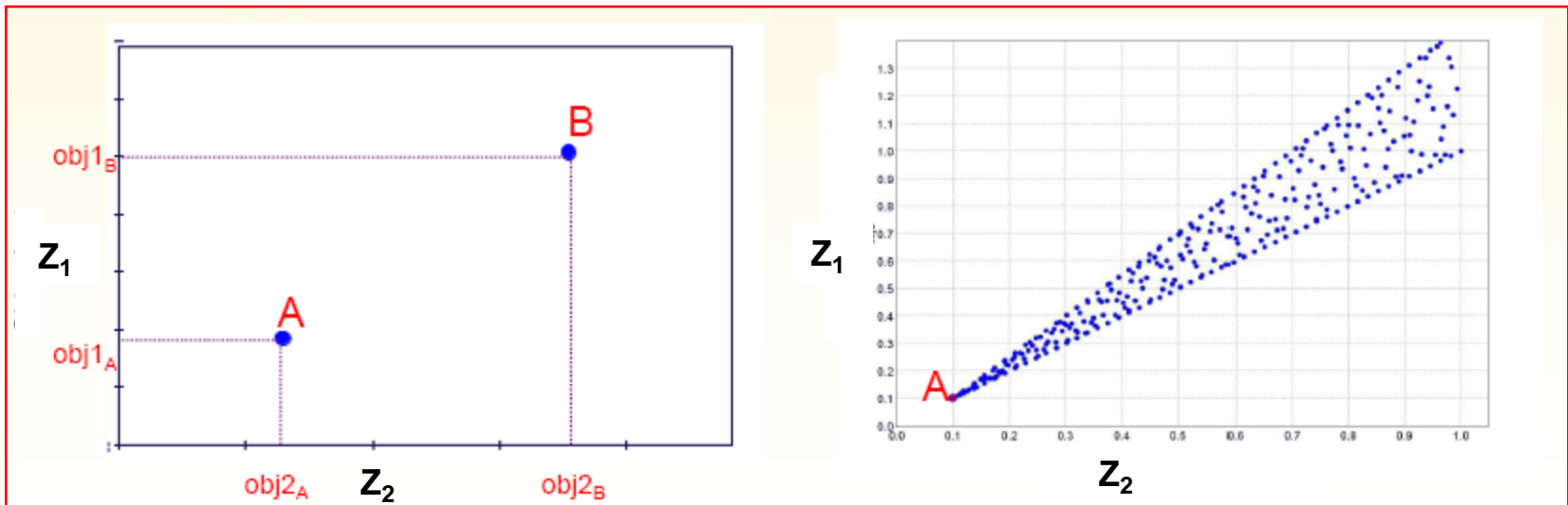
Single Objective Optimization (example: minimize $F(X)$). Then A is the best design point obtained **at the moment**. Then we have a **Simple Optimization**.



7. Multi-Objective Optimization

Multi-Objective Optimization (example: minimize non-conflicting Z_1 and Z_2)

When there is more than 1 Objective Function, but they **do not conflict** against each other, it means that maximizing one of them lead to maximizing the other one, and viceversa. Then, we have again a **Simple Optimization case**.

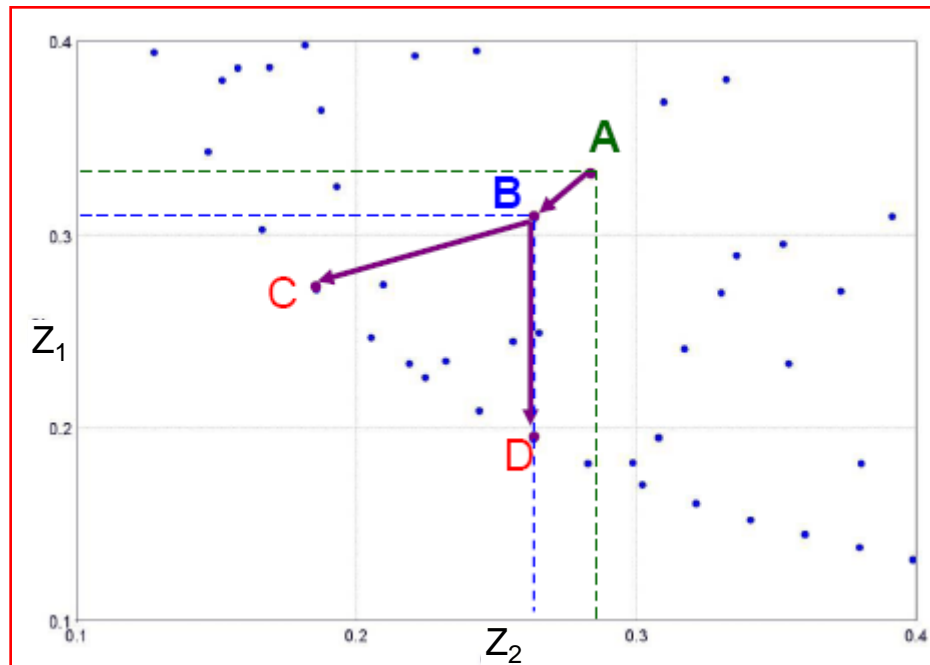


"A" dominates all the solutions

7. Multi-Objective Optimization

Multi-Objective Optimization (example: minimize conflicting Z_1 and Z_2)

If we try to minimize **two or more Objective Functions**, it may happen that there is not a unique optimum, but a compromise between both objectives or a boundary of "optima", name **Pareto Frontier**.



For example:

B dominates **A** because **B** is better than **A** for both objectives.

C & **D** dominate **A** & **B**, because the former are Pareto points. However, **C** & **D** do not dominate each other.

Which one is more important?

Ans. Later on ...

7. Multi-Objective Optimization

What are the Constraints and how do they affect the Optimization?

Constraints:

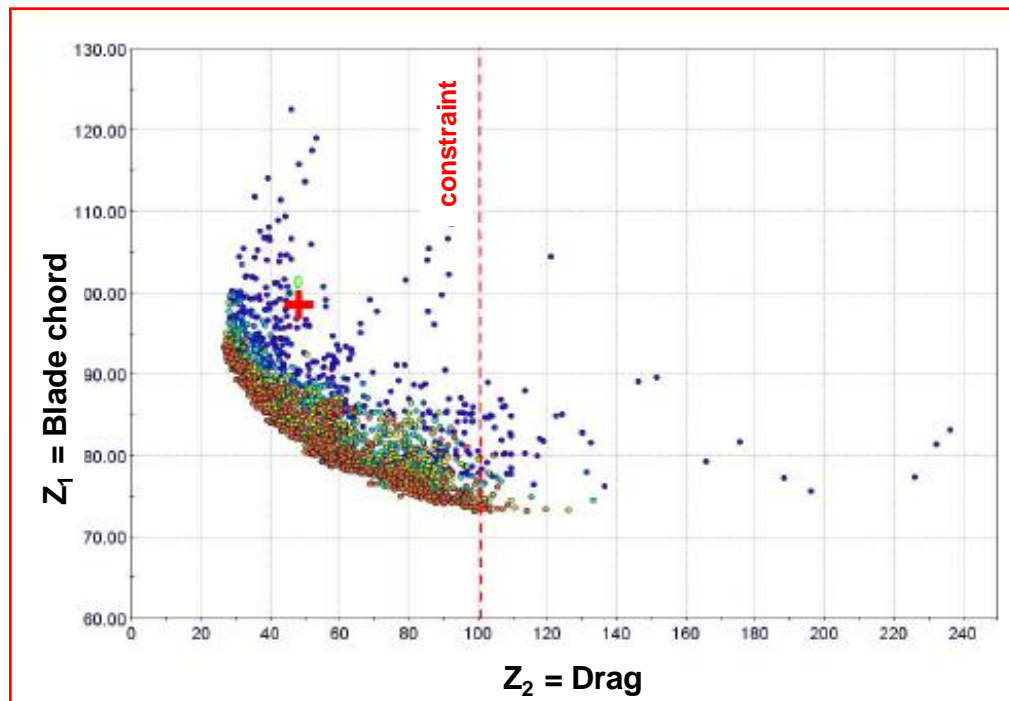
The constraints are quantities or limits mandatory to the project, e.g., limits or restrictions associated to functionality, standards, etc. These, as a whole, define the **feasibility region**.

