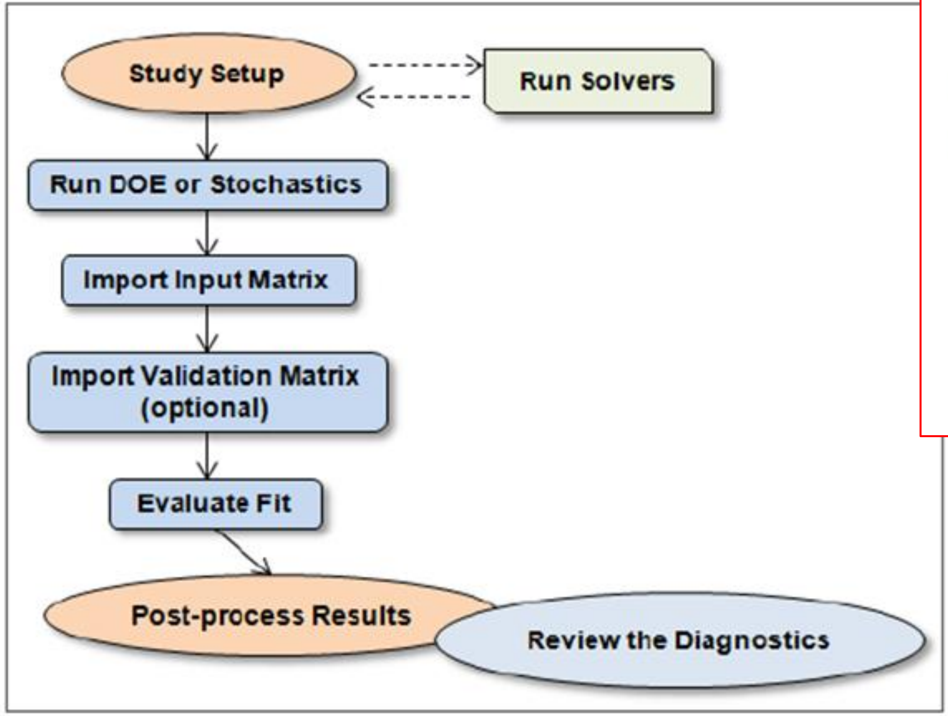
Ottimizzazione attraverso il CAE
- introduzione all'uso di Hyperstudy -

Metamodeling

(immagini e esempi presi dai tutorial Altair University)

Metamodeling
o superfici di regressione



D Fit - Concepts

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Fitting functions (Approximations) are **meta models** that represent the actual responses.

Why the need for a fit?

- Some simulations are computationally expensive which makes it impractical to rely on them exclusively for design studies. Use of a fit in such cases lead to substantial savings of computational resources.
- Optimization can fall into local minimum or maximum when the responses are nonlinear. Using approximate responses, the user can avoid this issue.

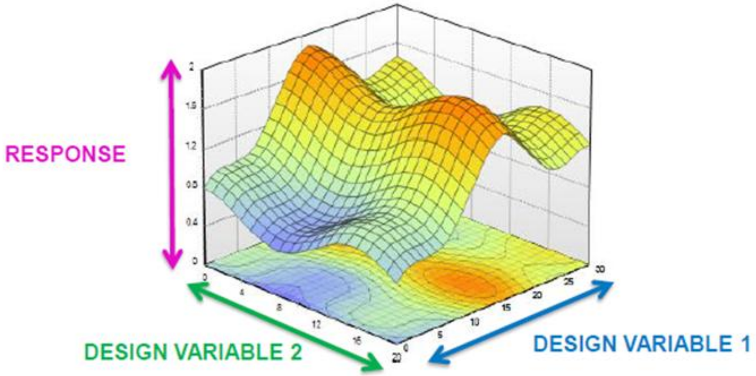
The challenge?

- When using a fit, the issue of a trade off between accuracy and efficiency is ever present.
- The question is how approximate the representation of the design space can be while remaining accurate enough.

Metamodeling - Concetti di base

RSM – Response Surface Method

- RSM techniques were originally developed to analyze experimental data which use **polynomial functions** computed to create **empirical models of the observed response values**
- The particular strength of RSM is its applicability to investigations where there are few observations because the physical experiment is both very expensive and very time consuming to perform.



D Fit - Terminology

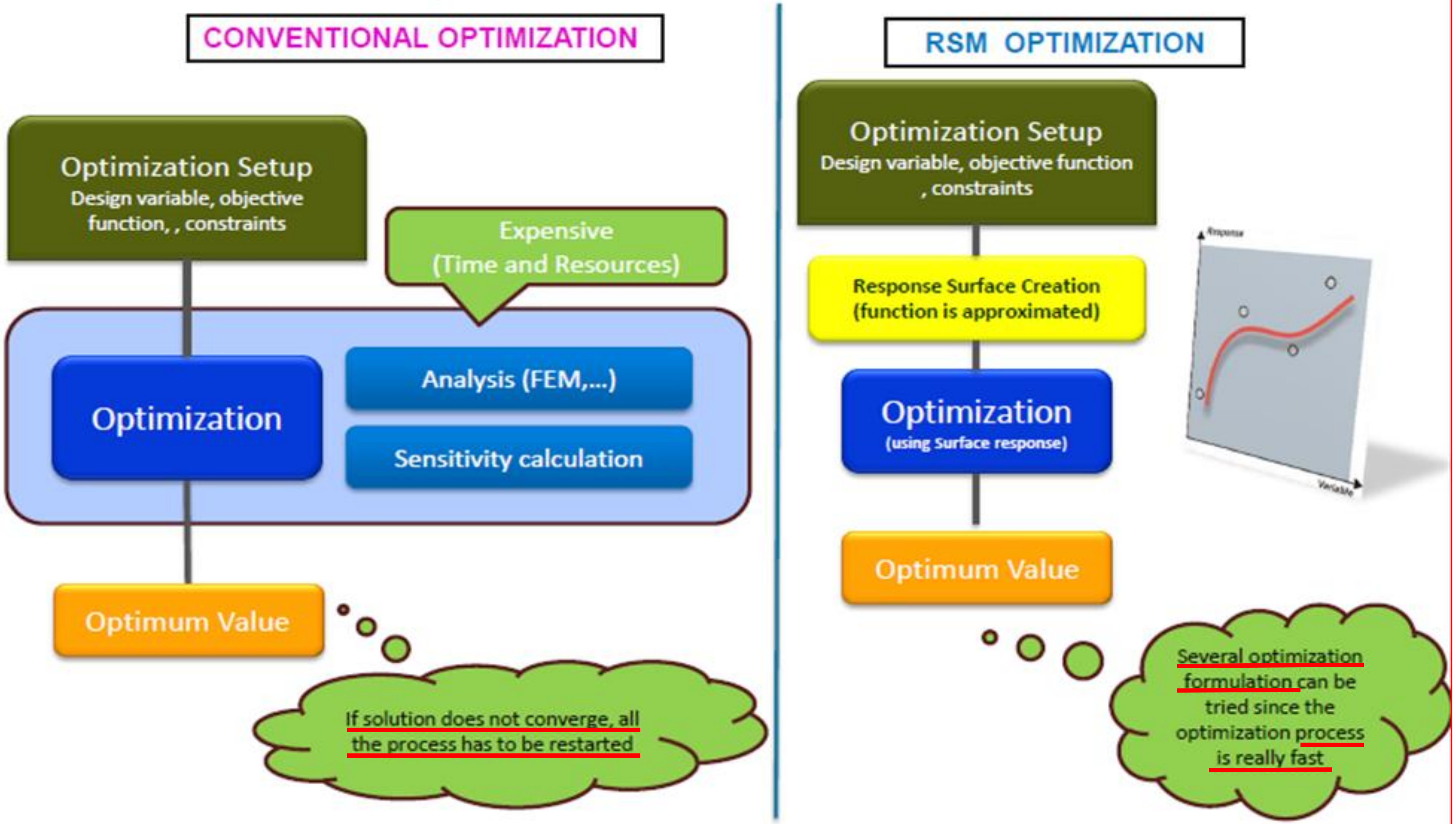
- ***Regression equation*** is the polynomial expression that relates the response of interest to the factors that were varied.
  Selection of the proper model is required to create an accurate approximation.
  However this requires *a- prior* knowledge of the behavior of the responses (linear, non linear, noisy …) and enough runs to feed the selected model and allow for a successful regression.
- ***Linear Regression model***
  $F(X) = a_0 + a_1X_1 + a_2X_2 +$ (error)
- ***Interaction Regression Model***
  $F(X) = a_0 + a_1X_1 + a_2X_2 + a_3X_1X_2 +$ (error)
- ***Quadratic Regression Model (2nd order)***
  $F(X) = a_0 + a_1X_1 + a_2X_2 + a_3X_1X_2 + a_4X_1^2 + a_5X_2^2 +$ (error)

Vettore coeff=inv$[X^T X]$ X^T(vettore run);
XT_1j=1 j=1,…,n
K+1 coefficienti
n run

A fit is only as good as the uniformity of the design sampling and, for example, a two-level parameter only has a linear relationship in the regression.

Higher order polynomials can be introduced by using more levels for the factors, but then, using more levels results in more runs.

