

Introductory Course: Using LS-OPT[®] on the TRACC Cluster

2.2a - User Defined Function - PERL or OCTAVE

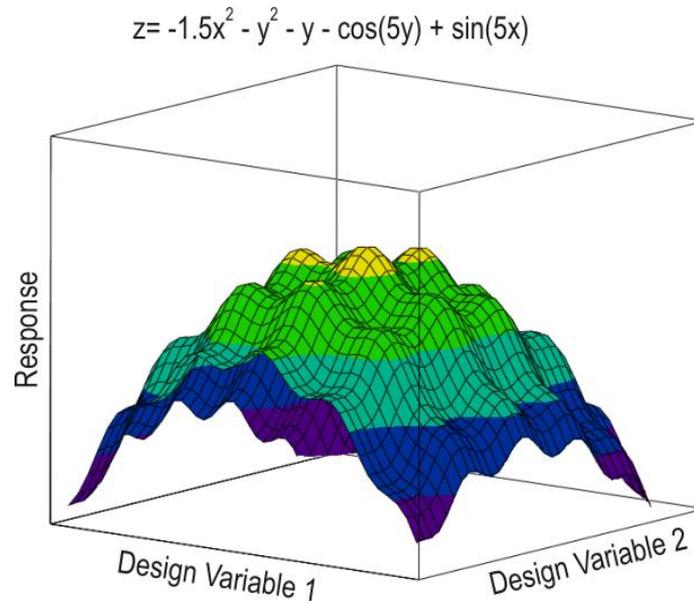
By: Cezary Bojanowski, PhD

Problem Description

- Objective: find global maximum of a function:

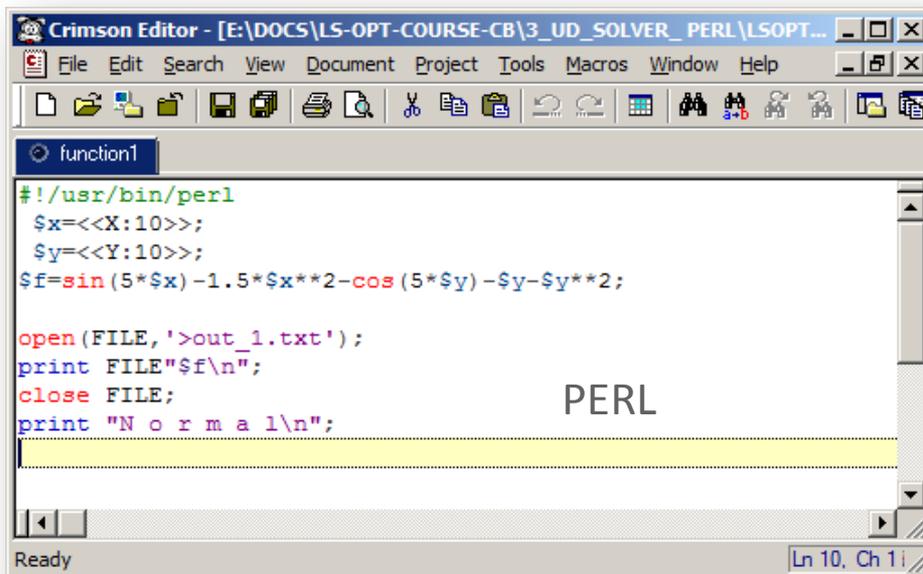
$$z = -1.5x^2 - y^2 - y - \cos(5y) + \sin(5x)$$

- Two design variables: x and y in the range $(-3, 3)$
- Use Perl (or OCTAVE) as a solver



Perl or OCTAVE script

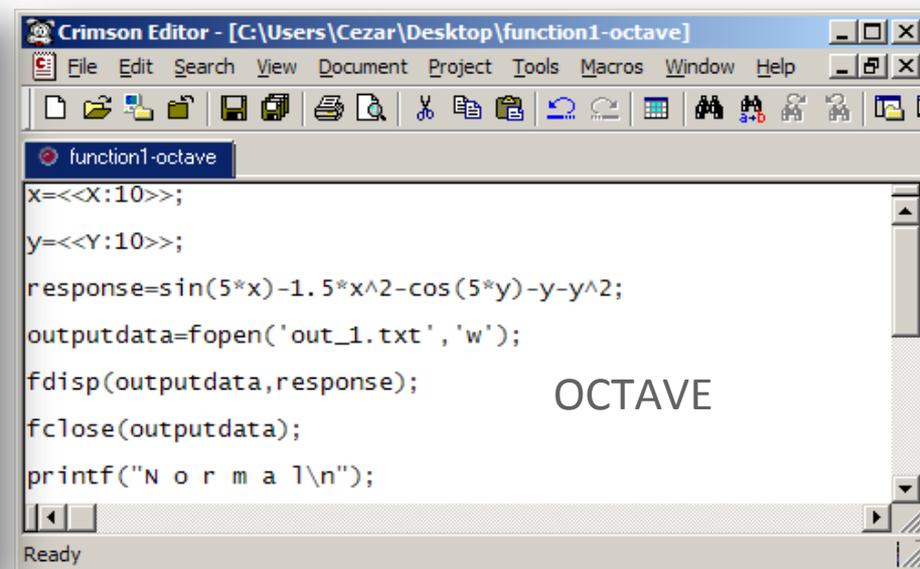
- LS-OPT is ignoring lines starting with "\$" – place the space in the front of variable definition in the Perl script
- The values of variables will be fed by LS-OPT® into the places between << >> signs in both codes
- The output will be written to file `out_1.txt`
- The string "N o r m a l" must be written to signify a normal termination



```
#!/usr/bin/perl
 $x=<<X:10>>;
 $y=<<Y:10>>;
 $f=sin(5*$x)-1.5*$x**2-cos(5*$y)-$y-$y**2;

open(FILE,'>out_1.txt');
print FILE"$f\n";
close FILE;
print "N o r m a l\n";
```

