

# Lecture 3

## Design of Experiments (DOE)

14.5 Release

A horizontal banner with a yellow background. It features four distinct 3D visualizations: blue fluid flow lines on the left, a purple gear with a glowing center, a green concentric circle pattern, and a stack of teal cubes on the right. Below these images is a dark teal bar containing four white text labels.

Fluid Dynamics

Structural Mechanics

Electromagnetics

Systems and Multiphysics

# Introduction to ANSYS

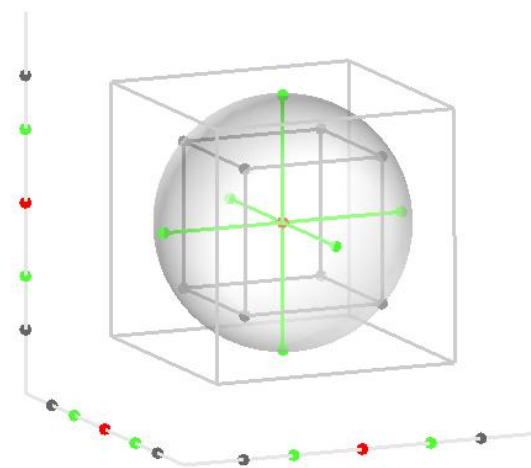
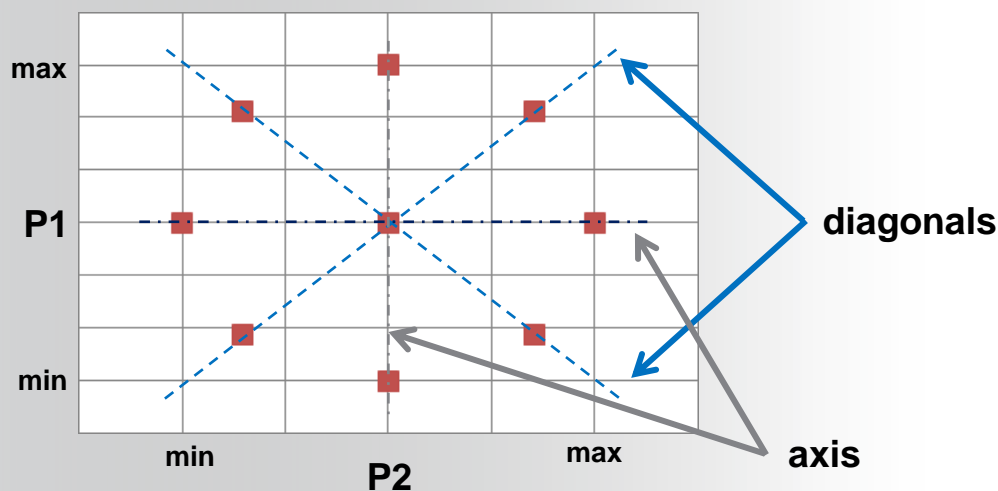
## DesignXplorer

# Available DOE schemes

1. Central Composite Design (CCD) [default]
2. Box Behnken Design
3. Optimal Space Filling Design
4. Custom + Sampling
5. Sparse Grid Initialization
6. Latin Hypercube Sampling Design