D Fit - RSM in Optimization



Metamodeling - Passi logici e metodi

D Fit - Using RSM

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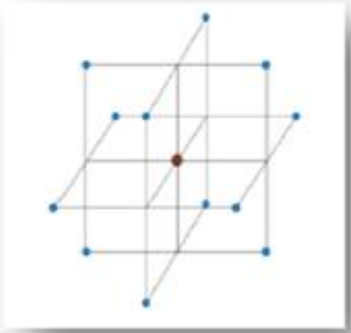
Step 1 → **Step 2** → **Step 3**

Step 1

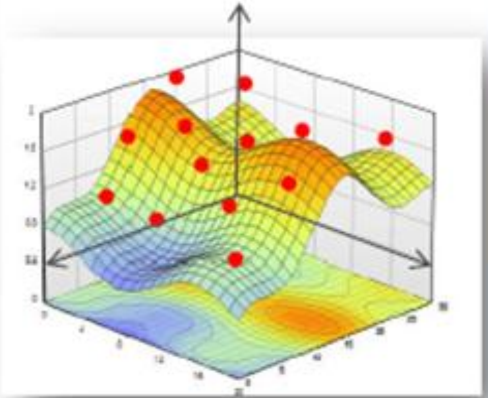
Creating an experimental design



- Latin HyperCube
- Hammersley
- User defined
- External Matrix

Step 2

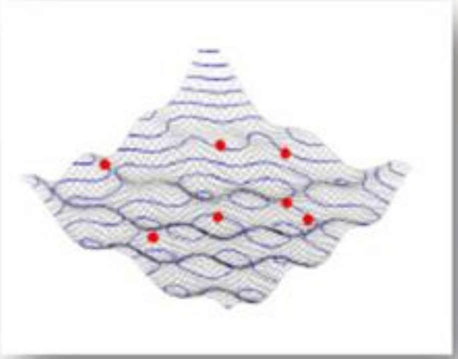
Build the surrogate model



- Least square
- Moving least square
- HyperKriging

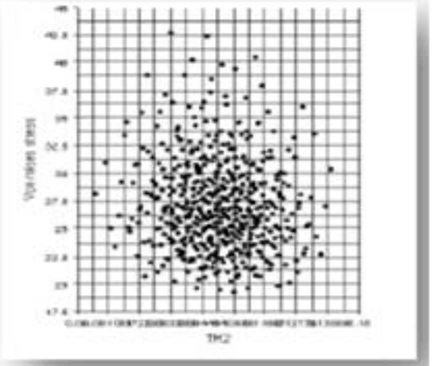
Step 3

Optimize based on surrogate model



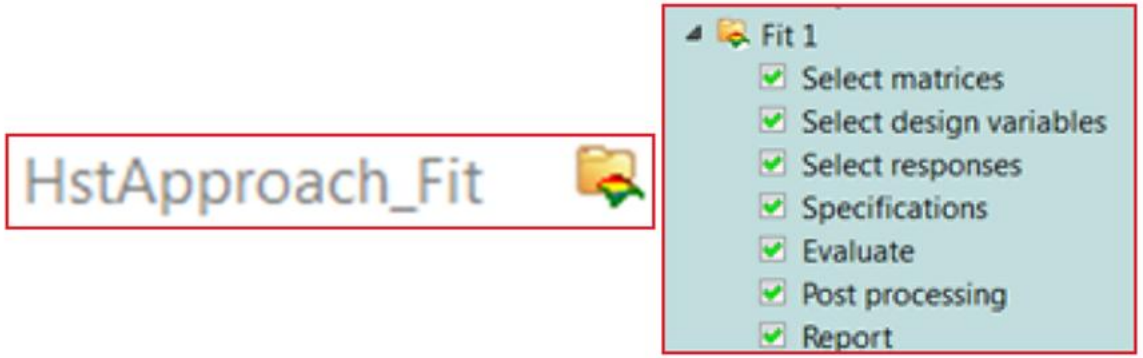
- Genetic Algorithm
- Sequential Quadratic Programming
- Adaptive Response Surface
- Method of Feasible Directions
- Sequential Optimization and Reliability Assessment
- Multi-Objective Genetic Algorithm
- Gradient-Based Method for Multi Objective Optimization
- External optimizers

Stochastic study based on surrogate model



- Random
- Latin HyperCube
- Hammersley

Metamodeling -
Passi logici in HyperStudy



D Fit - Process

The steps to set up a **Fit** Approach in HyperStudy are:

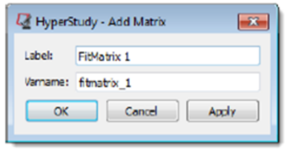
1. **Select Matrices (Fit)**
   - Import the run matrix
2. **Select Design Variables**
3. **Select Responses**
4. **Specifications**
   - Methods, Matrix, Regression Terms, Settings
5. **Evaluate**
6. **Post-Processing**
   - Residuals, Diagnostics, Trade-Off 1D, Trade-Off 2D/3D
   - Analysis of Variance (ANOVA, only on **Least Square Regression**)
7. **Report**
   - HTML, HyperWorks
   - Post-Processing
   - Spreadsheet (Fit Excel Plug-In)

Scelta del piano di partenza

D Fit – Select Matrices

1) Click ***Add Matrix*** button [Add Matrix]

2) In the **HyperStudy - Add** dialog, enter a label for the matrix in the **Label** field.



3) Click ***Apply*** or ***OK*** according to your needs

4) Once you add a matrix, define the following fields:

Select matrices — Add Matrix | Remove Matrix

	Active	Label	Varname	Type	Matrix Source	Matrix Origin	Status
1	☑	FitMatrix 1	fitmatrix_1	Input	Optimization 1 (opt_1)	OptStudyOptimization 1	Import Pending
2	☑	FitMatrix 2	fitmatrix_2	Input	Optimization 1 (opt_1)	OptStudyOptimization 1	Import Pending
3	☑	FitMatrix 3	fitmatrix_3	Input	Optimization 3 (opt_3)	OptStudyOptimization 3	Import Pending

5) Click ***Import Matrix*** button [Import Matrix] to import the data from the matrix(ces).

D Fit – Select Matrices

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This step is only required during a **Fit** approach.

Select matrices allows you to import and modify the design matrices and associated results for the creation of the approximation model. The matrix and results should be imported from an existing DOE or Stochastic approach and can be further edited on the fly.

Fit can import two types of matrices:

- **Input matrices**: the data will be used to create the fit and tune its parameters
- **Validation matrices**: the data will be used to assess the quality of the fit.

Specifications | Input Matrix | Validation Matrix | Regression Terms

	Include	Thickness	H2	I1	I2	Mass	Disp	Freq
1	☑	0.0023750	-0.5000000	-0.5000000	-0.5000000	2.2165600	0.0027033	322.54180
2	☑	0.0023750	-0.5000000	-0.5000000	0.5000000	2.4824000	0.0015447	351.47020
3	☑	0.0023750	-0.5000000	0.5000000	-0.5000000	2.4695000	0.0023253	300.41670
4	☑	0.0023750	-0.5000000	0.5000000	0.5000000	2.7342300	0.0013569	325.26170
5	☑	0.0023750	0.5000000	-0.5000000	-0.5000000	2.3873400	0.0022789	415.00990

- **Regression Terms**: If the imported matrices contain failed runs, the corresponding lines are made inactive the data will be used to assess the quality of the fit.

Specifications | Input Matrix | Validation Matrix | Regression Terms

	Active	Coefficient	Terms
1	☑	a0	intercept
2	☑	a1	dv_1^1
3	☑	a2	dv_2^1

D Fit – Select Design Variables

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This step is similar across the four approaches with the following exceptions.

For a **Fit**, you can:

- Select the design variables against which the approximation will be built. The design variables shown in the table in the work area are derived from the design variables present in the matrices (see **Select Matrices**, To import a design matrix). Some variables can be removed from the default table.

Define design variables | Details | Distributions | Link

Add Design Variable | Remove Design Variable

	Active	Label	Varname	Lower Bound	Initial	Upp
1	☑	Thickness	m_1_Thickness	0.0015000	0.0020000	0.00
2	☑	H2	m_1_H2	-1.0000000	0.0000000	1.00
3	☑	I1	m_1_I1	-1.0000000	0.0000000	1.00
4	☑	I2	m_1_I2	-1.0000000	0.0000000	1.00

D Fit – Select Responses

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Review your responses and exclude any of the responses from the approach by un-checking the response in the State column.

It is not possible to exclude responses in an optimization approach.

You can also change the evaluation source from its default entry of SOLVER to one of the Fits (if you have any Fit approaches defined prior to this approach).

Select responses

Add Response | Remove Response

	Active	Label	Varname	Expression	Evaluate From
1	☑	Mass	r_1	v_1[0]	Mass__MLSM (r_1_fit_5)
2	☑	Disp	r_2	v_2[0]	Disp__MLSM (r_2_fit_5)
3	☑	Freq	r_3	v_3[0]	Freq__MLSM (r_3_fit_5)

Evaluate From

Mass__MLSM (r_1_fit_5)
SOLVER
Mass__MLSM (r_1_fit_5)
Freq__MLSM (r_3_fit_5)

Scelta dei metodi di fitting

D Fit – Specifications Methods

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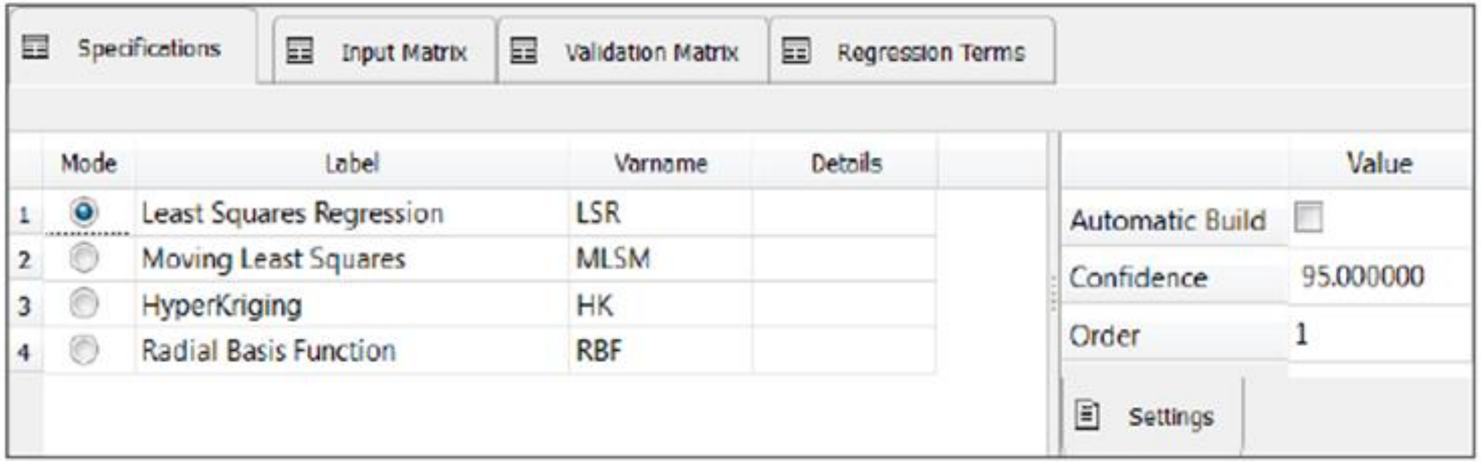
Fits methods:

- Least Squares Regression (LSR)
- Moving Least Squares Method (MLSM)
- HyperKriging (HK)
- Radial Basic Function (RBF)



In the **Input Matrix** and **Validation Matrix** tabs, the matrices selected when creating the **Fit** approach are displayed. The tables can be reviewed, and the values in the cells can be edited. Some lines can be removed from the selection. If the imported matrices contain failed runs, the corresponding lines are made inactive.