- **General constraints**
 - Maximum drag
 - Minimum lift
 - Minimum pressure drop
 - Function of variables
 - etc.
- **Constraints on variables**
 - Total weight (volume)
 - Width range
 - Explicit function of variables.
 - etc.

7. Multi-Objective Optimization

How do the constraints affect the Optimization?

Constraints may be dimensional (input variable), but also they might be associated to output variables (e.g., drag, lift, etc.)



For example:

Designs with a Drag force larger than 100 N are NOT viables.

7. Multi-Objective Optimization

How to deal with conflicting Multi-Objectives?

Weighting Functions:

- **n objectives** may be coupled as a simple objective, using weights:

$$F(x) = \sum_{i=1}^n \omega_i f_i(x)$$

- **Pros:**
 - Simple formulation.
 - Weights depend on Decision Maker judgement.
- **Cons:**
 - Weights depend on each problem and must be defined empirically.

7. Multi-Objective Optimization

Optimization in ANSYS-DX™: Goal Driven Optimization (GDO)

- **GDO may be invoked from:**
 - **Parameters set bar.** In this case, GDO will generate its own DP's using the known DoE and RSM techniques.
 - **Design of Experiments cell of a Response Surface.** In this case, GDO will share all data generated from the DoE.
 - **Response Surface cell of a Response Surface.** In this case, GDO will share all data generated from DoE and RSM.
- **Optimization options: Screening, MOGA and NLPQL**
- **Graphical Rating of Candidates:** as explained in Goodness of Fit section (6 scales: "****", "***", "**", "+", "++", "+++").

7. Multi-Objective Optimization

ANSYS-DX™ GDO: Screening

- Based on shifted **Hammersley sampling** algorithm.
- Conventional **Hammersley sampling** is a quasi-random generator, with low discrepancy (**high uniformity**). The quasi-random number generator uses the “radical inverse function” to produce numbers in the range (0, 1) .

7. Multi-Objective Optimization

ANSYS-DX™ GDO. Evolutionary Design → Genetic Algorithms

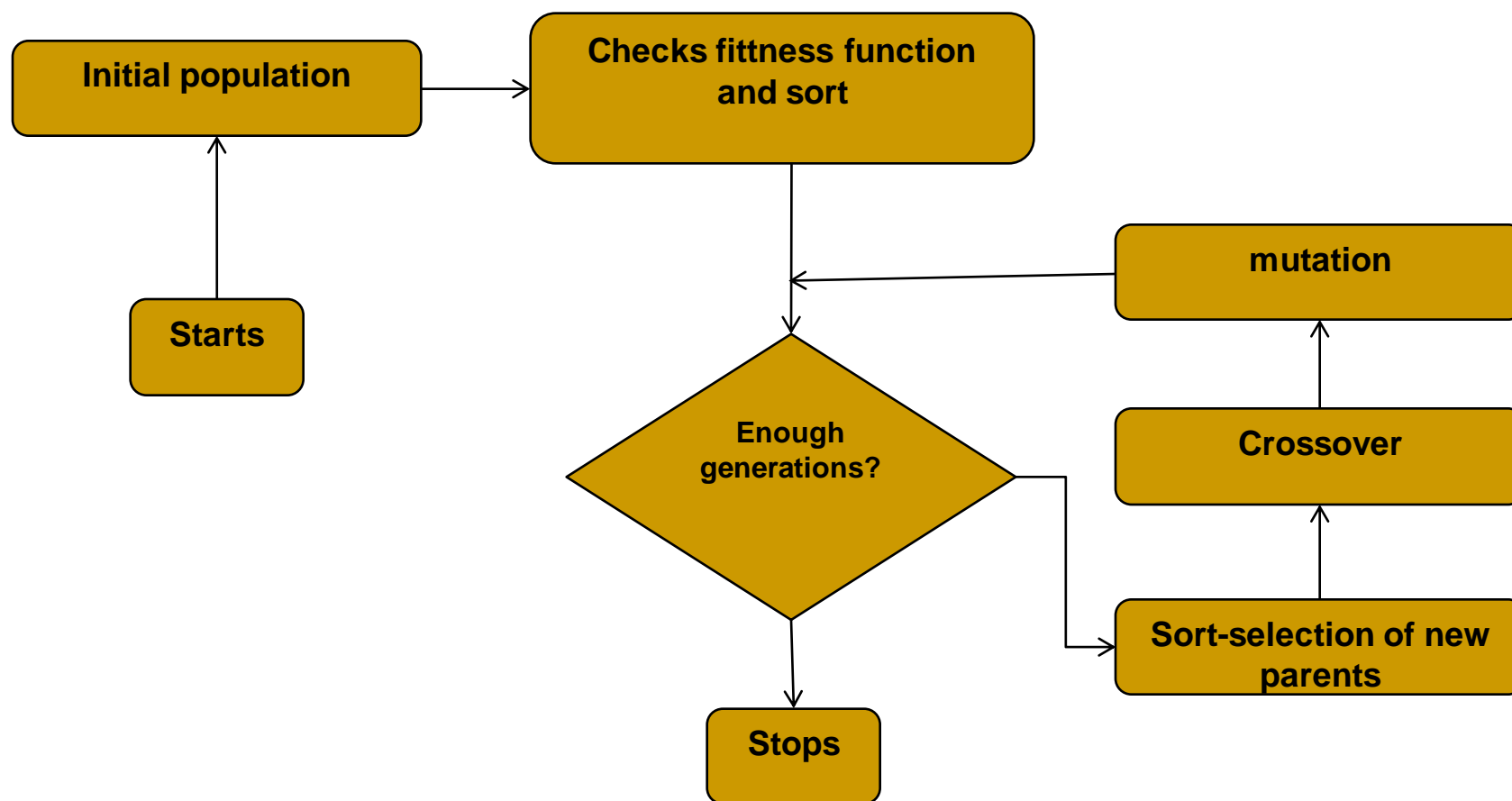
Steps:

- Select initial population (DoE-like).
- Check fitness of elements.
- **Selection and sorting** according to fitness.
- **Crossover** between better fitted samples.
- Random **mutation** according to set levels.
- Check **fitness** of elements and repeat until enough generations have been produced; then stop.