# Central Composite Design (CCD)

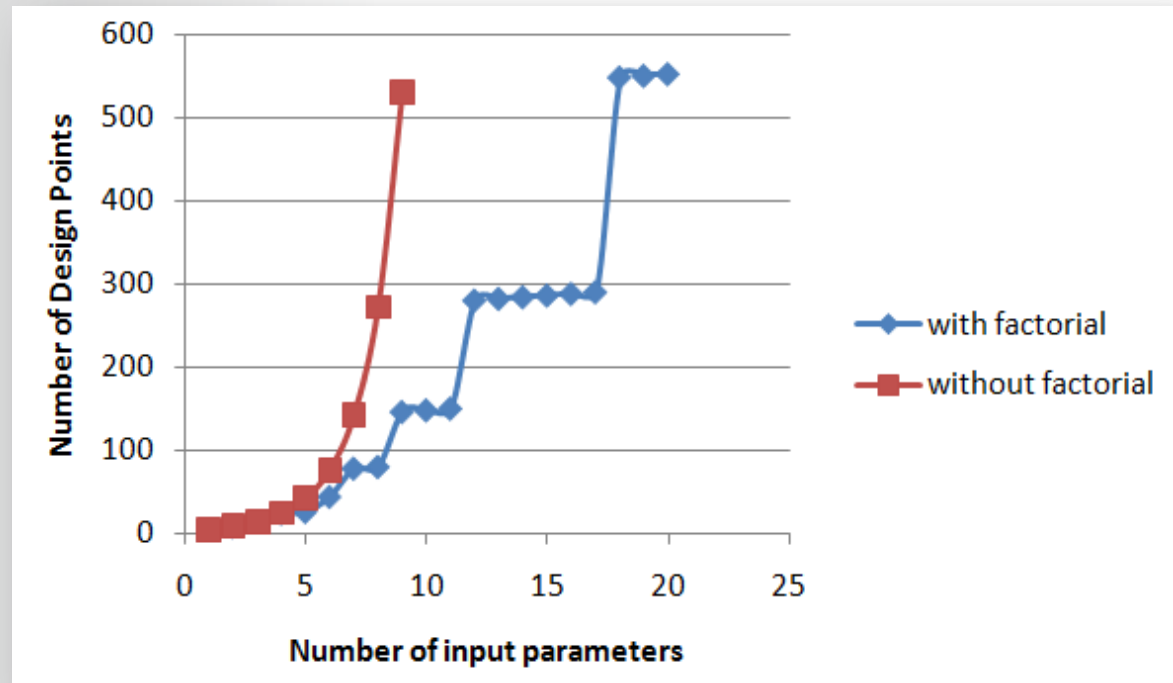
- Central Composite designs are five-level fractional factorial designs that are suitable for calibrating the quadratic response model
- A CCD consists of:
  - 1 center point
  - $2 \times N$  axis points located at the  $-a$  and  $+a$  positions on each axis of the selected input parameter
  - $2^{(N-f)}$  factorial points located at the  $-1$  and  $+1$  positions along the diagonals of the input parameter space [factorial number  $f$  discussed on next slide]



# Central Composite Design (CCD)

- Factorial (f) : In order to restrict the number of design points to a *reasonable* number some diagonal points are not included based on the factorial f

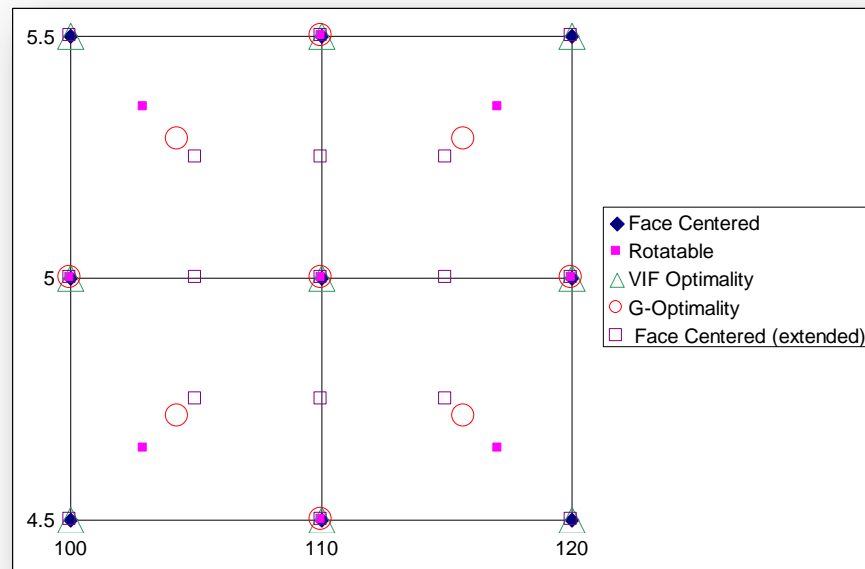
| Number of Parameters | f  | with factorial | without factorial |
|----------------------|----|----------------|-------------------|
| 1                    | 0  | 5              | 5                 |
| 2                    | 0  | 9              | 9                 |
| 3                    | 0  | 15             | 15                |
| 4                    | 0  | 25             | 25                |
| 5                    | 1  | 27             | 43                |
| 6                    | 1  | 45             | 77                |
| 7                    | 1  | 79             | 143               |
| 8                    | 2  | 81             | 273               |
| 9                    | 2  | 147            | 531               |
| 10                   | 3  | 149            | 1,045             |
| 11                   | 4  | 151            | 2,071             |
| 12                   | 4  | 281            | 4,121             |
| 13                   | 5  | 283            | 8,219             |
| 14                   | 6  | 285            | 16,413            |
| 15                   | 7  | 287            | 32,799            |
| 16                   | 8  | 289            | 65,569            |
| 17                   | 9  | 291            | 131,107           |
| 18                   | 9  | 549            | 262,181           |
| 19                   | 10 | 551            | 524,327           |
| 20                   | 11 | 553            | 1,048,617         |



# Central Composite Design (CCD)

- There are 5 types of CCDs available each with their own benefits and drawbacks.