Scelta dei metodi di fitting – Least Squares Regression

D Fit - Least Squares Regression (LSR)

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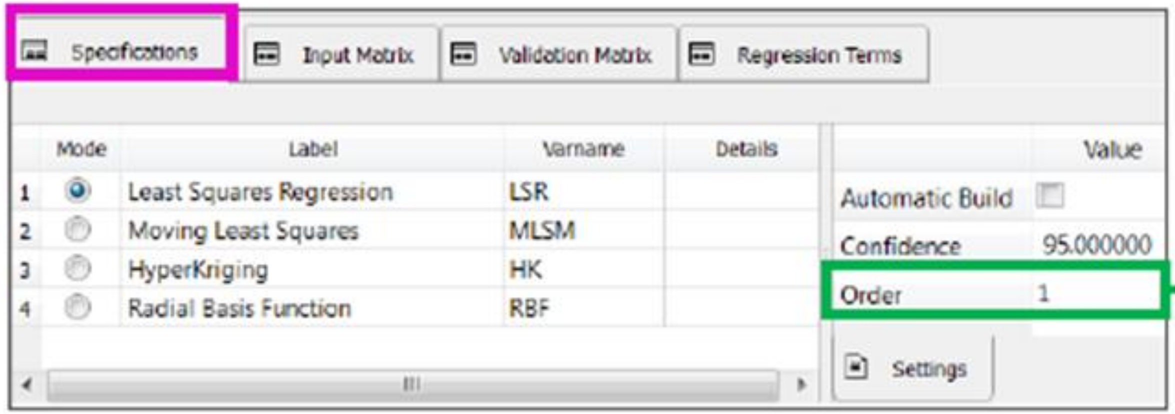
LSR method creates a regression polynomial of the chosen order such that the sum of the squares of the differences (residuals) between response values predicted by the regression model and the corresponding simulation model is minimized.

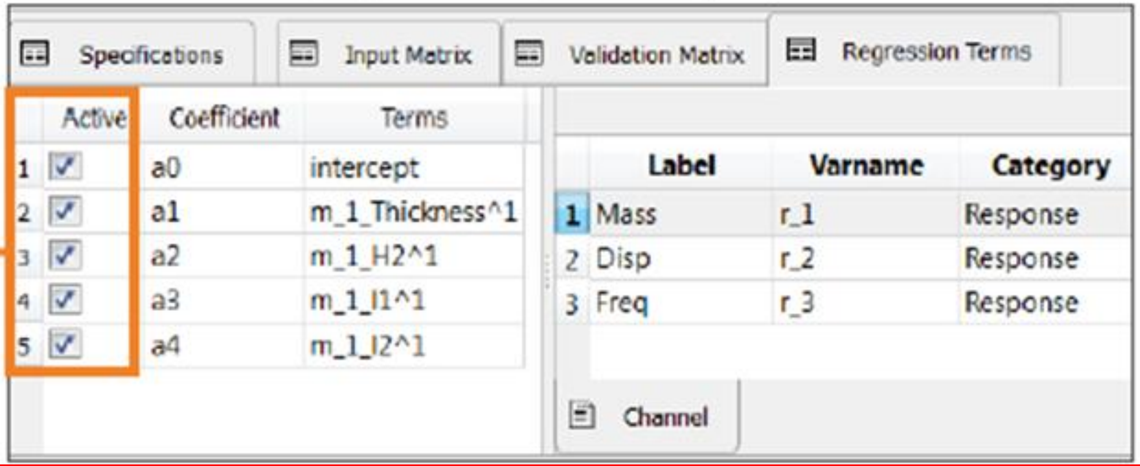
- **Usability Characteristics** → HyperStudy will create the least squares regression of any order
- **Settings** →



Can be any polynomial order, differentiator for HyperStudy

Can turn on/off, differentiator for HyperStudy.

If you want a higher order polynomial but do not have enough runs, can turns off the ones you think are not significant (very high order terms; high order interactions)



Scelta dei metodi di fitting – Moving Least Squares Method

D Fit - Moving Least Squares Method (MLSM)

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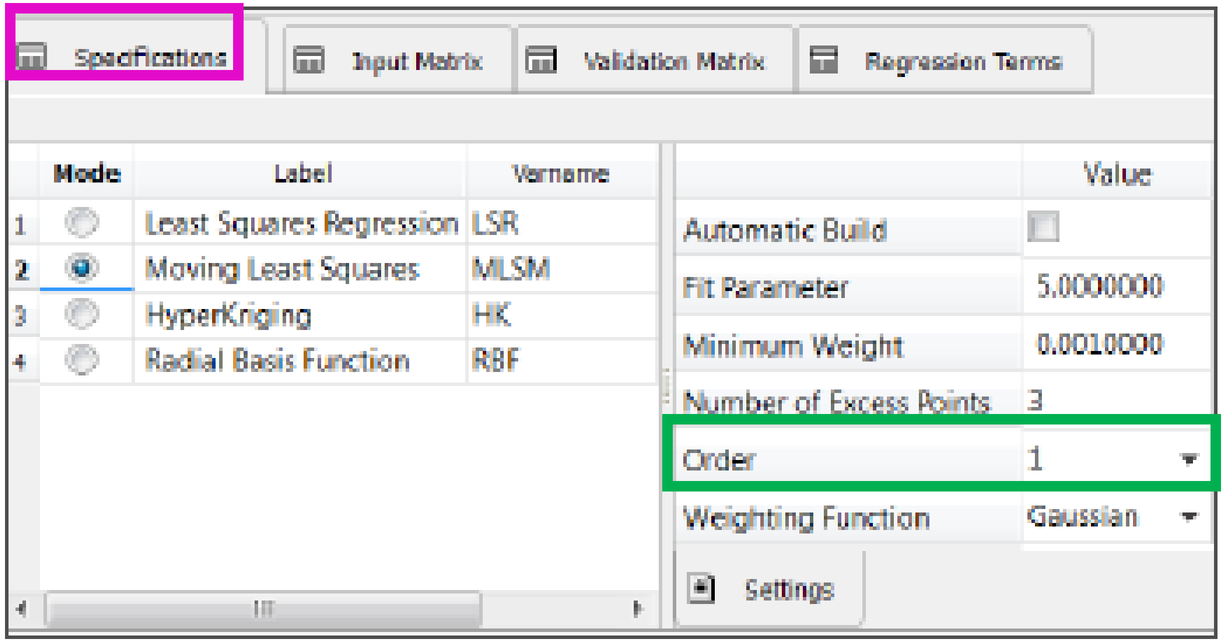
MLSM builds a weighted least squares model where the weights associated with the sampling points do not remain constant. They are functions of the normalized distance from a sampling point to a point *x*, where the surrogate model is evaluated. The weight, associated to a sampling point, decays (decay function) as the evaluation point moves away from it. For each point *x* it reconstructs a continuous function biased towards the region around that point.

- Usability Characteristics → Suggested to be used for non-linear and noisy responses.
- Settings →



Scelta dei metodi di fitting – Kriging

D Fit - HyperKriging (HK)

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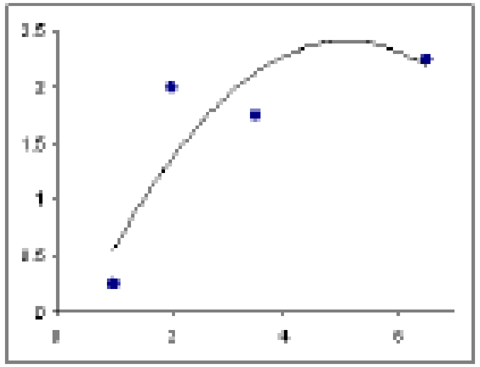
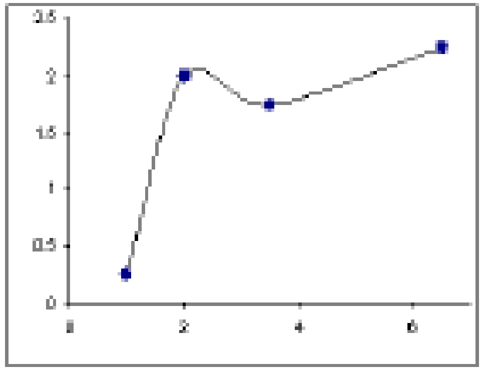
HyperKriging is a HyperStudy implementation of an approximation model building technique known as Kriging. Kriging was originally developed in the field of geostatistics and is attributed to the development of statistical techniques by mining engineer D.G. Krige. It is also known as Design and Analysis of Computer Experiments (DACE), which emphasizes that it models deterministic computer simulations.

- Usability Characteristics → Suitable for modeling highly nonlinear response data that does not contain numerical noise.