7. Multi-Objective Optimization

ANSYS-DX™ GDO. Evolutionary Design → Genetic Algorithms

Flow diagram:



7. Multi-Objective Optimization

ANSYS-DX™ GDO: MOGA (Multiple Optimization Genetic Algorithm)

- Mimics the evolutionary principles for living systems, obeying **Darwin's** idea of "**survival of the fittest**".
- **Genetic Algorithms** belongs to the more general family of **Evolutionary Algorithms (EA)** which generate solutions using a **meta-heuristic** model (based on experience-learning, rule-of-thumb, trial-and-error, etc).
- These methods have the ambition to solve optimization problems for which we **do not know a polynomial algorithm**.
- Based on a hybrid variant of the **Non-dominated Sorted Genetic Algorithm-II (NSGA-II)** , which is used for continuous variables.

But, how is the Evolutionary Theory applied to Optimization Genetic Algorithms?

7. Multi-Objective Optimization

ANSYS-DX™ GDO: MOGA

- Based on **NSGA-II** (Non-dominated Sorted Genetic Algorithm)
- **NSGA-II** is a Multiple Objective algorithm based on continuous variables, while original **MOGA** is for discrete spaces.
- Need to specify:
 - **number of initial samples** (if want to start from new set). Recommended **10 times input variables**, but less than 300.
 - **number of samples per iteration**. Samples iterated and updated at each iteration. Must be smaller than previous.
 - **maximum allowable Pareto percentage** with respect to samples. 50-70% is recommended.

7. Multi-Objective Optimization

ANSYS-DX™ GDO: MOGA

- Need to specify (cont'd):
 - **maximum number of iterations**, before the solver stops, unless the error target is met. It gives an idea of how long would it take for a full cycle.
 - **initial samples**. Use if a new set of samples has to be produced or else, use previous "Screening" samples.
- **PROS**: high robustness (in terms of finding global critical points) and good at handling multi-objective problems.
- **CONS**: low-convergence rate if accuracy is an issue.

7. Multi-Objective Optimization

ANSYS-DX™ GDO. Gradient-based Algorithms (GBA)

- Local maximum/minimum (accuracy ↑, robustness ↓).
- It gives the direction with highest increase of function:
→ convergence speed
- It is for **SINGLE-OBJECTIVE** non-linear problems. Derivatives:

Forward differences:

$$\left. \frac{\partial f}{\partial x_i} \right|_{x_m} \cong \frac{f(x_m + \Delta x_i) - f(x_m)}{\Delta x_i}$$

Central differences:

$$\left. \frac{\partial f}{\partial x_i} \right|_{x_m} \cong \frac{f(x_m + \Delta x_i) - f(x_m - \Delta x_i)}{2\Delta x_i}$$

Gradient

$$\vec{\nabla} f(x_o) = \left\{ \begin{array}{c} \frac{\partial f}{\partial x_1} \\ \cdot \\ \cdot \\ \frac{\partial f}{\partial x_n} \end{array} \right\}$$

7. Multi-Objective Optimization

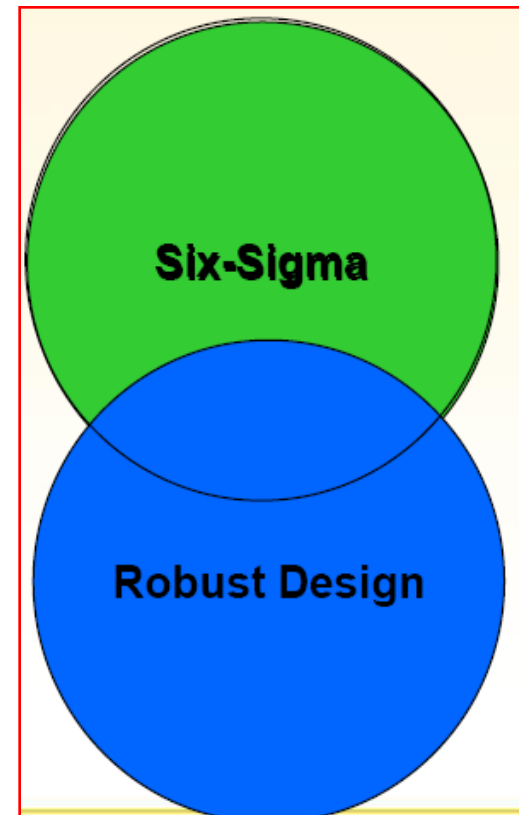
ANSYS-DX™ GDO: NLPQL

- Can only handle **one output parameter objective**; however, other output limits may be handled via constraints.
- User needs to specify:
 - ❑ **Allowable Convergence Percentage.** Larger → less convergence iterations and ↓ accuracy (but faster), and viceversa. 1E-06 is default, as typically error is scaled.
 - ❑ **Maximum number of iterations.**

7. Six Sigma Analysis (SSA) and Robust Design

Six Sigma and Robust Design

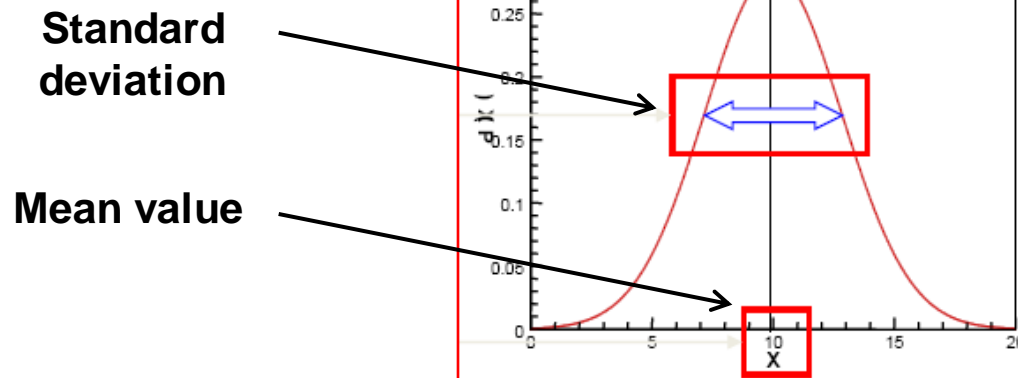
- **Six-Sigma (6σ):**
 - Group of best practices to systematically improve, via reduction of defects (Motorola, 1986).
 - Processes under Six-Sigma standards, generate less than 3.4 defective parts per million units.
- **Robust Design:**
 - Includes uncertainties during the design stage to guarantee robustness. Applies Six-Sigma principles.



6. Six Sigma Analysis (SSA) and Robust Design

What does Robust Design mean?