PERL

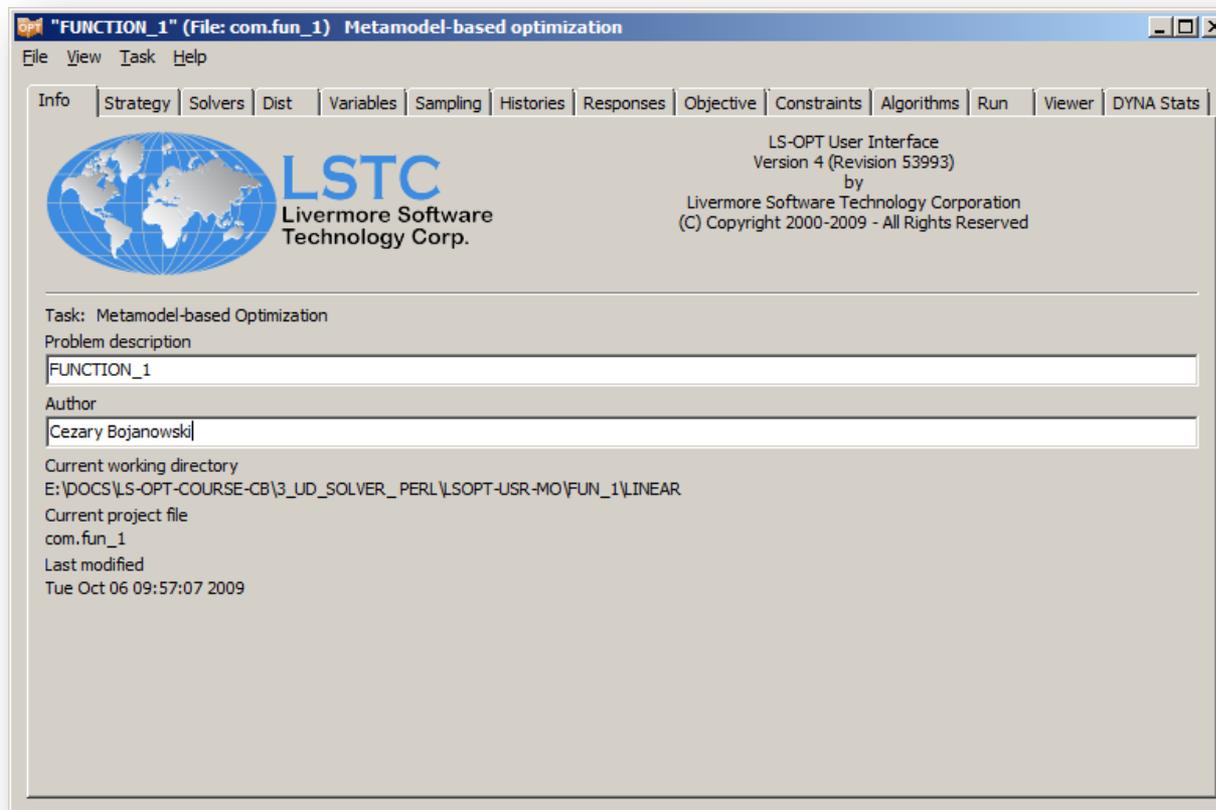


```
x=<<X:10>>;
y=<<Y:10>>;
response=sin(5*x)-1.5*x^2-cos(5*y)-y-y^2;
outputdata=fopen('out_1.txt','w');
fprintf(outputdata,response);
fclose(outputdata);
printf("N o r m a l\n");
```