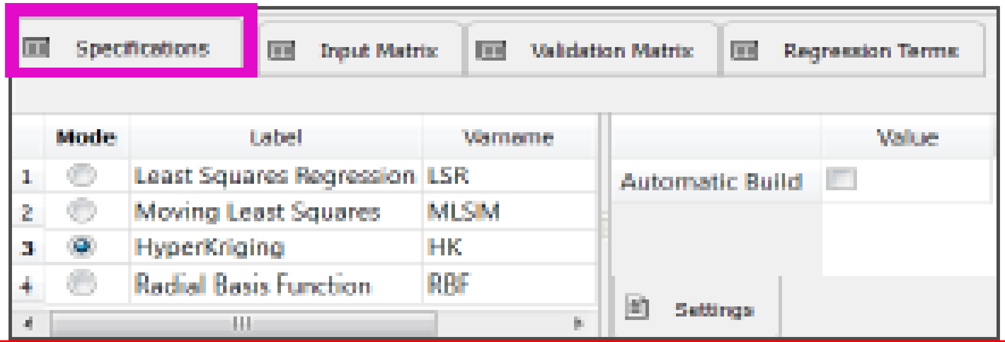


Least squares quadratic regression



Kriging model

- Settings →



Scelta dei metodi di fitting – Radial Basis Functions

D Fit - Radial Basis Functions (RBF)

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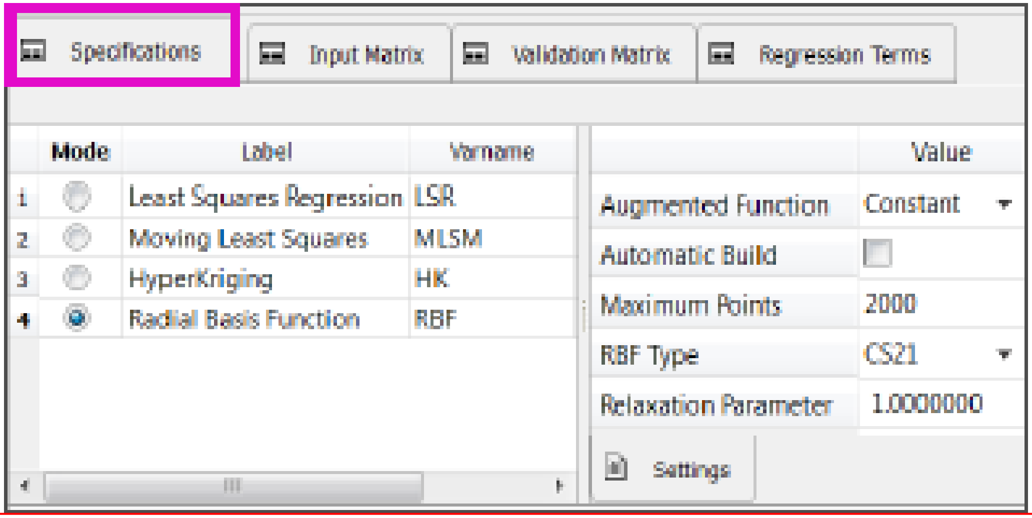
RBF method is a Fit method that uses linear combinations of basis functions. Typical basis functions are linear, cubic, thin-plate spline, Gaussian, multiquadric, and inverse-multiquadric. These basis functions are observed to be accurate for highly nonlinear responses but not for linear responses. To remedy this deficiency, in HyperStudy, a RBF model is augmented with a polynomial function:

$$f(x)=\sum_{i=1}^{n}\lambda_i\phi\left(\left\|x-x_i\right\|\right)$$

- Usability Characteristics → RBF tries to go through the exact sampling points, and in general, the residuals are small, if not zero.
- Settings →



Scelta dei metodi di fitting – confronto

D Fit – Specifications Methods Summary

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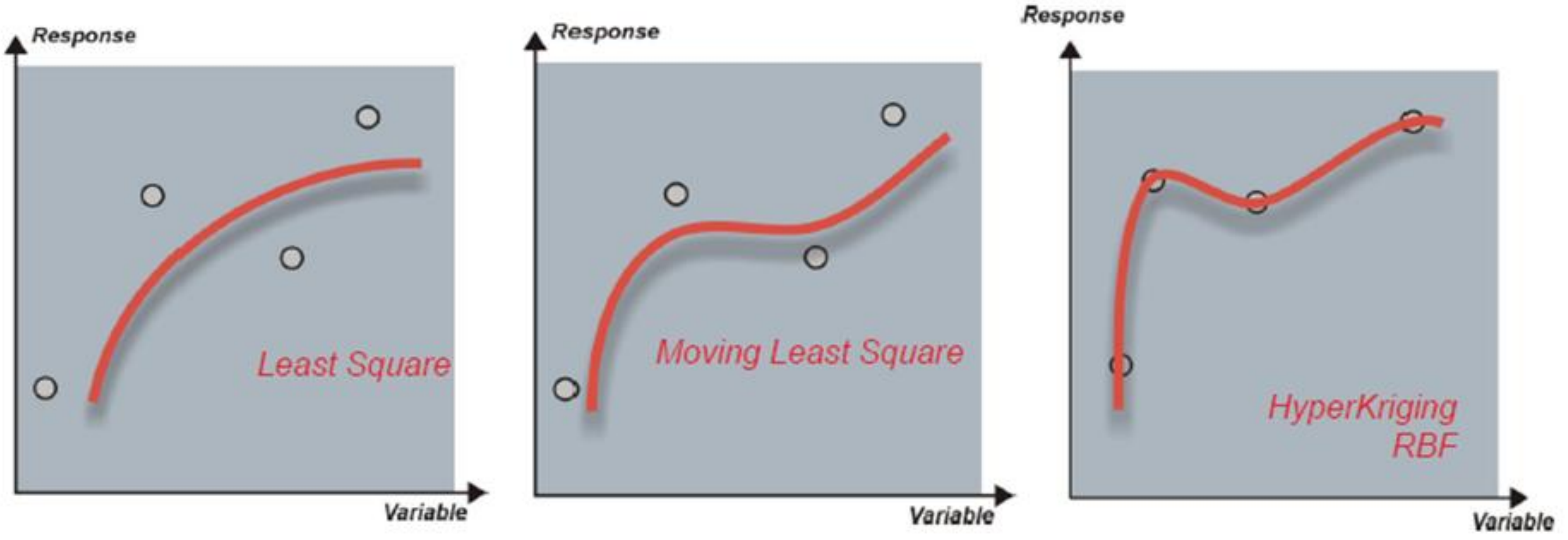
Type	Equation Available	Application
Least Square Regression	Yes	Nonlinear (e.g. second order) with noise
Moving Least Squares	No	Highly non-linear behavior with noise
HyperKriging	No	Highly non-linear behavior without noise
Radial Basis Functions	No	Highly non-linear behavior without noise



Come si vede Kriging è un metodo interpolante, quindi è conforme al DACE

D Fit - Evaluate

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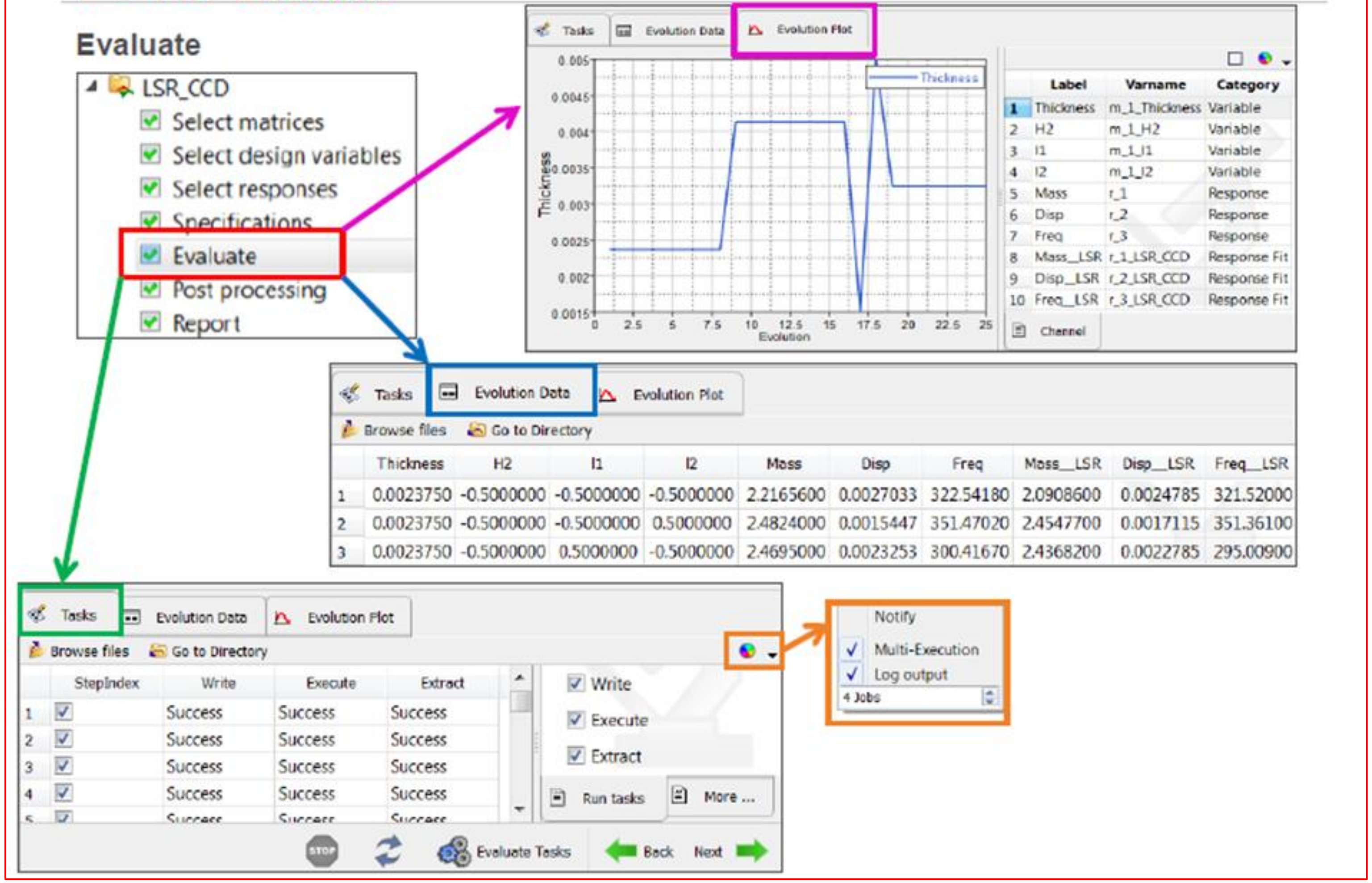