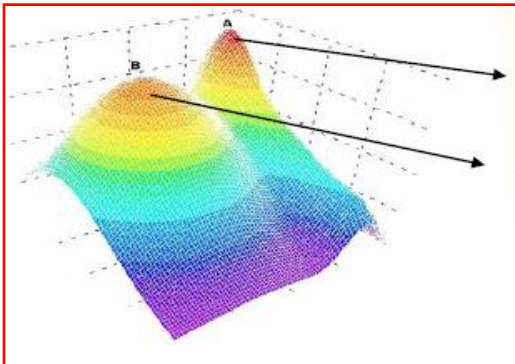
- In many engineering problems the design parameters may be known only within **certain tolerance**.
- In many problems, parameters are described by a **probabilistic distribution**.



6. Six Sigma Analysis (SSA) and Robust Design

Robust Designs

- The **uncertainties** in the **input** parameters is reflected on the system **outputs**. For example, a good solution for deterministic input data, may not be **robust** to small variations.
- The **robustness** of a solution is defined as the response quality to be insensible to variation in input parameters.
- A Robust design optimization aims at robust solutions using Six-Sigma principles.



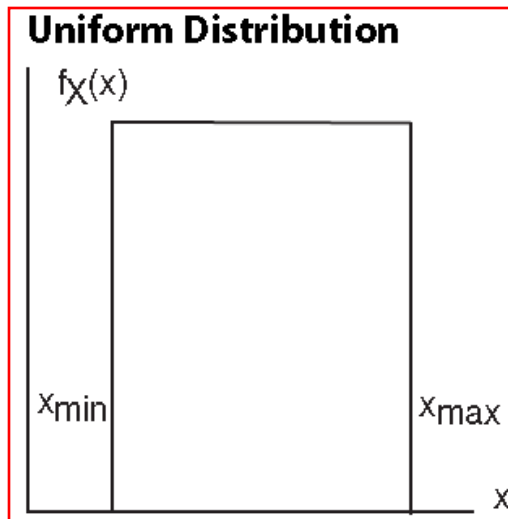
Best solution (if robustness is not an issue)

Best solution (if Robust Design is the goal)

6. Six Sigma Analysis (SSA) and Robust Design

Six-Sigma Analysis (SSA) in ANSYS-DX™

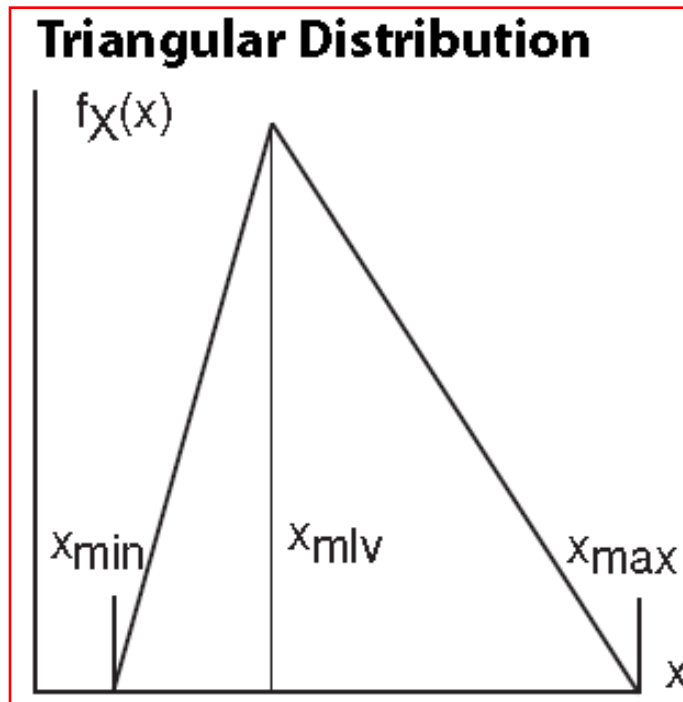
- Requires mean value and specify statistical distribution function of randomness.
- Statistical distribution functions available: ***Uniform, Triangular, Normal, Truncated Normal, Lognormal, Exponential, Beta and Weibull.***
- For example, if a given input variable has a histogram like this:



User must specify X_{\min} , X_{\max} , and applies for cases with similar likelihood for all possible values of random variable.

6. Six Sigma Analysis (SSA) and Robust Design

Six-Sigma Analysis (SSA) in ANSYS-DX™

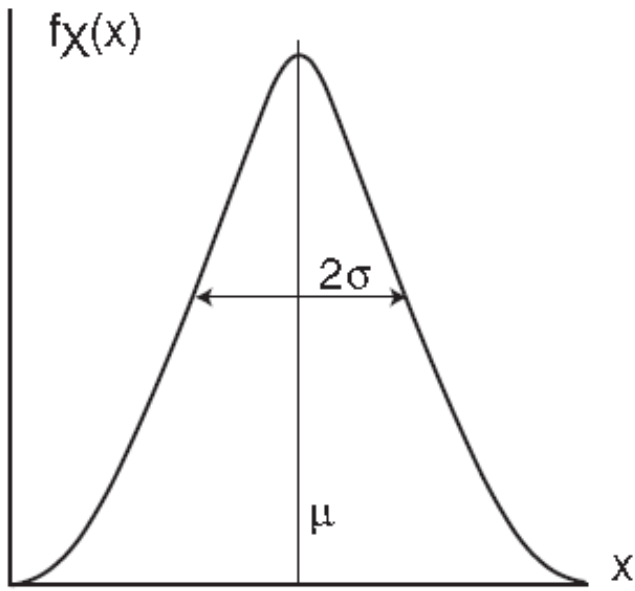


- User must specify X_{min} , X_{max} and most likely value limit X_{mlv} .
- Applies when for cases when actual data is unavailable. For instance, based on opinion of experts.

6. Six Sigma Analysis (SSA) and Robust Design

Six-Sigma Analysis (SSA) in ANSYS-DX™

Gaussian (Normal) Distribution

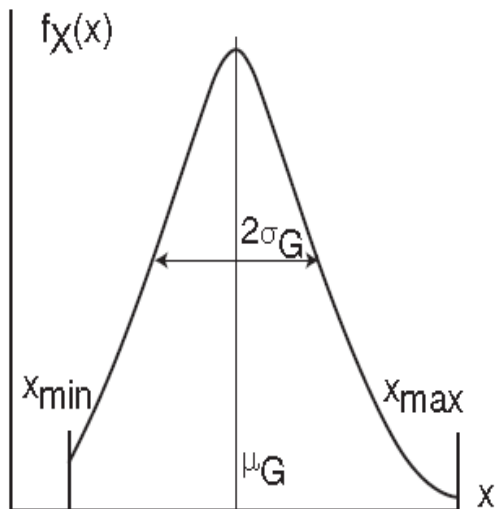


- User must specify mean value “ μ ” and standard deviation “ σ ”.
- Applies for scattering of truly random variables.