- 1. Auto Defined (default):** Automatically switches between the G-Optimal (if the number of input variables is 5) or VIF-optimal otherwise
- 2. Face Centered:** 3 levels, not rotatable. Benefit is that it gets sampling points at all extremes.
- 3. Rotatable:** 5 levels and rotatable. Drawback, does not get sampling points at all extremes. Rotatable is preferred since prediction variance is the same for any two locations that are the same distance from the design center
- 4. VIF (Variance Inflation Factor) Optimality:**  
Maximizes orthogonality
- 5. G-Optimality:** Minimizes leverage

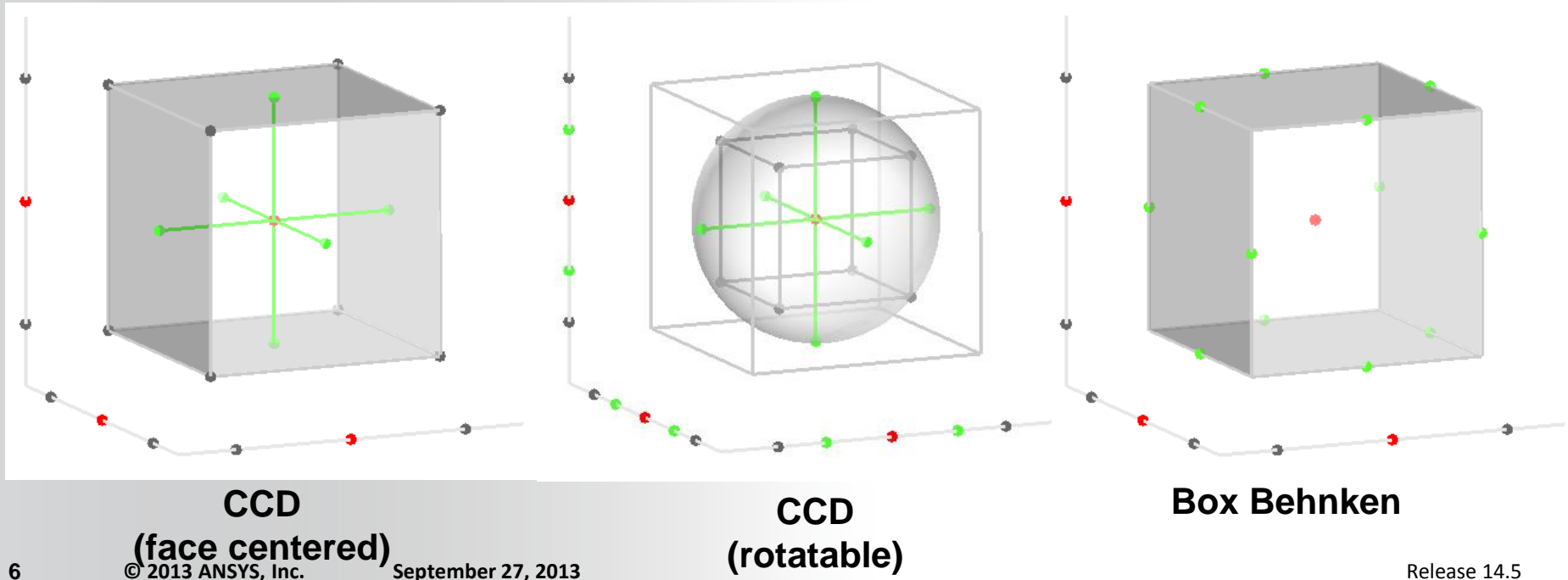


•For 2 parameters, the standard CCD schemes are based on 9 points.

•The “extended” face centered is made of 17 points (note: there is also a 17 points Rotatable scheme).