In questo caso non serve il <<purge >> perché non sono stati lanciati nuovi DOE di simulazione

Postprocessing

D Fit - Post-Processing

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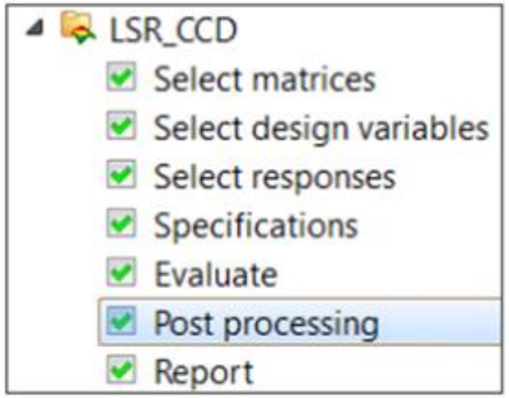
Post processing options for the approaches of a study are split into two groups; one group is available regardless of approach, and another group provides approach-specific options.

Run Summary, **Statistics**, **Histogram, Box Plot** and the **Scatter plots** (**2D and 3D**) are available across all approaches. Any approach-specific post processing options will appear in a second group of tabs.

The Fit-specific **Post-Processing** includes **Residuals**, **Diagnostics**, **Trade-Off 1D**, **Trade-Off 2D/3D** and **Analysis of Variance (ANOVA).**

In the **Explorer** select ***Post-processing*** step, [✓ Post processing] to proceed with Fit Post-Processing.

- **Run Summary**
- **Statistics**
- **Histograms**
- **Box Plot**
- **Scatter 2D**
- **Scatter 3D**
- …



Postprocessing

D Fit - Post-Processing

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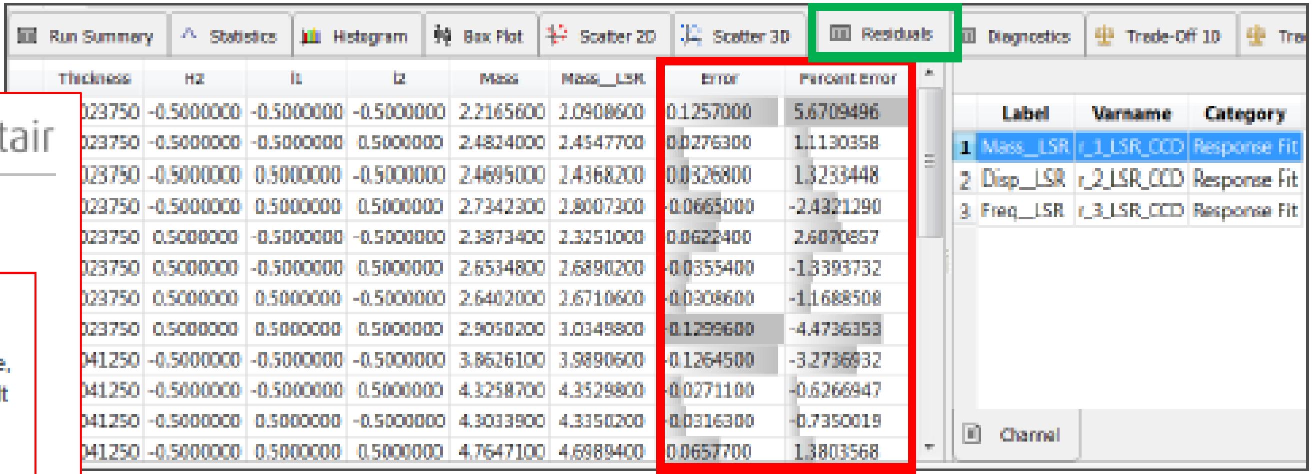
Residuals

For each run of the input matrix, error (and percentage) between the original response and the approximation is listed.
Using the find and sort capabilities of the tables, it is then possible to search for specific cases.



The difference between the response value from the solver and the response value from the response surface is the error, or the residual. The residual plot can be used to determine which runs are generating more error in the model.

D Fit - Post-Processing

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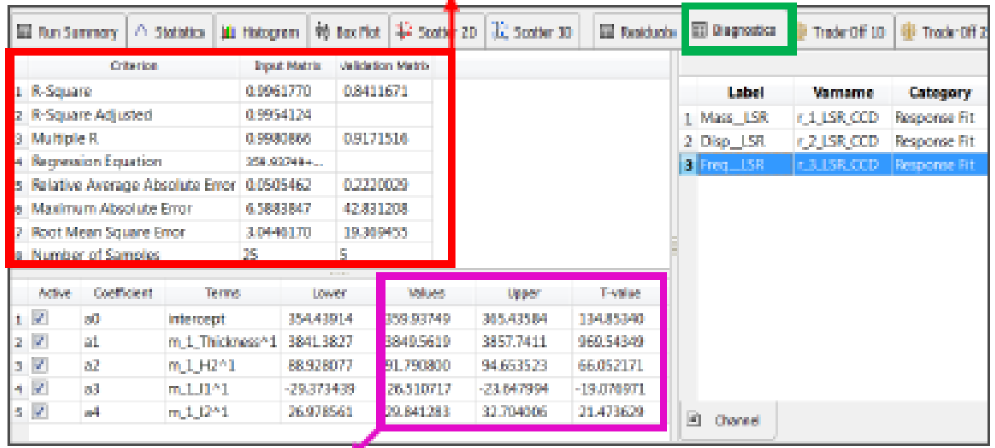
Diagnostics

Diagnostics help in the assessment of the accuracy of the approximate model.

R-Square, ***R-Square Adjusted*** and ***Multiple R*** are statistical terms indicating the accuracy of the approximations:

- ***R-Square*** predicts how well a regression approximates real data points.
- ***R-Square Adjusted*** is a modification of R-Square that takes number of data points into account. Unlike R-Square, R-Square Adjusted increases only is the new term improves the model more than would be expected by chance. It can be negative and will always be less than or equal to R-Square.
- ***Multiple R*** is the correlation coefficient. It indicates relationship between the approximation and the data.



Range for coefficients for the corresponding confidence limit
We have 95% confidence that the intercept value is between ~40 and ~89.

Postprocessing

D Fit - Post-Processing

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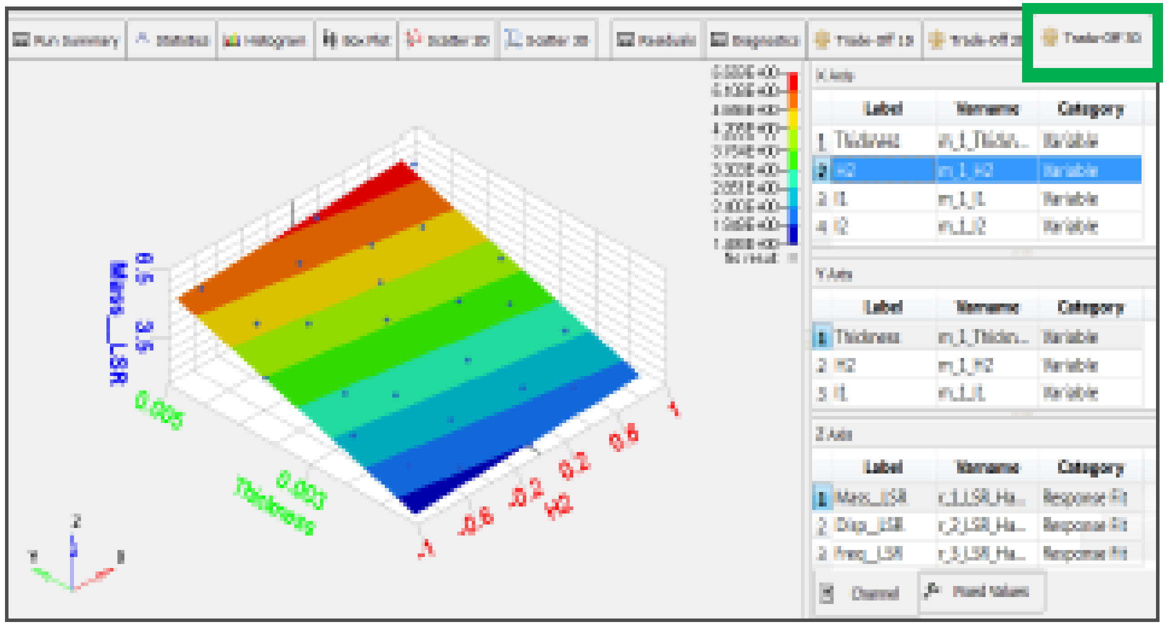
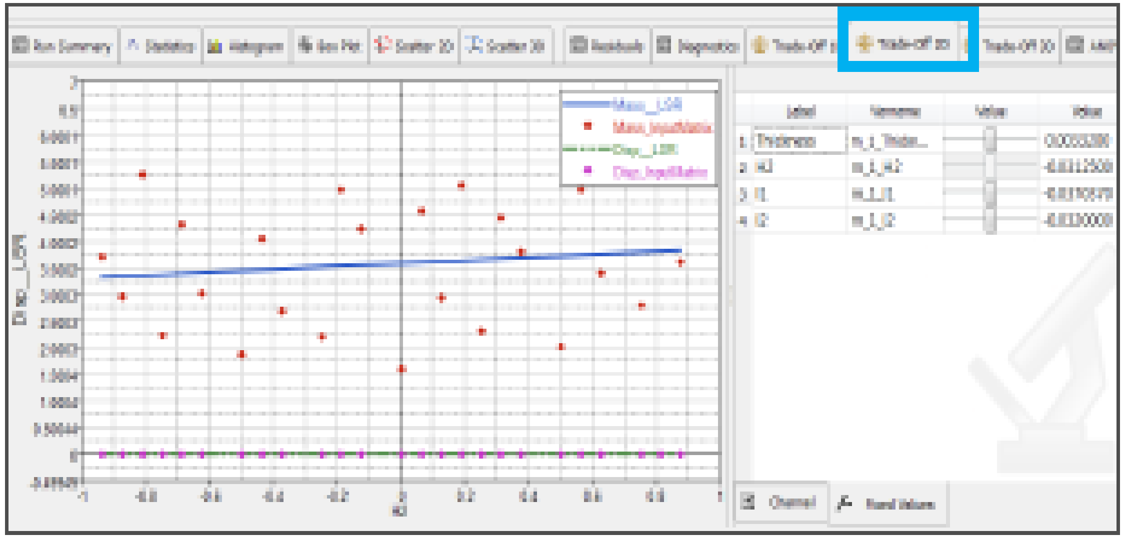
Trade-Off 2D/3D