6. Six Sigma Analysis (SSA) and Robust Design

Six-Sigma Analysis (SSA) in ANSYS-DX™

Truncated Gaussian (Normal) Distribution

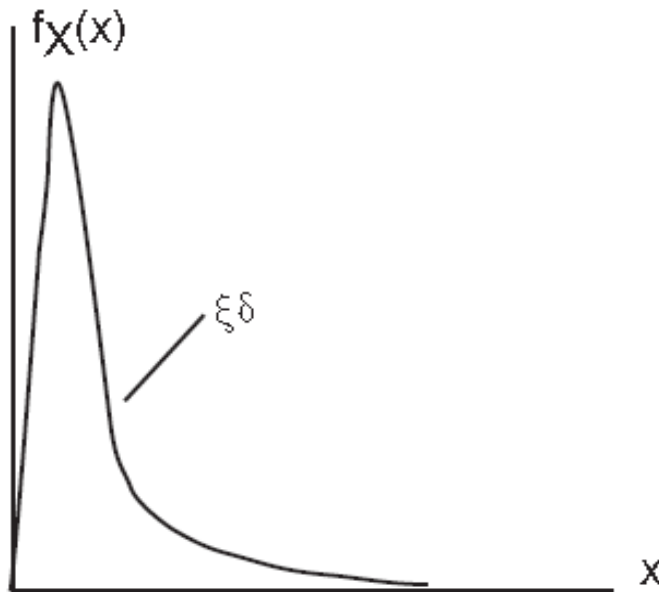


- User must specify mean value “ μ ” and standard deviation “ σ ”. But also, the user specifies lower and higher limits, X_{min} and X_{max} , respectively.
- Applies for scattering of truly random variables, when a lower and higher limits are established by quality control.

6. Six Sigma Analysis (SSA) and Robust Design

Six-Sigma Analysis (SSA) in ANSYS-DX™

Lognormal Distribution



- User must specify the logarithmic mean value “ ξ ” and the logarithmic deviation “ δ ”, calculated as:

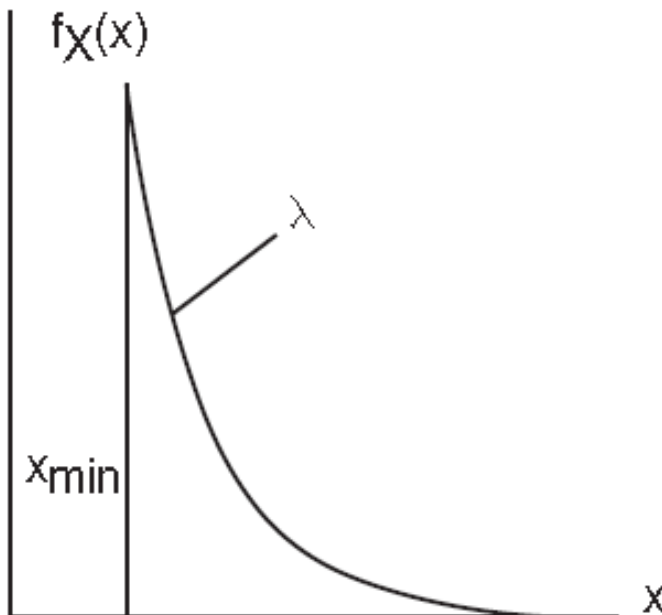
$$f(x, \xi, \delta) = \frac{1}{\sqrt{2\pi \cdot x \cdot \sigma}} \cdot \exp \left(-\frac{1}{2} \left(\frac{\ln x - \xi}{\delta} \right)^2 \right)$$

- Appropriate for scattered data for which the $\ln(X)$ follows a normal distribution.

6. Six Sigma Analysis (SSA) and Robust Design

Six-Sigma Analysis (SSA) in ANSYS-DX™

Exponential Distribution

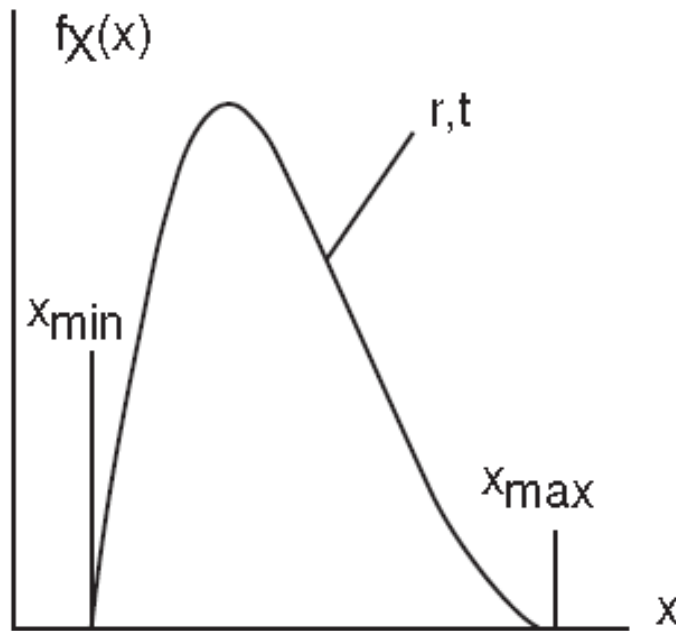


- User must specify the decay parameter “ λ ” and the lower limit x_{min} .
- Applies to cases for which the probability density decays as the random variable grows. For example in time-phenomena, among others.

6. Six Sigma Analysis (SSA) and Robust Design

Six-Sigma Analysis (SSA) in ANSYS-DX™

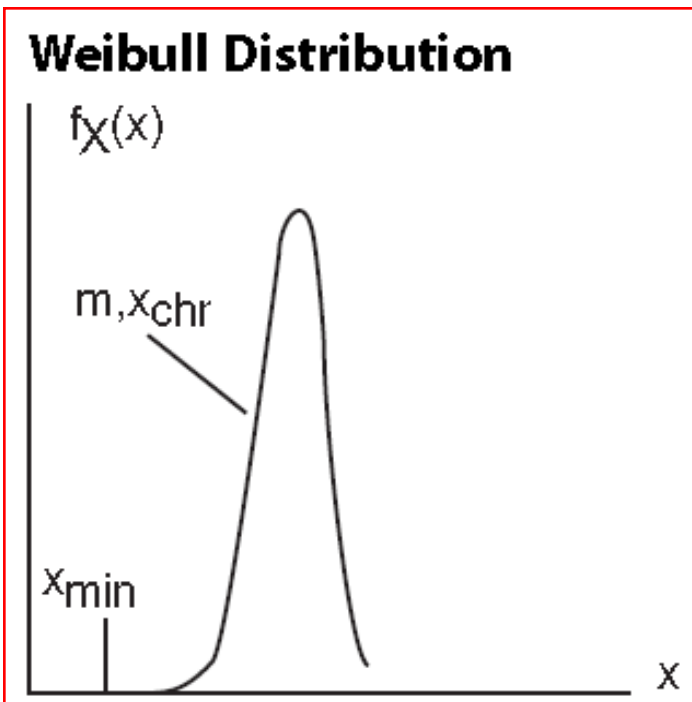
Beta Distribution



- User must provide shape parameters “r” and “t”, and lower/upper limits of variable, X_{\min} , X_{\max} , respectively.
- Applies to random variables bounded on both sides. This case occurs mostly on random variables that follow normal distribution after being subject to a linear operation (e.g., subtraction of a geometric magnitude).