OCTAVE

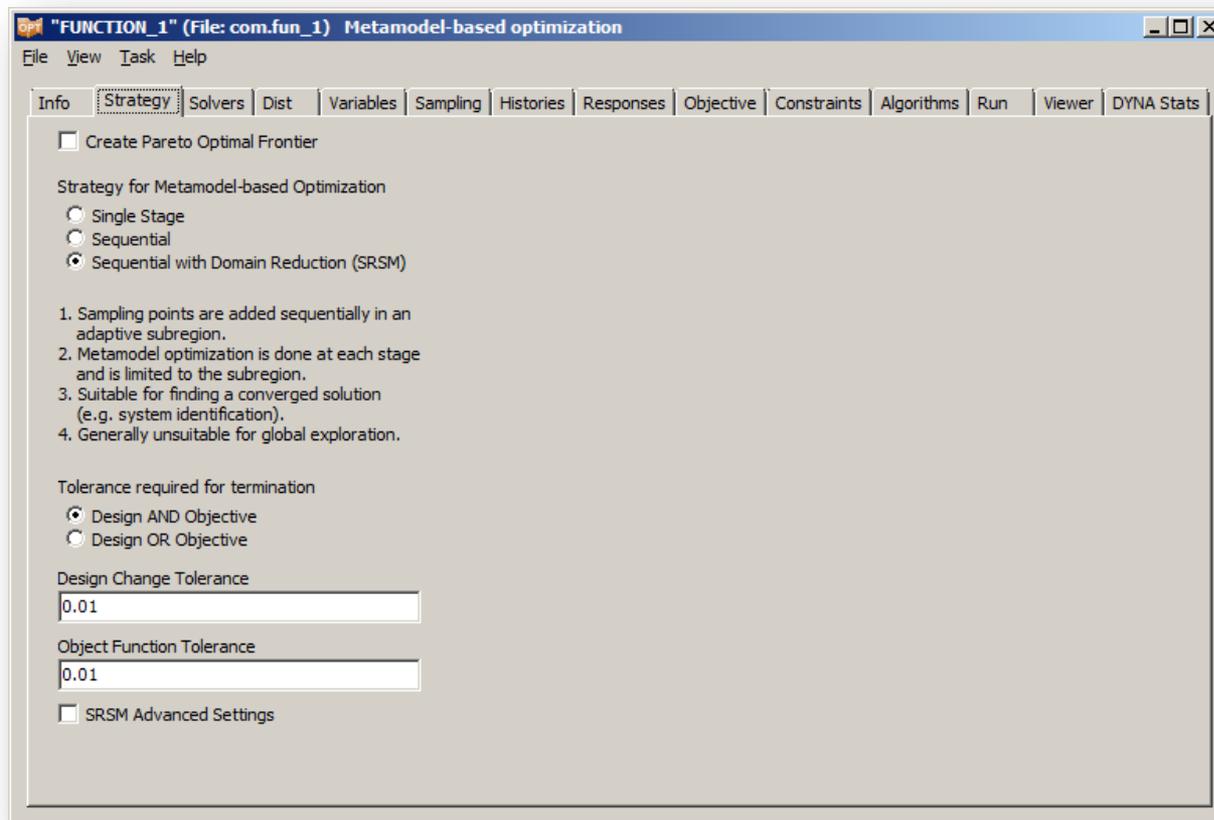
Info Panel

- Define problem `FUNCTION_1` and
- Save file as `com.fun_1`



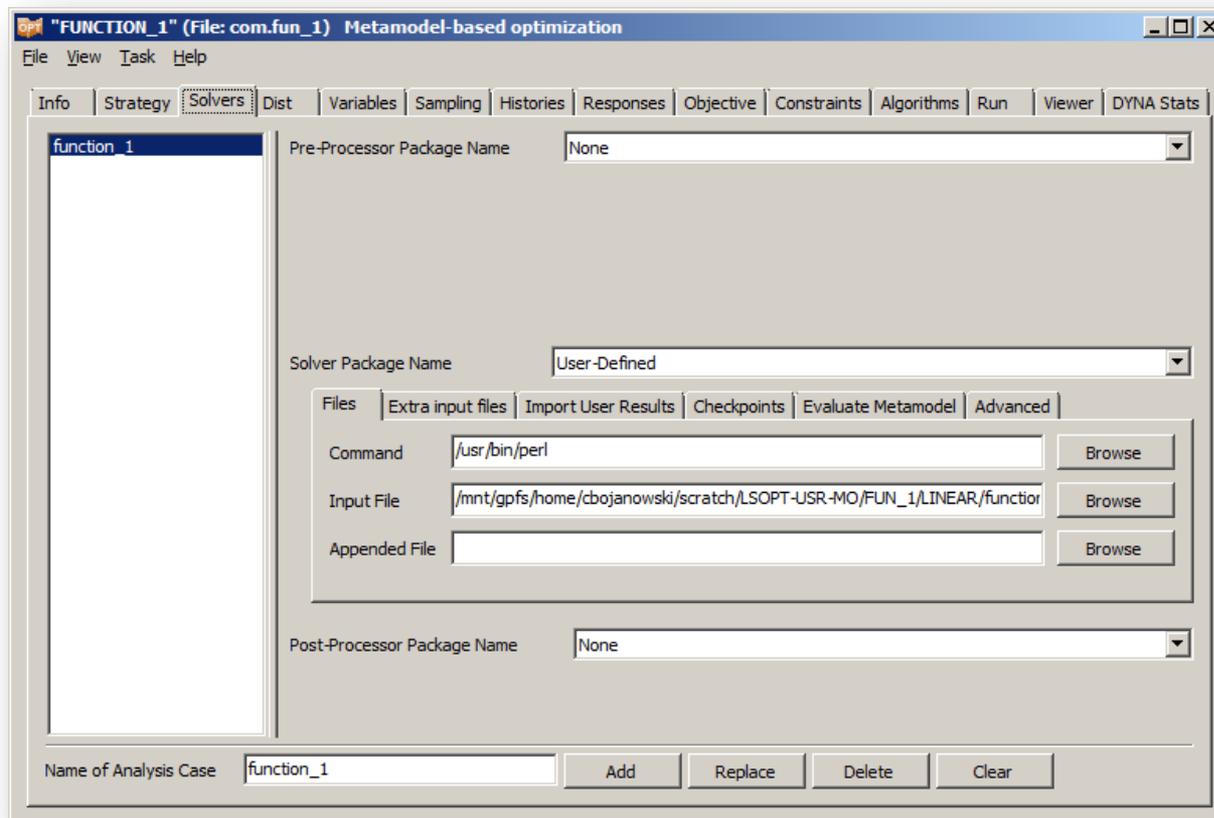
Strategy Panel

- In the Strategy Panel choose Sequential with Domain Reduction
- Leave defaults for stopping criteria



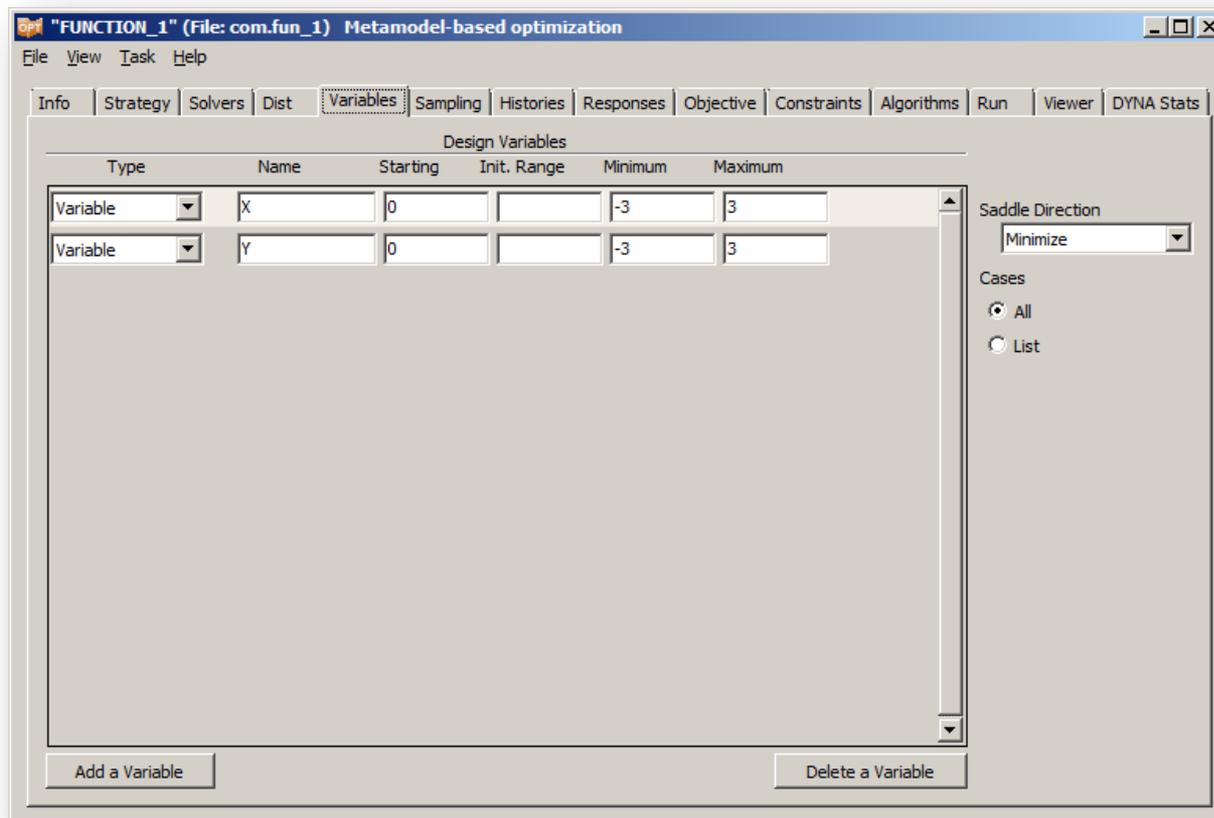
Solvers Panel

- In the Solvers panel enter `/usr/bin/perl` (`/usr/bin/octave`) for Command
- Browse the file `function1` (or `function1-octave`) for your Input file
- For Name of the Analysis Case enter `function_1` and press Add
- The rest of the input is the same for both Perl and OCTAVE