The Trade-Off 2D/3D tabs are an extension of the Trade-Off 1D tab.

In both of these tabs:

- Responses are selected in the Channel tab (right-hand panel).
- Variables are modified using the Fixed Values tab (right-hand panel). The sliders in the Value column, can be used to modify the other design variables, while studying the response throughout the design space.
- Displays plots of response vs. design variables.





D Fit - Post-Processing

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Analysis of Variance (ANOVA)

ANOVA is a useful technique for estimating error variance and for determining the relative importance of various factors.

In HyperStudy, the ANOVA is performed only on **Least Square Regression**.

The ANOVA is plotted as the **Percentage contribution** of each design variable, the interaction and the **Error**.

The following quantities are computed in the process of performing the ANOVA:

DoF	- Degrees of freedom, Number of terms in the approximation.
SS	- Sum of Square
MSS	- Mean sum of squares (MSS = SS/DoF)
%	- Percentage contribution.
F0	- F0 value (F0 = MSS(Variable)/MSS(Error)).

Run Summary | Statistics | Histogram | Box Plot | Scatter 2D | Scatter 3D | Residuals | Diagnostics | Trade-Off 1D | Trade-Off 2D | Trade-Off 3 | ANOVA

	Variables	Degrees Of Freedom	Sum Of Squares	Mean Squares	Mean Squares Percent	F Value
1	m_1_Thickness	1	21.619055	21.619055	92.131113	4793.2620
2	m_1_H2	1	0.3292243	0.3292243	1.4030124	72.993865
3	m_1_I1	1	0.7181368	0.7181368	3.0603903	159.22148
4	m_1_I2	1	0.7946048	0.7946048	3.3862636	176.17554
5	Error	20	0.0902060	0.0045103	0.0192210	N/A
6	Total	24	23.551227	N/A	100.00	N/A

	Label	Varname	Category
1	Mass_LSR	r_1_LSR_CCD	Response Fit
2	Disp_LSR	r_2_LSR_CCD	Response Fit
3	Freq_LSR	r_3_LSR_CCD	Response Fit

Channel

Reporting

D Fit - Reporting

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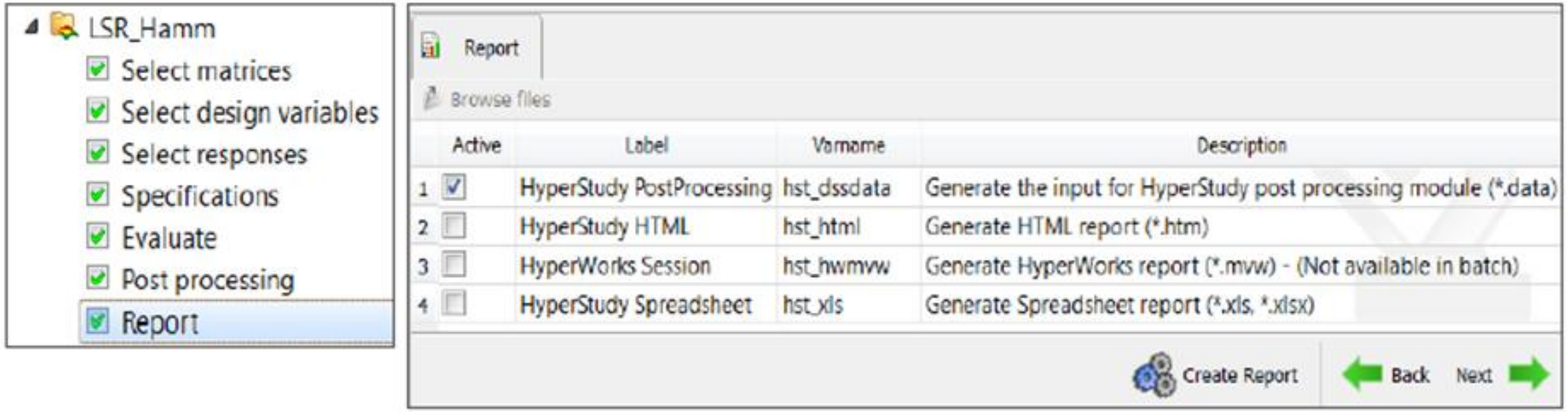
Reporting

There are currently four reporting options for all approaches:

- **HTML** - Generates a HTML report and opens it in your default web browser
- **HyperWorks** - Generates a HyperWorks report and opens it in HyperWorks Desktop.
- **Post-Processing** tool (review help) - Launches the post-processing and data mining tool
- **Spreadsheet** - Generates a spreadsheet report and opens it in Excel. For a Fit approach, Trade-off 1D post-processing can be reported to Excel spreadsheets, which allows you to do trade-off studies in Excel, independent of HyperStudy. For more information on this feature, refer to ***Fit Excel Plug-In***.

In the **Explorer** select ***Report*** step [Report], to proceed with Fit Reporting.



Reporting

D Fit - Reporting

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Reporting (…continue)

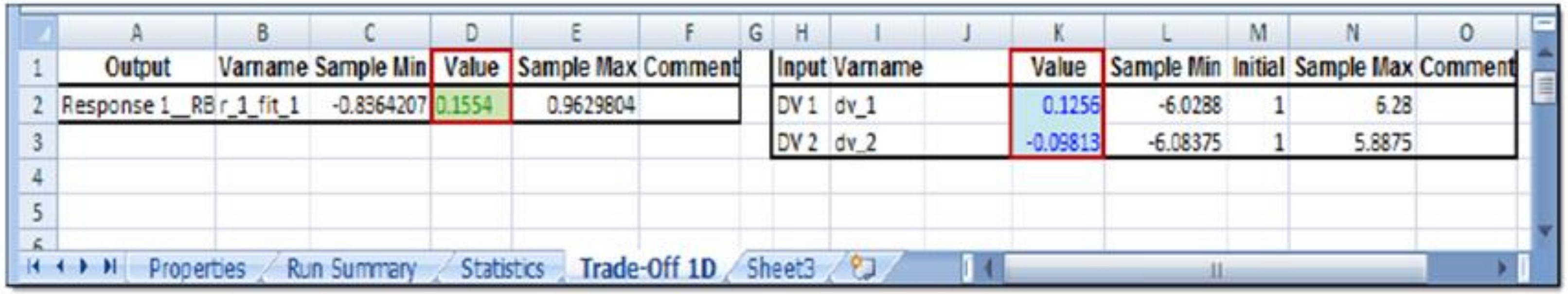
- **Fit Excel Plug-In**

For a **Fit** approach, you can generate a **Trade-off 1D** post-processing report to **Excel** spreadsheets. This specific report allows you to do trade-off studies in Excel, independent of HyperStudy. In order to use this feature, you add the HstAddinFit add-in to Excel.
Fit Excel report: Trade-Off 1D tab is a reflection of the corresponding **Trade-Off 1D** tab (HyperStudy). From the Trade-Off 1D tab in Excel, you can adjust the design variable values on the right-hand side to change the predicted responses values displayed on the left-hand side.

1) Select the ***HyperStudy Spreadsheet*** check box.

2) Click ***Create Report***. HyperStudy generates an Excel report and opens it in Excel.

3) In the Excel report, click the ***Trade-Off 1D*** tab.



	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O
1	Output	Varname	Sample Min	Value	Sample Max	Comment		Input	Varname		Value	Sample Min	Initial	Sample Max	Comment
2	Response 1__RB	r_1_fit_1	-0.8364207	0.1554	0.9629804			DV 1	dv_1		0.1256	-6.0288	1	6.28	
3								DV 2	dv_2		-0.09813	-6.08375	1	5.8875	
4															
5															

4) To verify that the same values occur in the response prediction columns for the same set of design variables, simultaneously adjust the values within HyperStudy and the Excel report.