6. Six Sigma Analysis (SSA) and Robust Design

Six-Sigma Analysis (SSA) in ANSYS-DX™

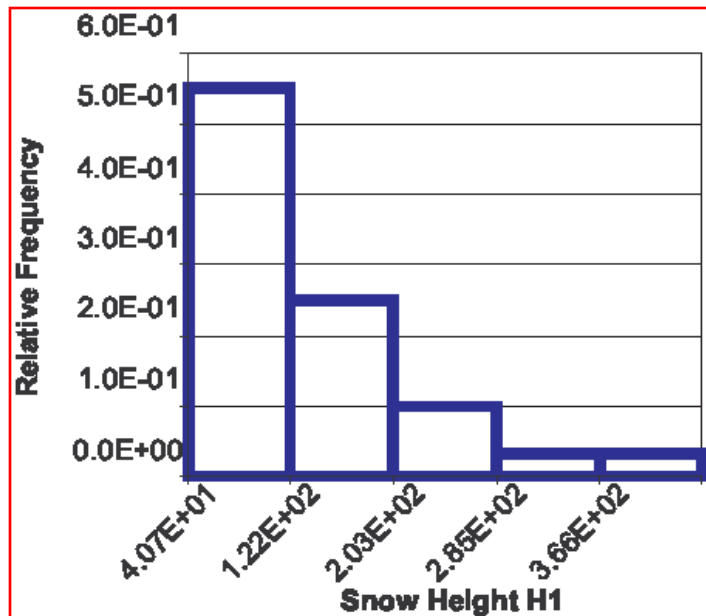


- User must provide Weibull characteristic parameter X_{chr} , Weibull exponent “ m ”, and the minimum value X_{min} ($m=2$ gives Rayleigh distribution).
- Applies to strength/related lifetime parameters. Used for wind velocities, giving a 2-year data collection, for example.

6. Six Sigma Analysis (SSA) and Robust Design

Six-Sigma Analysis (SSA) in ANSYS-DX™

- **Example.** If a given input variable has a histogram like this:



Then, the most appropriate statistical distribution will be the **Exponential**.

6. Six Sigma Analysis (SSA) and Robust Design

Six-Sigma Analysis (SSA) Input-to-Output Transformation (1/2)

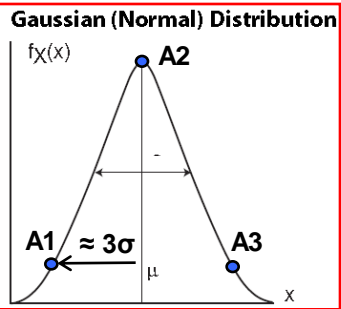
- **Probability operation rules**

- **Mutually** exclusive events A and B (can't occur simultaneously).
 - $P(A \text{ and } B) = 0$
 - $P(A \text{ or } B) = P(A) + P(B)$
- **Non-Mutually** exclusive events A and B (can occur simultaneously).
 - $P(A \text{ or } B) = P(A) + P(B) - P(A \text{ and } B)$ (always valid)
- **Independent** events A and B: $P(A \text{ and } B) = P(A) * P(B)$
- In ANSYS-DX™ **Input Parameters** are treated as **independent variables** (events) in $6\sigma^*$.

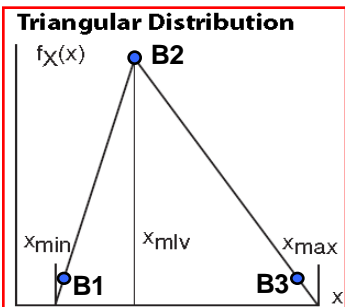
6. Six Sigma Analysis (SSA) and Robust Design

Six-Sigma Analysis (SSA) Input-to-Output Transformation (2/2)

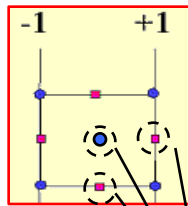
Input Parameter A



Input Parameter B

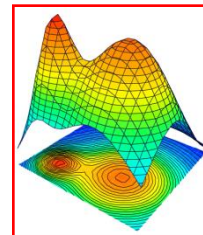


DoE

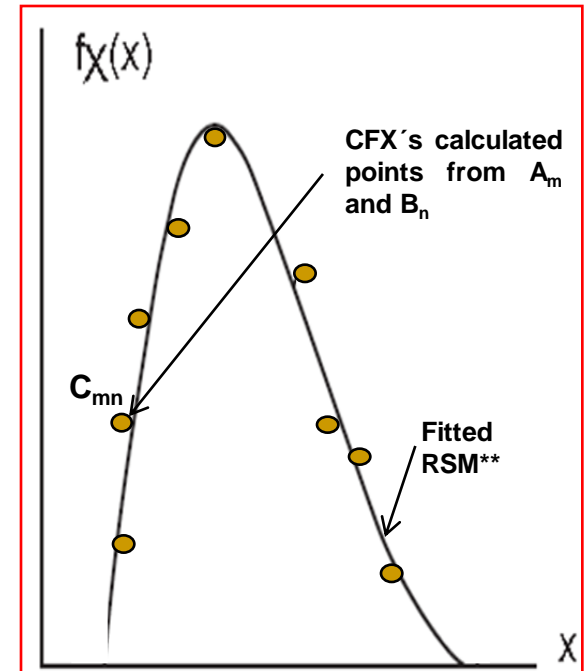


ANSYS-CFX™

RSM → 6σ



Output Parameter C



- Each DP has a combined probability $P(A \text{ and } B) = P(A) \cdot P(B)$.
- Therefore, Point A1B1 produces, via CFX, an Output Point C11 with Probability: $P(C11) = P(A1) \cdot P(B1)$.
- System non-linearity may stretch or shrink location of output points in probability density plot wrt mean input-output location.

(*) CCD or another DoE sampling, as previously shown.

(**) As before, points will lie on fitted curve when using Kriging

6. Six Sigma Analysis (SSA) and Robust Design

Six-Sigma Analysis (SSA) Output Analysis in ANSYS-DX™

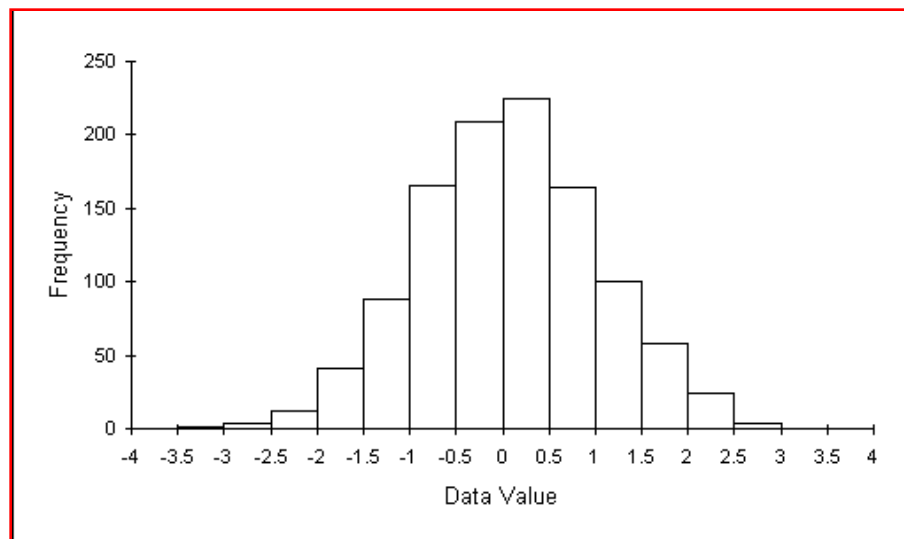
- **Histogram**
- **Cumulative Distribution Function**
- **Probability Table**
- **Statistical Sensitivities**