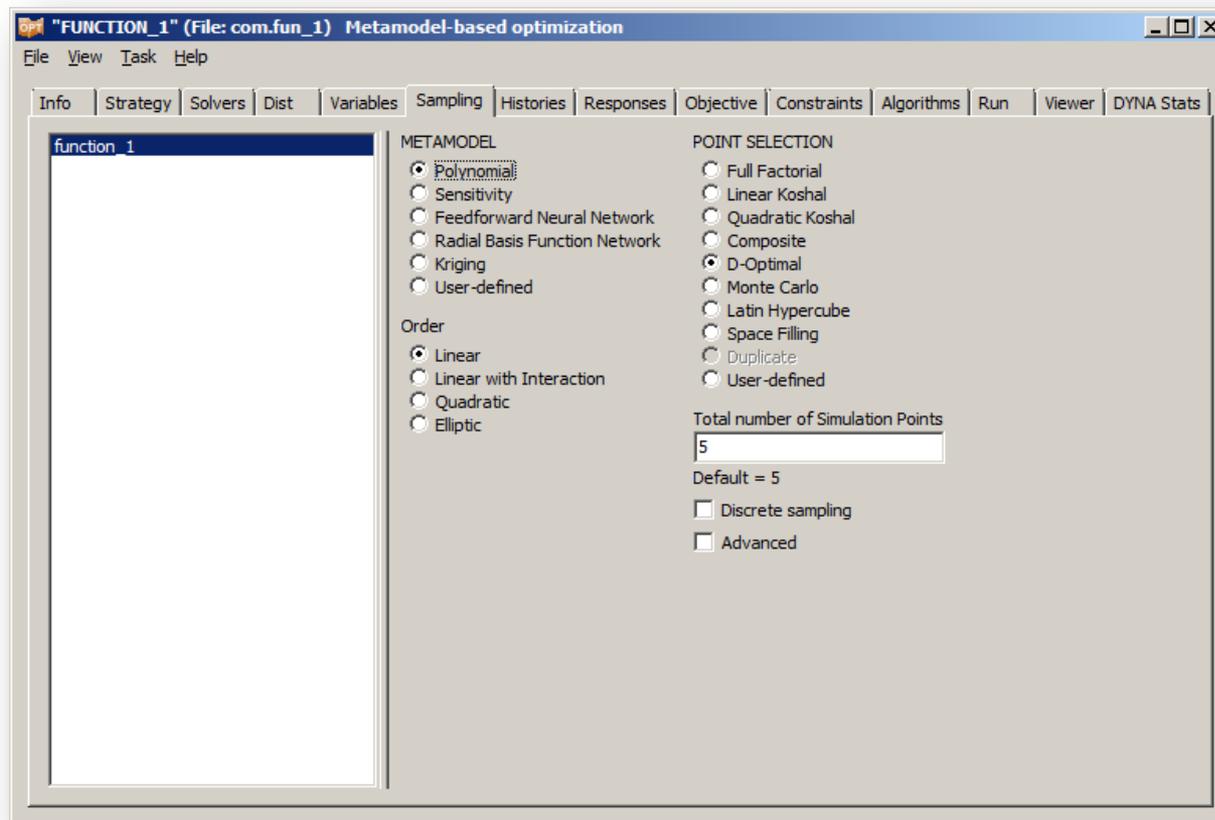
Variables Panel

- In the Variables tab select Type Variable
- Define variable **X** starting at **0** with min bound **-3** and max bound **3**
- Add a Variable
- For name enter **Y** with the same starting value and bounds as **X**