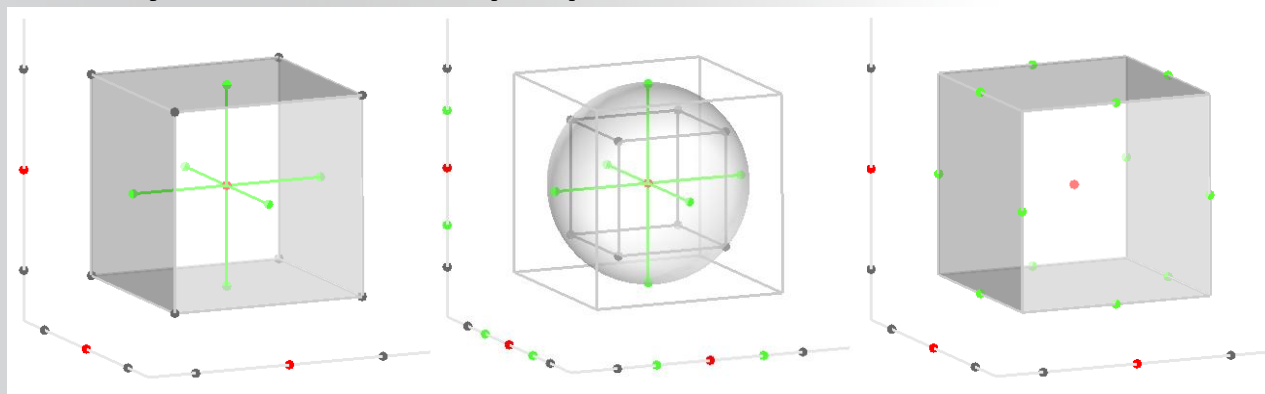
# Box-Behnken Design

- The Box-Behnken design is a three-level quadratic design that does not contain fractional factorial design
- the sample combinations are treated such that they are located at midpoints of edges formed by any two factors
- Rotatable (or near rotatable)



# Box-Behnken Design

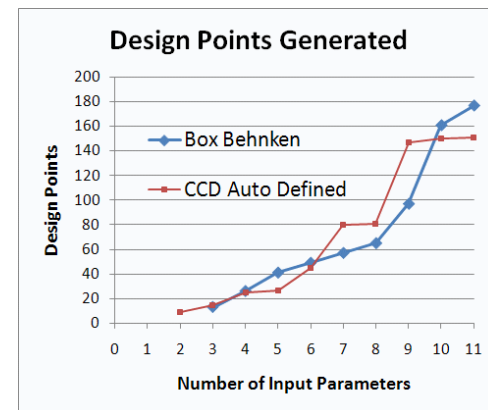
- Advantage over CCD:
  - Requires fewer DPs than full factorial CCD
  - Generally requires fewer DPs than fractional factorial CCD
  - By avoiding the corners of the design space, Box-Behnken allows user to work around extreme factor combinations
- Disadvantage from CCD:
  - The prediction at the extremes (corner points) is poor
  - Only three levels for per parameter



**CCD**  
(face centered)

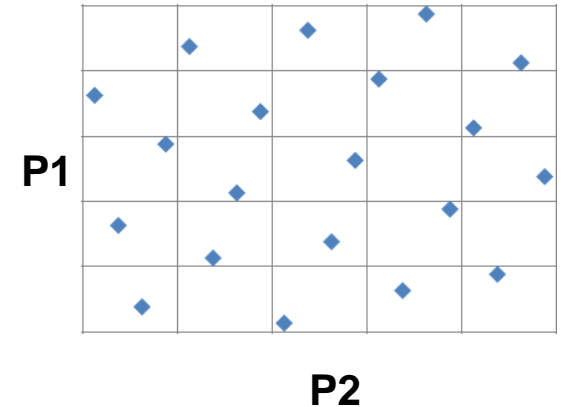
**CCD**  
(rotatable)

**Box Behnken**



# Optimal Space Filling

- Due to the noise associated with physical experimentation, classical DOE's (e.g. CCD) would focus on parameter settings near the perimeter of the design region
- Computer simulation is not subject to this constraint (or at least not as much).
- A space filling scheme distributes the design parameters equally throughout the design space
- Objective is to gain the maximum insight with the fewest number of points
- Very useful when the computation time available is limited (user can specify the number of points)
- The coverage of the design space is not homogeneous. Corners and/or mid-points are not necessarily included.
- Some randomness is included in the choice of the starting point