6. Six Sigma Analysis (SSA) and Robust Design

Six-Sigma Analysis (SSA) Output Analysis in ANSYS-DX™

Histogram (for inputs-outputs):

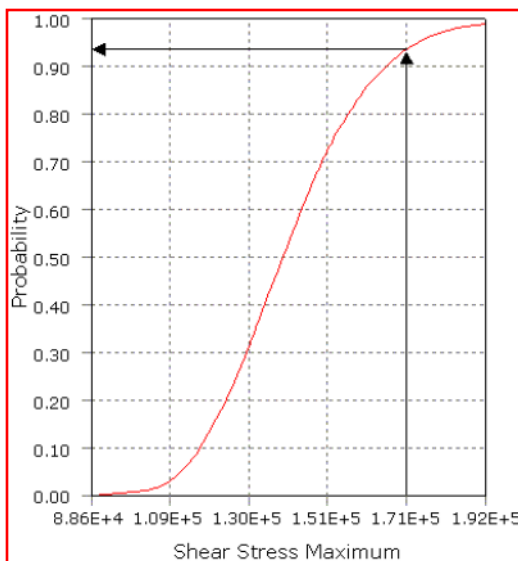
- Derived by dividing the global range between **min-value** and **max-value**, into **intervals** of **equal length**.
- It shows the fidelity of the sampling process (check if loops are enough, for example).



6. Six Sigma Analysis (SSA) and Robust Design

Six-Sigma Analysis (SSA) Output Analysis in ANSYS-DX™

- **Cumulative Distribution Function** (for inputs-outputs).
 - Assesses the reliability or the **failure probability** of a component or product.
 - Basically, evaluates the probability of a given output parameter of exceeding or being under a **threshold value**.



- **Example:** the figure shows that there is a 93% probability of having stress smaller than 1.71E+5.

6. Six Sigma Analysis (SSA) and Robust Design

Six-Sigma Analysis (SSA) Output Analysis in ANSYS-DX™

Probability Table. Provides probabilities of input or output parameters as a Table (similar to Cumulative Distribution Function).

	A	B	C
1	P1 - DXLENGTH	Probability	Sigma Level
2	43.97	0.0059075	-2.462
3	44.8	0.022859	-1.998
4	45.631	0.043931	-1.7060
5	46.461	0.077687	-1.4208
6	47.292	0.13522	-1.0830
7	48.122	0.2242	-0.7581
8	48.952	0.33403	-0.42881
9	49.783	0.46503	-0.087763
10	50.613	0.59335	0.23617
11	51.443	0.71737	0.57505
12	52.274	0.81430	0.89414
13	53.104	0.89377	1.2468
14	53.934	0.94418	1.5909
15	54.765	0.96858	1.8604
16	55.595	0.98111	2.0771
17	56.425	0.98945	2.2717
18	57.256	0.99309	2.462
*	New Parameter Value		

" σ "-distance from mean

Quantile-Percentile

Percentile-Quantile

	A	B	C
1	Probability	Sigma Level	P1 - DXLENGTH
2	0.0059075	-2.462	43.97
3	0.01	-2.3263	44.229
4	0.02275	-2	44.797
5	0.025	-1.96	44.857
6	0.05	-1.6449	45.854
7	0.1	-1.2816	46.793
8	0.15866	-1	47.487
9	0.3	-0.5244	48.718
10	0.5	0	50.025
11	0.7	0.5244	51.318
12	0.84134	1	52.512
13	0.9	1.2816	53.228
14	0.95	1.6449	54.105
15	0.975	1.96	55.127
16	0.97725	2	55.287
17	0.99	2.3263	56.664
18	0.99309	2.462	57.256
*	New Probability Value	New Sigma Level	

6. Six Sigma Analysis (SSA) and Robust Design

Six-Sigma Analysis (SSA) Output Analysis in ANSYS-DX™

Probability Table. Analysis:

Percentile-Quantile

	A	B	C
1	Probability	Sigma Level	P1 - DXLENGTH
2	0.0069075	-2.462	43.97
3	0.01	-2.3263	44.229
4	0.02275	-2	44.797
5	0.025	-1.96	44.857
6	0.05	-1.6449	45.854
7	0.1	-1.2816	46.793
8	0.15866	-1	47.487
9	0.3	-0.5244	48.718
10	0.5	0	50.025
11	0.7	0.5244	51.318
12	0.84134	1	52.512
13	0.9	1.2816	53.228
14	0.95	1.6449	54.185
15	0.975	1.96	55.127
16	0.97725	2	55.287
17	0.99	2.3263	56.664
18	0.99309	2.462	57.256
*	New Probability Value	New Sigma Level	

"σ"-distance
from mean

- 6σ (SSA) is very useful after performing Optimization, as a tool to determine the robustness of the chosen design.

- We can check, writing in lowest row-cell, the value of Probability 6σ ($P=0.9999966$) and we'll get the the value of the Output Parameter (OP) at such a limit. All values larger than this, will be in the "3.4/1000000 defects tolerated". Any customer specification lower than this OP, satisfies 6σ .