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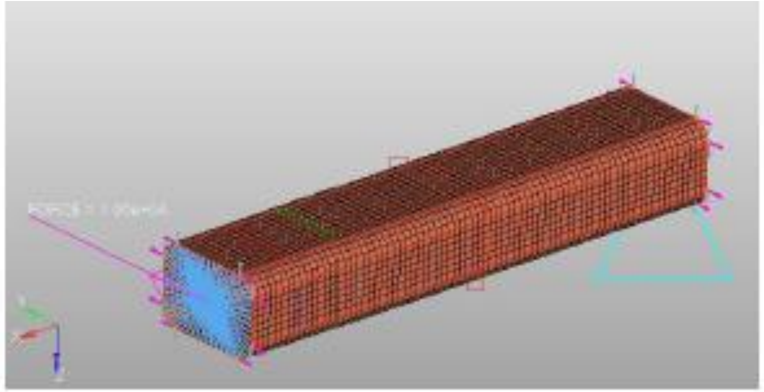

D Fit - Exercise 3a

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Input file:

This exercise uses the completed study from Exercise 2b, Study_2b_complete.xml. Alternatively, you can begin from a file in the tutorials set, Study_3a, Study-3A-BASE-FILES (Study-3A-base-files-archive.hstx).

Goal:

To create an approximation from DOEs performed in HyperStudy. The quality of the DOE and inputs to the approximation will determine the amount of error in the resulting approximation surface.

Variables:

PSHELL Thickness, Shapes, H2, I1, I2

Define Fits:

Create Fits and compare the error and the quality of the approximation for each method

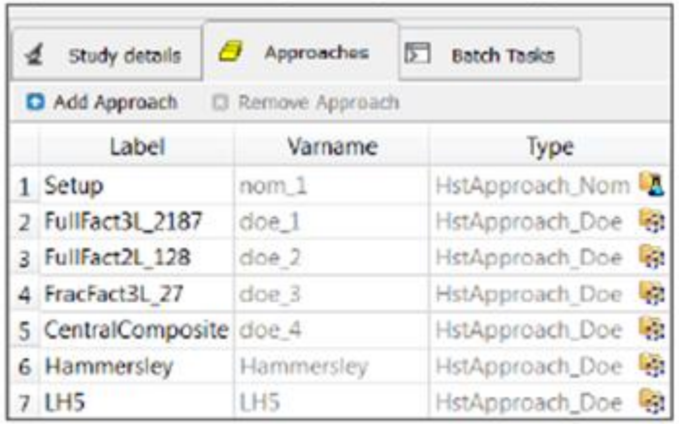
Responses:

[No responses for this exercise]

D Fit - Exercise 3a Major Steps

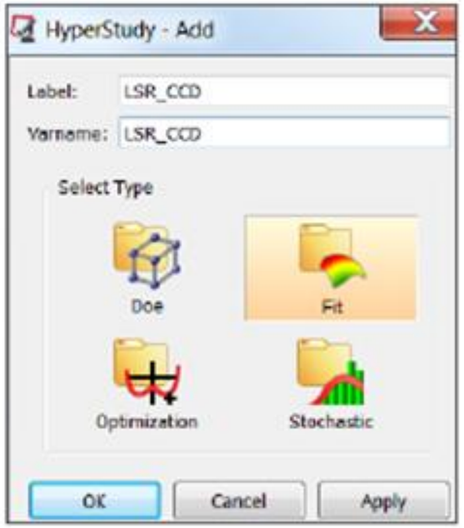
Altair

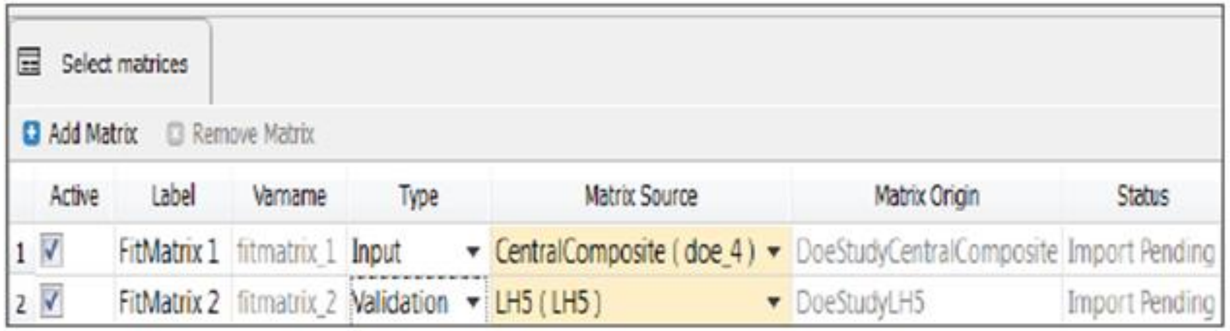
1) Open the existing study within HyperStudy (**Study-3a-base-files-archive.hstx**)



2) Add new Fit (Approximations) to the study

a] Fit (Approximation): Select matrices





D Fit - Exercise 3a

Altair

2) Add new Fit (Approximations) to the study

b] Fit (Approximation): Select design variables and Responses

Define design variables | Details | Distributions | Link Variables

Add Design Variable | Remove Design Variable

	Active	Label	Varname	Lower Bound	Initial	Upper Bound	Comment
1	☑	Thickness	m_1_Thickness	0.0015000	0.0020000	0.0050000	...
2	☑	H2	m_1_H2	-1.0000000	0.0000000	1.0000000	...
3	☑	I1	m_1_I1	-1.0000000	0.0000000	1.0000000	...
4	☑	I2	m_1_I2	-1.0000000	0.0000000	1.0000000	...

Select responses

Add Response | Remove Response

	Active	Label	Varname	Expression
1	☑	Mass	r_1	v_1[0] ...
2	☑	Disp	r_2	v_2[0] ...
3	☑	Freq	r_3	v_3[0] ...

c] Run Fit (Approximation): *Specifications* → *Mode* tab, choose Least Squares Regression

Input Matrix tab, ***Include*** column, set all flag on

Specifications | Input Matrix | Validation Matrix | Regression Terms

	Mode	Label	Varname	Details
1	◉	Least Squares Regression	LSR	
2	○	Moving Least Squares	MLSM	
3	○	HyperKriging	HK	
4	○	Radial Basis Function	RBF	

	Value
Automatic Build	☐
Confidence	95.000000
Order	1

Settings

Specifications | Input Matrix | Validation Matrix | Regression Terms

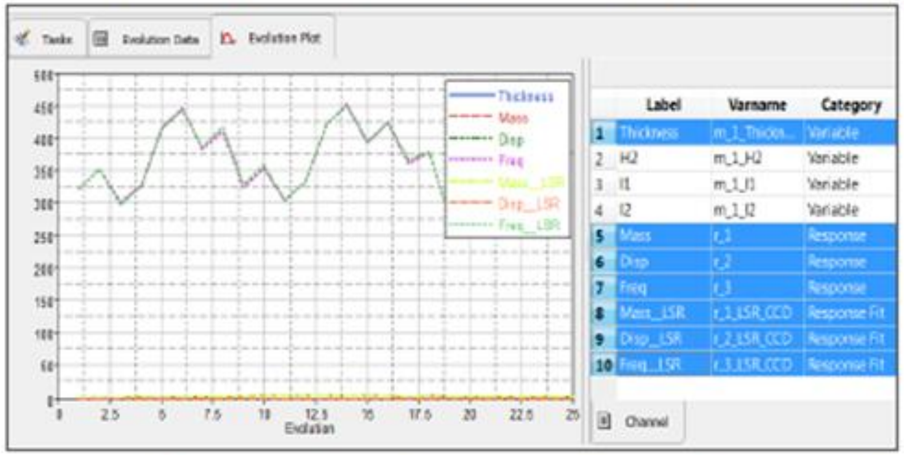
	Include	Thickness	H2	I1	I2	Mass	Disp	Freq
1	☑	0.0023750	-0.5000000	-0.5000000	-0.5000000	2.2165600	0.0027033	322.54180
2	☑	0.0023750	-0.5000000	-0.5000000	0.5000000	2.4824000	0.0015447	351.47020
3	☑	0.0023750	-0.5000000	0.5000000	-0.5000000	2.4695000	0.0023253	300.41670
4	☑	0.0023750	-0.5000000	0.5000000	0.5000000	2.7342300	0.0013569	325.26170

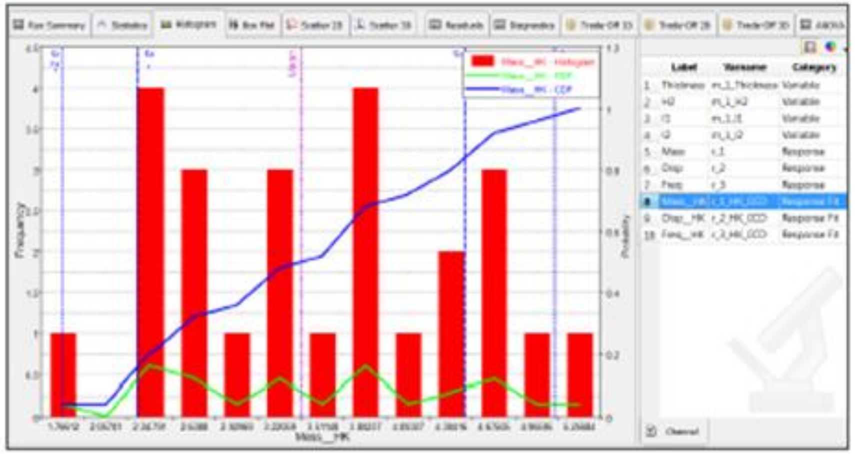
D Fit - Exercise 3a

Altair

2) Add new Fit (Approximations) to the study

d] Fit (Approximation): Evaluate and Post-Processing





3) Add 5 more Fit to the study with the following table

Label	Approximation Type
MLSM_CCD	Moving Least Squares Method
HK_CCD	HyperKriging
LSR_Hamm	Least Squares Regression
MLSM_Hamm	Moving Least Squares Method
HK_Hamm	HyperKriging