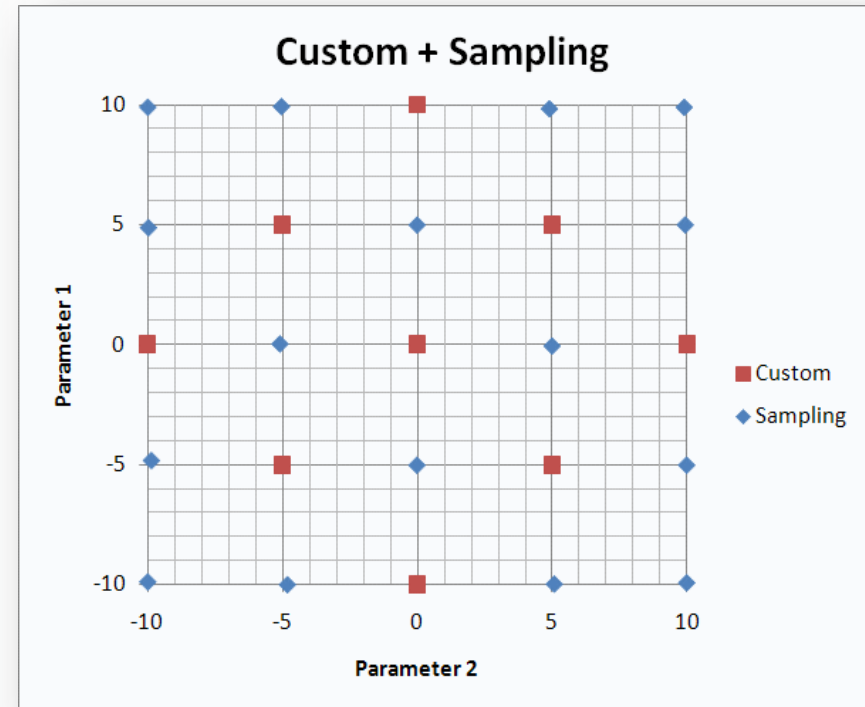




# Optimal Space Filling

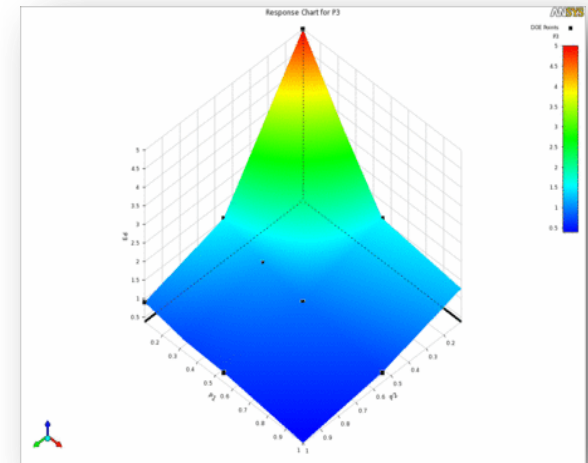
- **Advantage:**
  - Allows user to specify number of design points
  - Better space filling capabilities so it is more appropriate when a more complex meta modeling technique such as Kriging, Non-Parametric Regression or Neural Networks is desired
- **Disadvantage:**
  - The extremes are not necessarily covered
  - Selecting too few design points can result in a low quality of response prediction

- Allows the user to create its own DOE scheme
- A table of input parameters values can be created instead of the default DOE
- Can import design point values from an external CSV file
- An existing DOE can be enriched with user defined points
- Can add sampling to automatically fill the design space efficiently



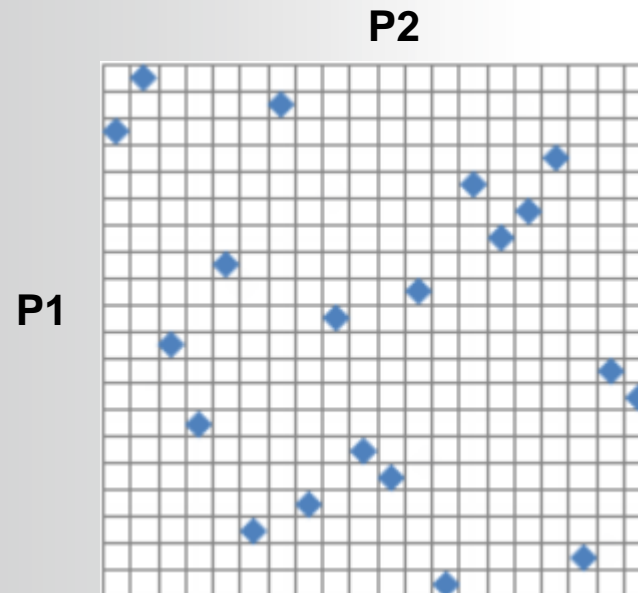
# Sparse Grid Initialization

- This must be used if creating a sparse grid response surface
- Consists of 1 center point and  $2*n$  axis points
- The sparse grid response surface is an adaptive meta-model driven by the accuracy that you request. It automatically refines the matrix of design points where the gradient of the output parameters is higher in order to increase the accuracy of the response surface.
- More details in the response surface lecture



# Latin Hypercube Sampling Design

- LHS algorithm is an advanced form of the Monte Carlo sampling method that avoids clustering samples.
- The points are randomly generated in a square grid across the design space, but no two points share input parameters of the same value.