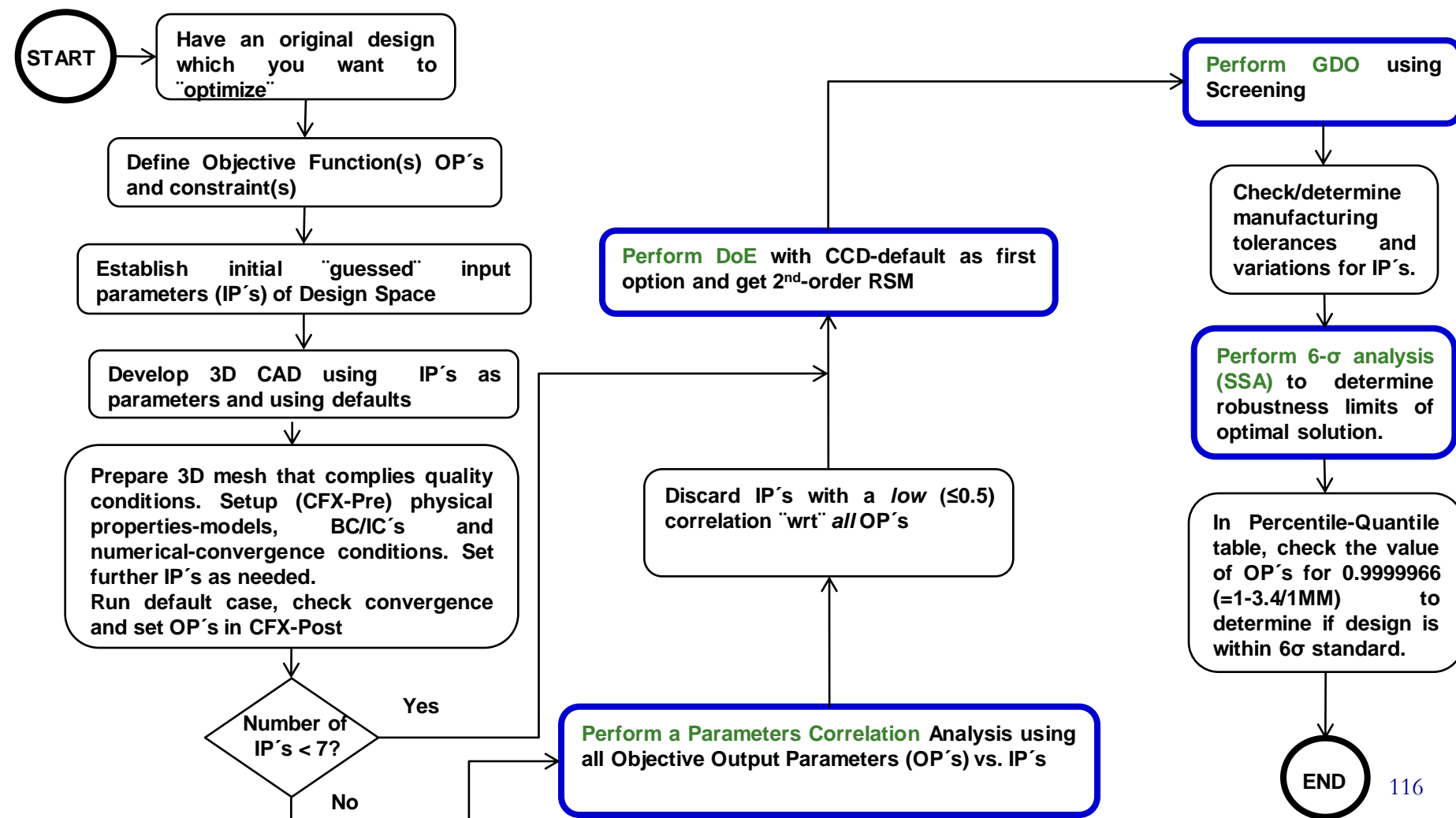
- Same for the lower bound ($P=3.4/1000000$).

6. Six Sigma Analysis (SSA) and Robust Design

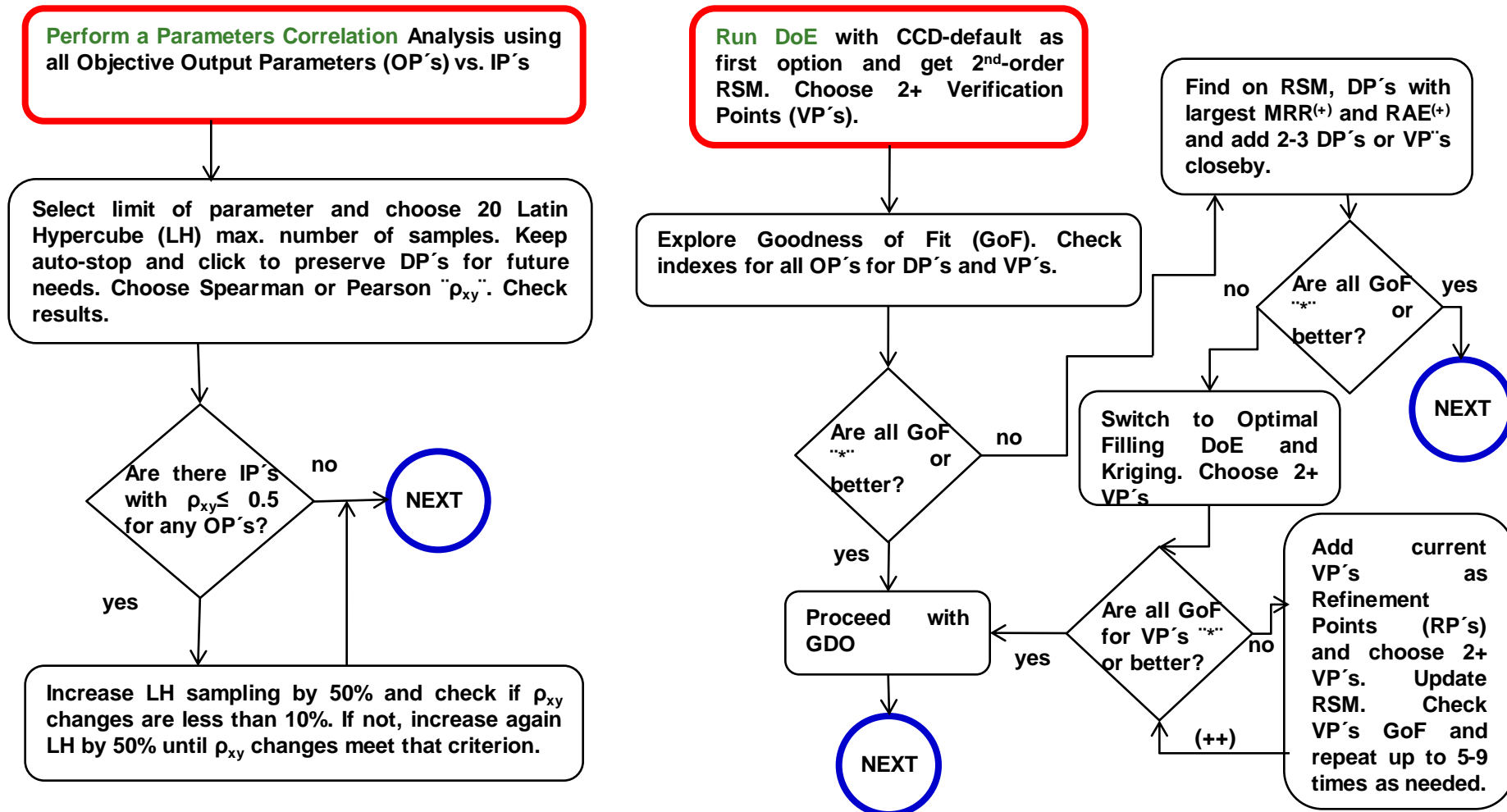
Six-Sigma Analysis (SSA) Output Analysis in ANSYS-DX™

- **Statistical Sensitivities.** Charts to help improving design towards a better quality design. It's available for any continuous output parameter.
- Changes of output parameters vs. input parameter change:
 - **Mean value** (average of a set of values)
 - **Standard deviation** (dispersion of data around the mean)
 - **Sigma Level** (measure of data dispersion from the mean)
 - **Skewness** (asymmetry of data around the mean)
 - **Kurtosis** (relative peakedness or flatness of distribution)
 - **Shannon Entropy** (complexity and predictability)
 - **Taguchi Signal-to-Noise ratios**
 - **Minimum and Maximum values**

Guidelines to perform CFD Optimization + 6 σ -Analysis (1/3)



Guidelines to perform CFD Optimization + 6 σ -Analysis (2/3)



Guidelines to perform CFD Optimization + 6 σ -Analysis (3/3)