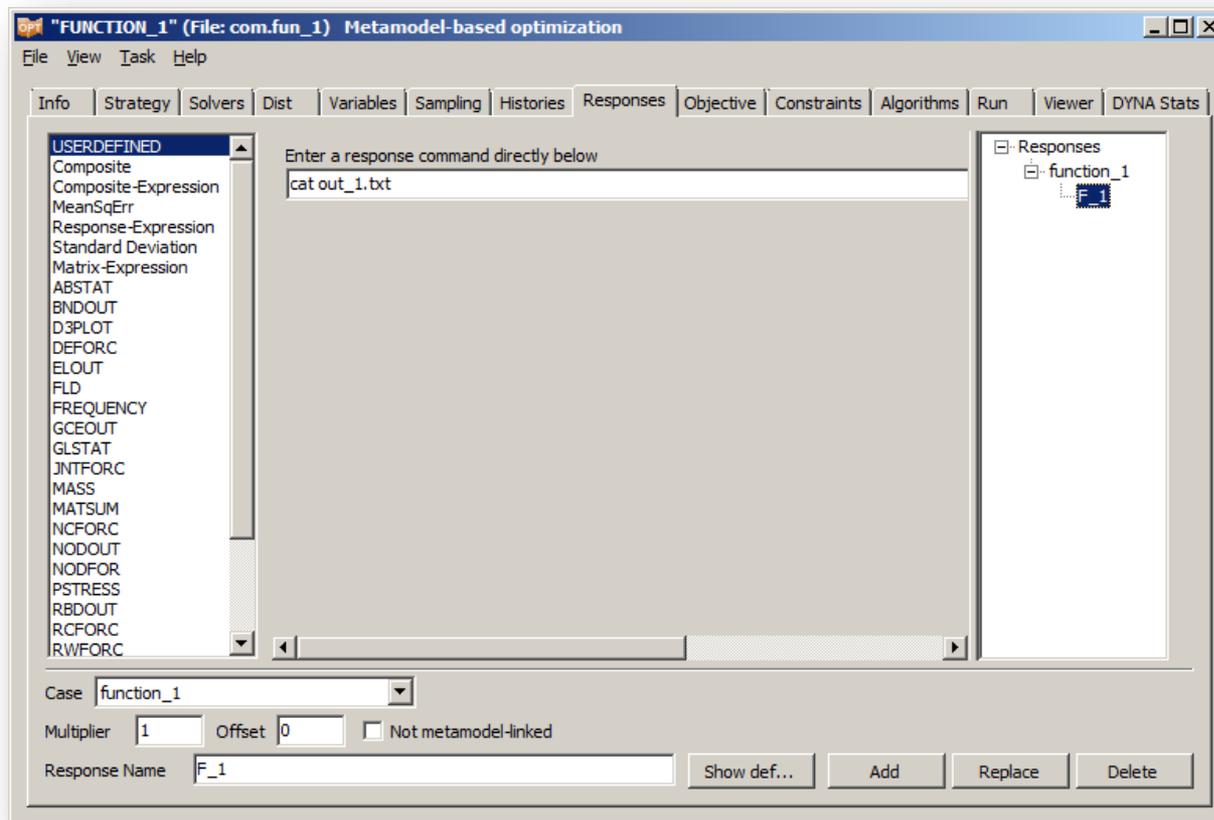
Sampling Panel - Linear Metamodel

- Select Sampling tab
- Choose Polynomial Metamodel with Linear Order
- For point selection method pick D-Optimal with Default number of simulations