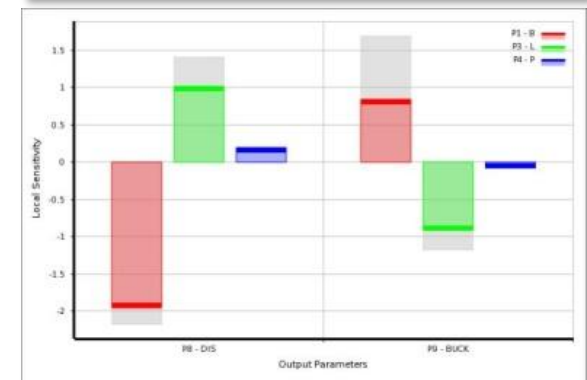
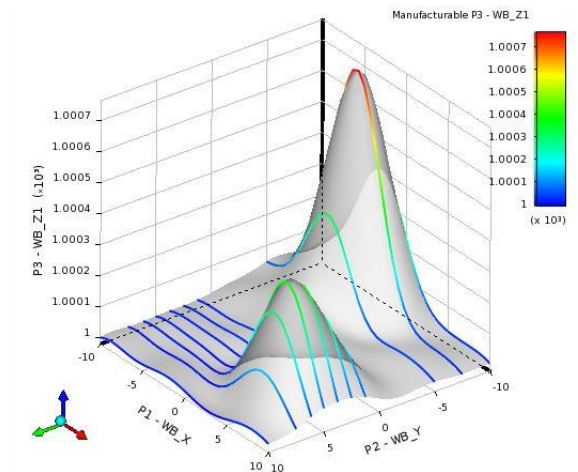
# Additional Settings

## Manufacturable Values

- Use to represent real world manufacturing or production constraints.
  - Only values that realistically represent manufacturing capabilities are included in the post-processing analysis
  - Verification points and optimization candidates will all be “manufacturable”

|    | A                         | B                                   |
|----|---------------------------|-------------------------------------|
| 1  | Property                  | Value                               |
| 2  | General                   |                                     |
| 3  | Units                     |                                     |
| 4  | Type                      | Design Variable                     |
| 5  | Classification            | Continuous                          |
| 6  | Values                    |                                     |
| 7  | Initial Value             | 1                                   |
| 8  | Lower Bound               | -10                                 |
| 9  | Upper Bound               | 10                                  |
| 10 | Use Manufacturable Values | <input checked="" type="checkbox"/> |
| 11 | Number Of Levels          | 6                                   |

|   | A         | B                     |
|---|-----------|-----------------------|
| 1 | Name      | Manufacturable Values |
| 2 | Level 1   | 0.125                 |
| 3 | Level 2   | 0.25                  |
| 4 | Level 3   | 0.75                  |
| 5 | Level 4   | 1                     |
| 6 | Level 5   | 1.5                   |
| 7 | Level 6   | 2                     |
| * | New Level |                       |



# Additional Settings

## Update Order

- Sort your design points to improve the update efficiency
  - Can reduce the number of system updates needed
- Automatically Optimize Update Order
- Manually adjust the order with the sort column

Table of Schematic C2: Design of Experiments (Central Composite Design : Auto Defined)

|    | A    | B   |               |
|----|------|---|---------------|
| 1  | Name | P1 - inlethot_velocity (m s <sup>-1</sup> ) | P2 - inletcol |
| 2  | 1    | 2.5   | 1             |
| 3  | 2    | 2.25  | 1             |
| 4  | 3    |   |               |
| 5  | 4    |   |               |
| 6  | 5    |   |               |
| 7  | 6    |   |               |
| 8  | 7    |   |               |
| 9  | 8    |   |               |
| 10 | 9    |   |               |

Context menu options:

- Copy
- Paste
- Set Update Order by Row
- Show Update Order
- Optimize Update Order
- Import Design Points...
- Insert as Design Point
- Export Data
- Copy all Design Points from the Parameter Set
- Expand All
- Collapse All