Study details · Approaches · Batch Tasks

Add Approach · Remove Approach

	Label	Varname	Type
1	Setup	nom_1	HstApproach_Nom
2	FullFact3L_2187	doe_1	HstApproach_Doe
3	FullFact2L_128	doe_2	HstApproach_Doe
4	FracFact3L_27	doe_3	HstApproach_Doe
5	CentralComposite	doe_4	HstApproach_Doe
6	Hammersley	Hammersley	HstApproach_Doe
7	LHS	LHS	HstApproach_Doe
8	LSR_CCD	LSR_CCD	HstApproach_Fit
9	MLSM_CCD	MLSM_CCD	HstApproach_Fit
10	HK_CCD	HK_CCD	HstApproach_Fit
11	LSR_Hamm	LSR_Hamm	HstApproach_Fit
12	MLSM_Hamm	MLSM_Hamm	HstApproach_Fit
13	HK_Hamm	HK_Hamm	HstApproach_Fit

D Fit - Exercise 3a

Altair

4) Fit (Approximation): setting changes (Type and Responses)

- Select Fit «**LSR_Hamm**», select ***Hammersley*** DOE as Matrix source and Run it.
- Set the other Fits according to the following table:

Fit Label	Specification (Approximation Mode)	Responses (flag on only)	Matrix Source (Import Doe)
MLSM_CCD	Moving Least Squares Method	All	Central Composite
HK_CCD	HyperKriging	All	Central Composite
LSR_Hamm	Least Squares Regression	Mass, Displacement, Frequency	Hammersley
MLSM_Hamm	Moving Least Squares Method	Mass, Displacement, Frequency	Hammersley
HK_Hamm	HyperKriging	Mass, Displacement, Frequency	Hammersley

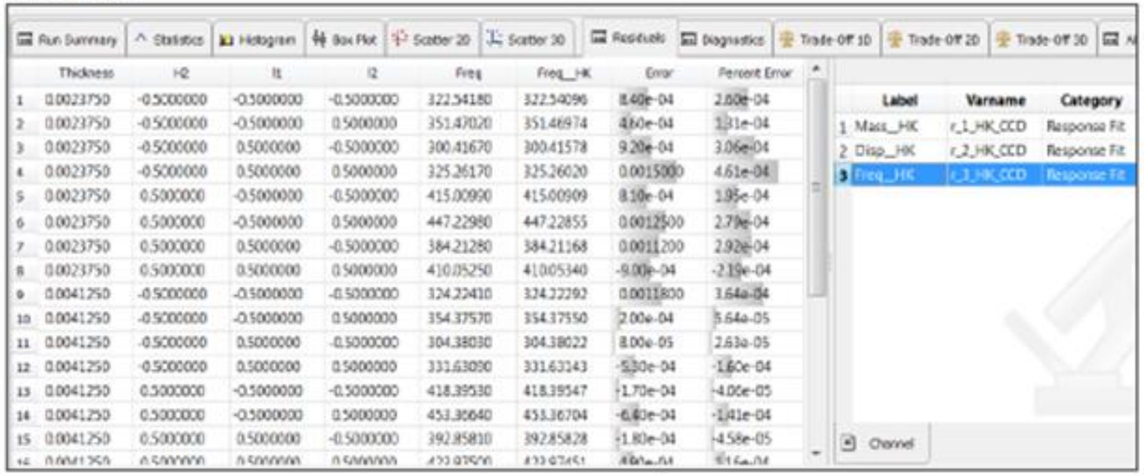
- Select the best method (Compare the error and the quality of the approximation for each method)

D Fit - Exercise 3a

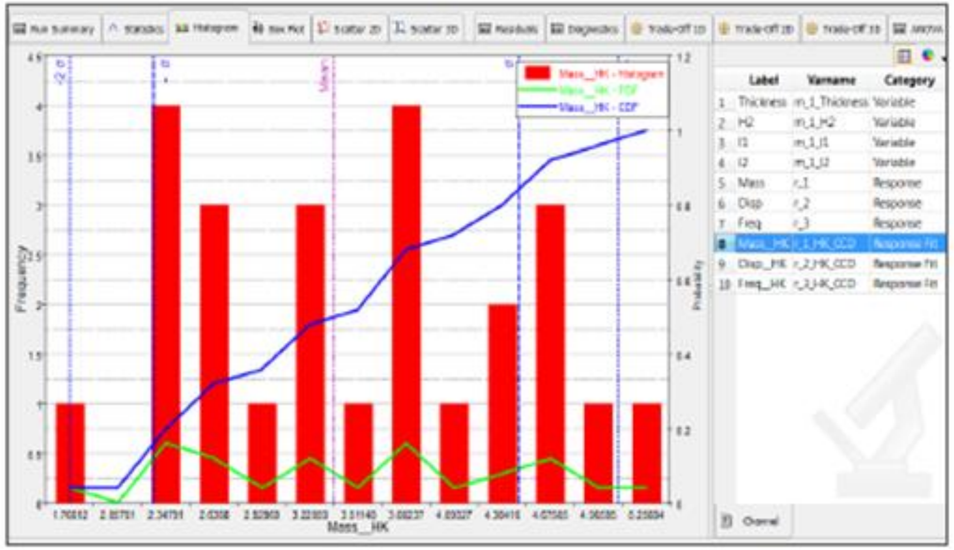
Altair

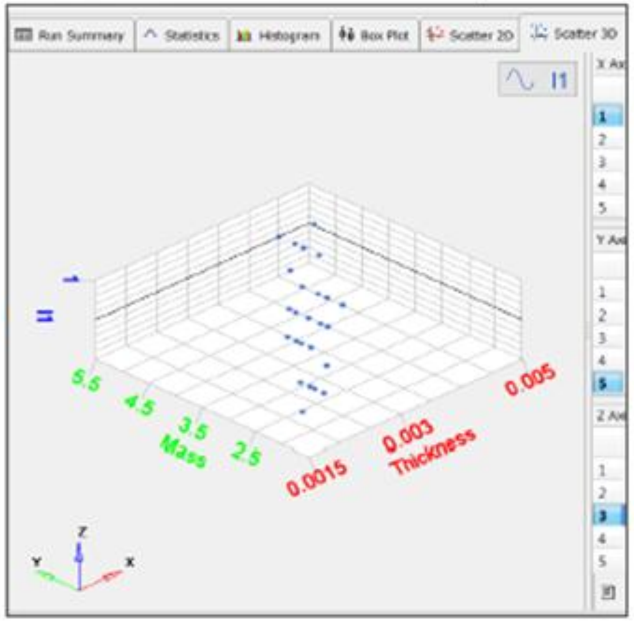
5) Post Process the Fits

a] Residuals



b] Scatter 3D & Histograms



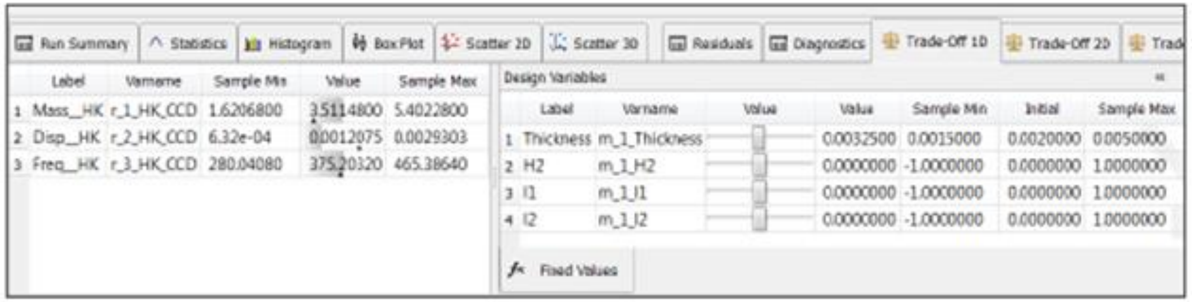


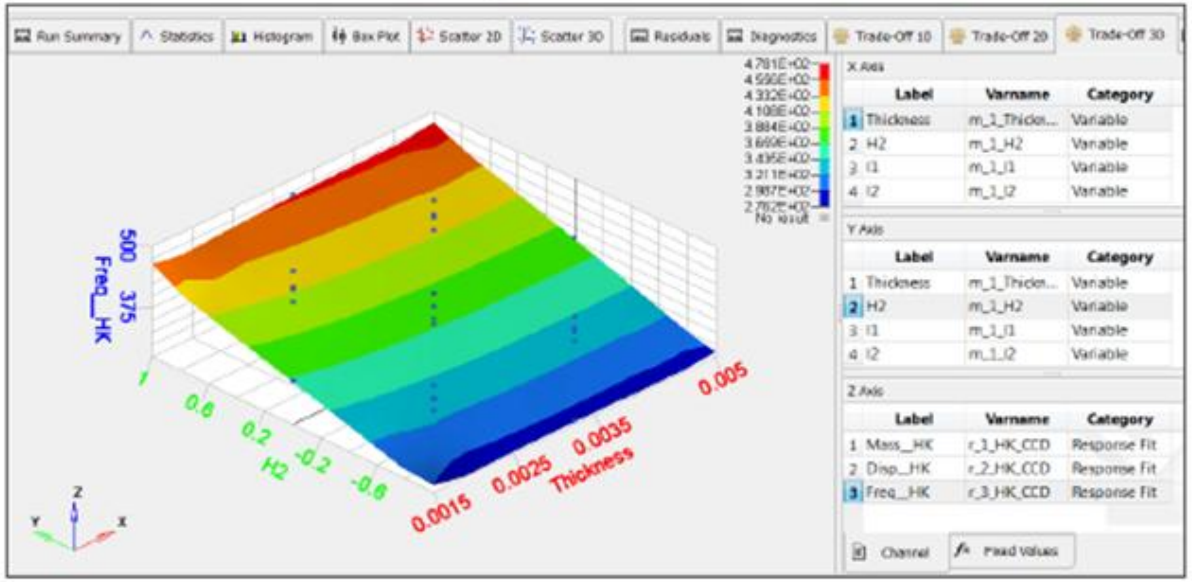
D Fit - Exercise 3a

Altair

5) Post Process the Fits

c] Trade-Off 1D





- Trade-Off is available only if you flag on the “Autobuild” option in the Specifications tab.

6) Save the Study