Table of Schematic C2: Design of Experiments (Central Composite Design : Auto Defined)

|    | A    | B            |
|----|------|--------------|
| 1  | Name | Update Order |
| 2  | 1    | 1            |
| 3  | 2    | 2            |
| 4  | 3    | 3            |
| 5  | 4    | 4            |
| 6  | 5    | 5            |
| 7  | 6    | 6            |
| 8  | 7    | 7            |
| 9  | 8    | 8            |
| 10 | 9    | 9            |

Table of Schematic C2: Design of Experiments (Central Composite Design : Auto Defined)

|    | A    | B            |
|----|------|--------------|
| 1  | Name | Update Order |
| 2  | 1    | 5            |
| 3  | 2    | 2            |
| 4  | 3    | 8            |
| 5  | 4    | 4            |
| 6  | 5    | 6            |
| 7  | 6    | 1            |
| 8  | 7    | 7            |
| 9  | 8    | 3            |
| 10 | 9    | 9            |

Default

- **Fewest design points**
  - Custom/Optimal space filling
- **Most design points**
  - Sparse Grid \*
  - Custom/Optimal space filling
- **Use with highly non-linear response**
  - Sparse Grid \*
  - Custom/optimal space filling
  - Any DOE + Kriging (with auto-refinement)
- **Coverage of extremes / even distribution**
  - CCD
  - Box-Behnkan
  - Custom

## Good default choice:

- **DOE: CCD (default)**
- **Response surface: Kriging (with auto-refinement)**

\* Few design points are created during the DOE but many refinement points are automatically generated with the response surface

- Appendix



- **Orthogonality**

- The degree to which the main effect and interaction estimates of interest are dependent of each other

|       | P1 | P2 |
|-------|----|----|
| Run 1 | 1  | 1  |
| Run 2 | -1 | -1 |

Not orthogonal because you can only estimate the combined effect of P1 and P2

|       | P1 | P2 |
|-------|----|----|
| Run 1 | 1  | 1  |
| Run 2 | 1  | -1 |
| Run 3 | -1 | 1  |
| Run 4 | -1 | -1 |

Orthogonal because you can estimate the independent effect of P1 and P2

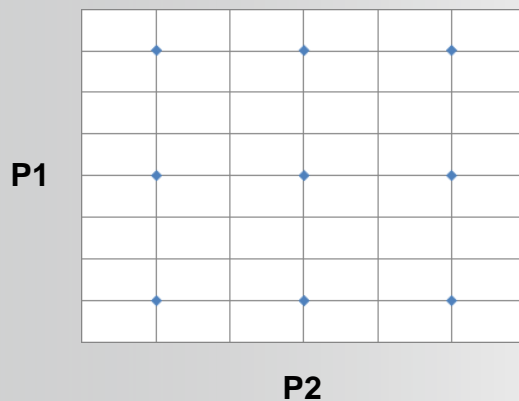
- **Leverage**

- The opportunity of sample points to have abnormal influence on the outcome.
  - E.g. A point made at an extreme value such that the lack of neighbouring observations means that the fitted regression model will pass close to that particular observation

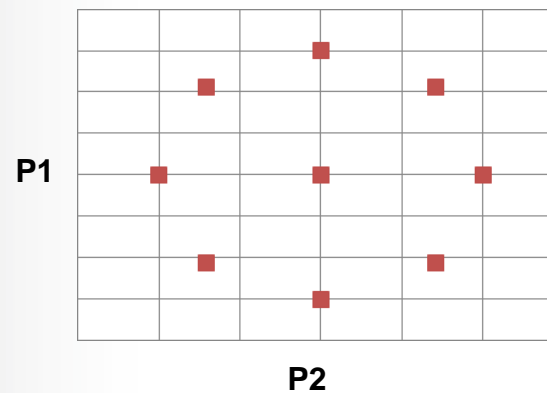
- Rotatable

- The degree to which the experimental design matrix is biased in any direction

**Not rotatable**



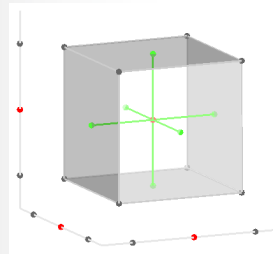
**rotatable**



## Example of how diagonals are removed

- Design Points = 5
- Minimum value for each parameter is 3
- Maximum value for each parameter is 3
- Face centered CCD
- Factorial  $f=1$
- In this example, DX keeps the design points with one 3, three 3's, and five 3's. It drops the design points with zero 3's, two 3's, and four 3's.

| P1 | P2 | P3 | P4 | P5 |             |
|----|----|----|----|----|-------------|
| 2  | 2  | 2  | 2  | 2  | center axis |
| 1  | 2  | 2  | 2  | 2  |             |
| 3  | 2  | 2  | 2  | 2  |             |
| 2  | 1  | 2  | 2  | 2  |             |
| 2  | 3  | 2  | 2  | 2  |             |
| 2  | 2  | 1  | 2  | 2  |             |
| 2  | 2  | 3  | 2  | 2  |             |
| 2  | 2  | 2  | 1  | 2  |             |
| 2  | 2  | 2  | 3  | 2  |             |
| 2  | 2  | 2  | 2  | 1  |             |
| 2  | 2  | 2  | 2  | 3  | diagonals   |
| 1  | 1  | 1  | 1  | 3  |             |
| 3  | 1  | 1  | 1  | 1  |             |
| 1  | 3  | 1  | 1  | 1  |             |
| 3  | 3  | 1  | 1  | 3  |             |
| 1  | 1  | 3  | 1  | 1  |             |
| 3  | 1  | 3  | 1  | 3  |             |
| 1  | 3  | 3  | 1  | 3  |             |
| 3  | 3  | 3  | 1  | 1  |             |
| 1  | 1  | 1  | 3  | 1  |             |
| 3  | 1  | 1  | 3  | 3  |             |
| 1  | 3  | 1  | 3  | 3  |             |
| 3  | 3  | 1  | 3  | 1  |             |
| 1  | 1  | 3  | 3  | 3  |             |
| 3  | 1  | 3  | 3  | 1  |             |
| 1  | 3  | 3  | 3  | 1  |             |
| 3  | 3  | 3  | 3  | 3  |             |



| P1 | P2 | P3 | P4 | P5 |             |
|----|----|----|----|----|-------------|
| 2  | 2  | 2  | 2  | 2  | center axis |
| 1  | 2  | 2  | 2  | 2  |             |
| 3  | 2  | 2  | 2  | 2  |             |
| 2  | 1  | 2  | 2  | 2  |             |
| 2  | 3  | 2  | 2  | 2  |             |
| 2  | 2  | 1  | 2  | 2  |             |
| 2  | 2  | 3  | 2  | 2  |             |
| 2  | 2  | 2  | 1  | 2  |             |
| 2  | 2  | 2  | 3  | 2  |             |
| 2  | 2  | 2  | 2  | 1  |             |
| 2  | 2  | 2  | 2  | 3  | diagonals   |
| 1  | 1  | 1  | 1  | 1  |             |
| 1  | 1  | 1  | 1  | 3  |             |
| 1  | 1  | 1  | 3  | 1  |             |
| 1  | 1  | 3  | 1  | 1  |             |
| 1  | 3  | 1  | 1  | 1  | zero 3's    |
| 3  | 1  | 1  | 1  | 1  |             |
| 1  | 3  | 1  | 1  | 1  |             |
| 3  | 1  | 1  | 1  | 1  |             |
| 1  | 1  | 1  | 3  | 3  |             |
| 1  | 1  | 3  | 1  | 3  | one 3's     |
| 1  | 3  | 1  | 1  | 3  |             |
| 3  | 1  | 1  | 1  | 3  |             |
| 1  | 3  | 1  | 3  | 3  |             |
| 3  | 1  | 3  | 1  | 3  |             |
| 1  | 3  | 3  | 1  | 3  | two 3's     |
| 3  | 3  | 1  | 1  | 3  |             |
| 1  | 3  | 3  | 3  | 1  |             |
| 3  | 3  | 3  | 1  | 1  |             |
| 1  | 3  | 3  | 3  | 3  |             |
| 3  | 3  | 3  | 3  | 1  | three 3's   |
| 3  | 3  | 3  | 1  | 3  |             |
| 3  | 3  | 1  | 3  | 3  |             |
| 3  | 1  | 3  | 3  | 3  |             |
| 1  | 3  | 3  | 3  | 3  |             |
| 3  | 3  | 3  | 3  | 3  | four 3's    |
| 3  | 3  | 3  | 3  | 1  |             |
| 3  | 3  | 3  | 1  | 3  |             |
| 3  | 3  | 1  | 3  | 3  |             |
| 3  | 1  | 3  | 3  | 3  |             |
| 1  | 3  | 3  | 3  | 3  | five 3's    |
| 3  | 3  | 3  | 3  | 3  |             |