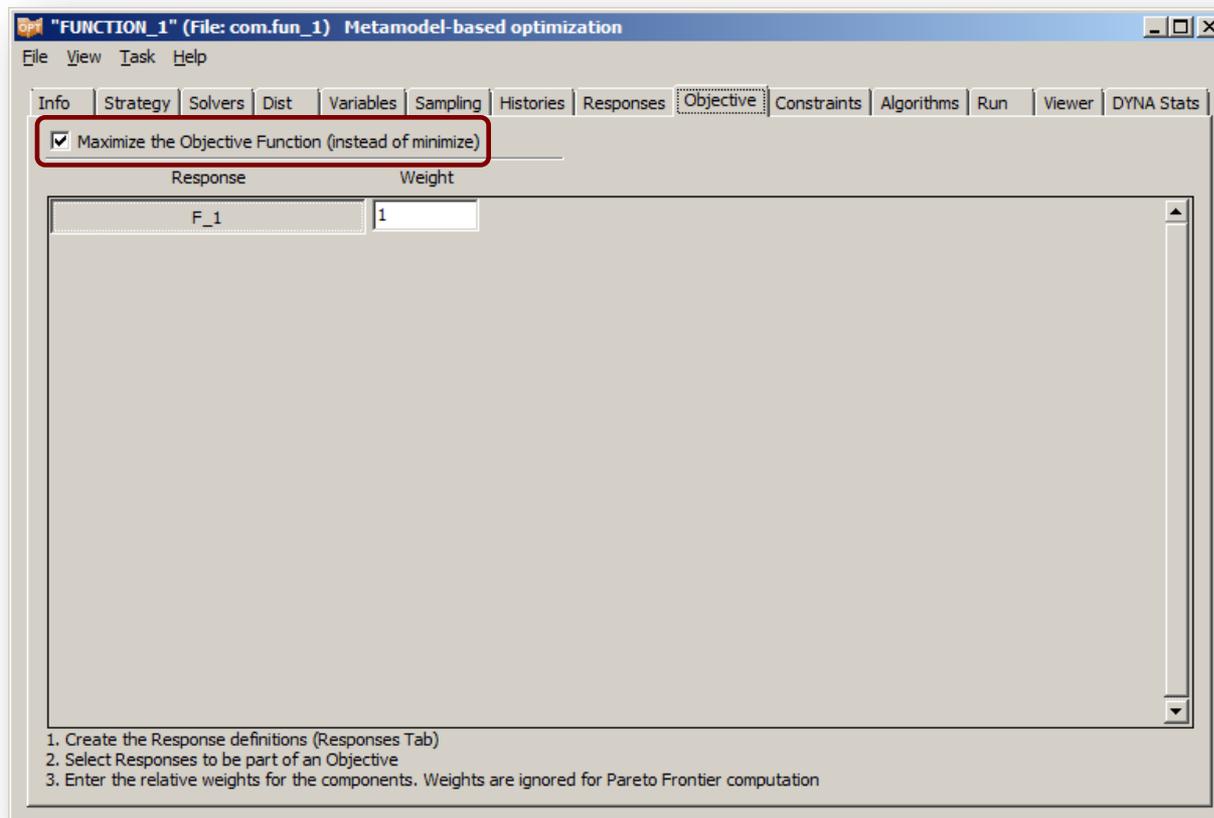
Responses Panel

- In the Responses panel choose **USERDEFINED**
- The response is written to the file **out_1.txt**; use **cat** command to read it
- Type Response command **cat out_1.txt**
- Type Response name **F_1** and push the Add button



Objective Panel

- In the Objective panel select **F_1** as your objective
- Make sure to check Maximize the Objective Function



Run Panel

- This time leave None for QUEUING software
- Request 10 iterations
- Leave 1 in Concurrent Jobs window
- Wait for 51 jobs to be finished

The screenshot shows the 'FUNCTION_1' Metamodel-based optimization software interface. The window title is "FUNCTION_1 (File: com.fun_1) Metamodel-based optimization". The 'Run' tab is active, displaying the following information:

Job ID	PID	Progress
1	(20220)	Normal Termination
2	(20225)	Normal Termination
3	(20233)	Normal Termination
4	(20238)	Normal Termination
5	(20243)	Normal Termination
6	(20266)	Normal Termination

QUEUING settings:

- QUEUING: None
- Concurrent Jobs: 1
- Case: function_1

SEQUENTIAL OPTIMIZATION settings:

- Number of iterations: 10
- Omit last verification run
- Clean Start from Iteration

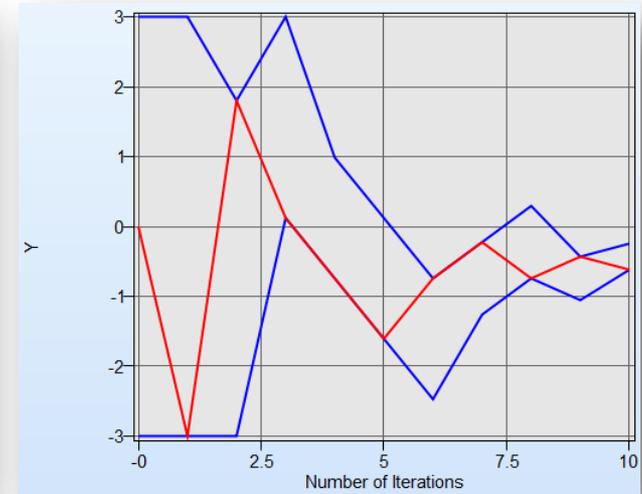
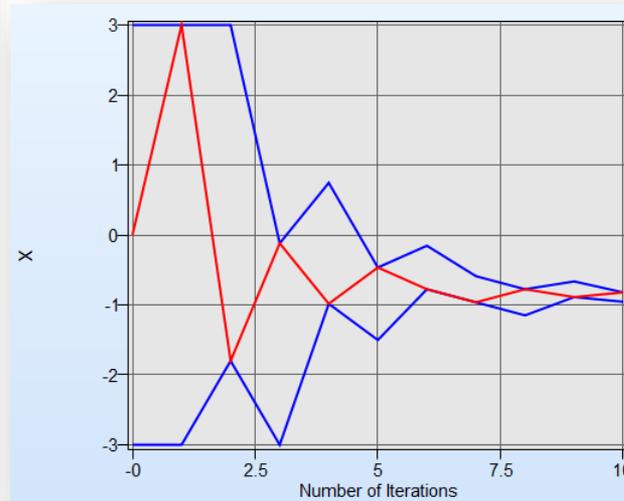
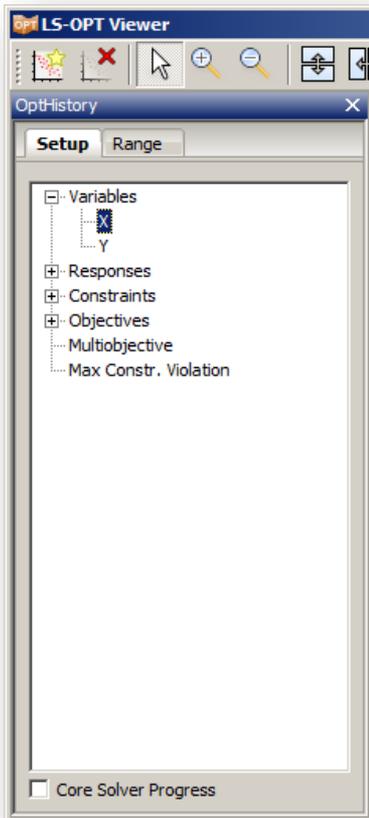
Time Step options:

- Kinetic Energy
- Internal Energy
- Total Energy
- Energy Ratio
- Global X Velocity
- Global Y Velocity
- Global Z Velocity
- Total CPU Time
- Time to Completion

The plot area shows "No Processes Selected" with a y-axis from 0 to 1 and an x-axis from 0 to 1.

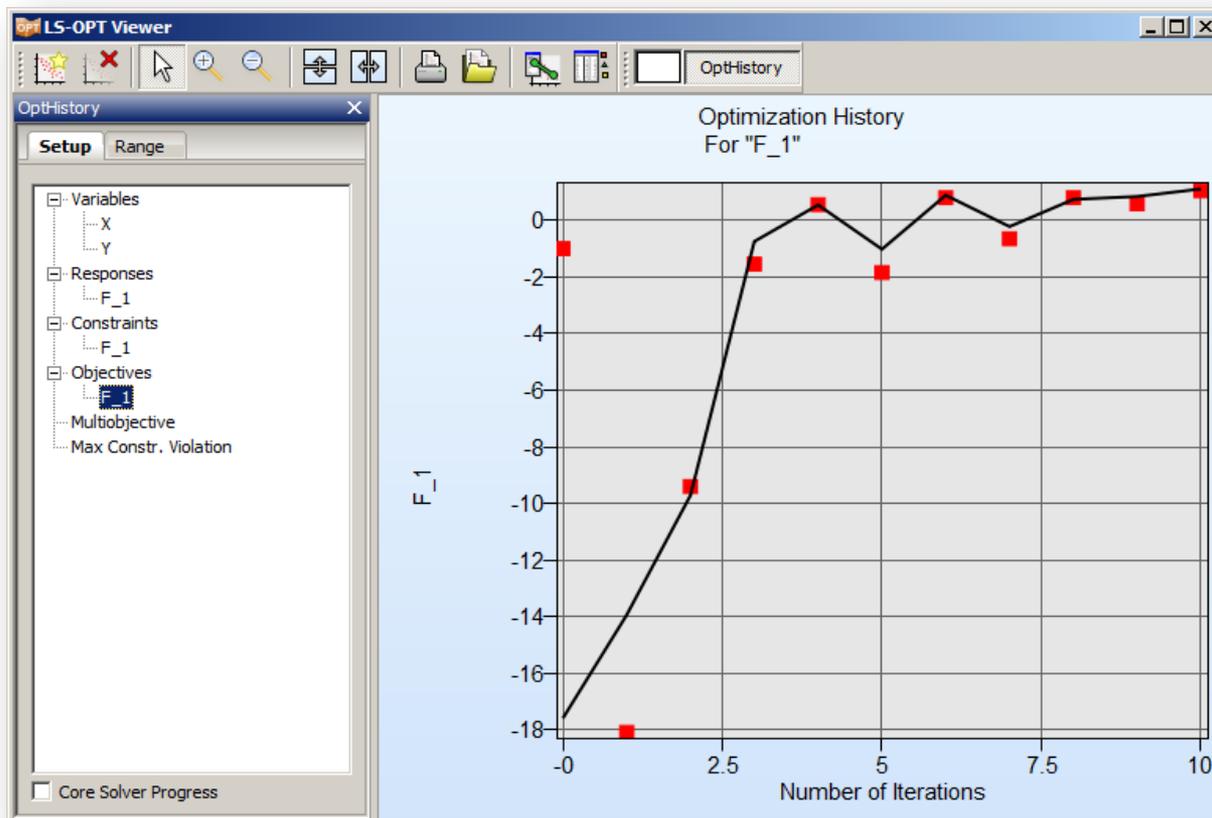
Viewer - Optimization History

- Go to Viewer Panel
- Select Optimization History from the pop-up window
- From the variables select **X**, then **Y**



Viewer - Optimization History

- From the Setup tab in Optimization History window Select **F_1** from Objectives
- Indicate with the cursor the last point on the graph
- Read from Point Selection window the values of design variables for the optimal design

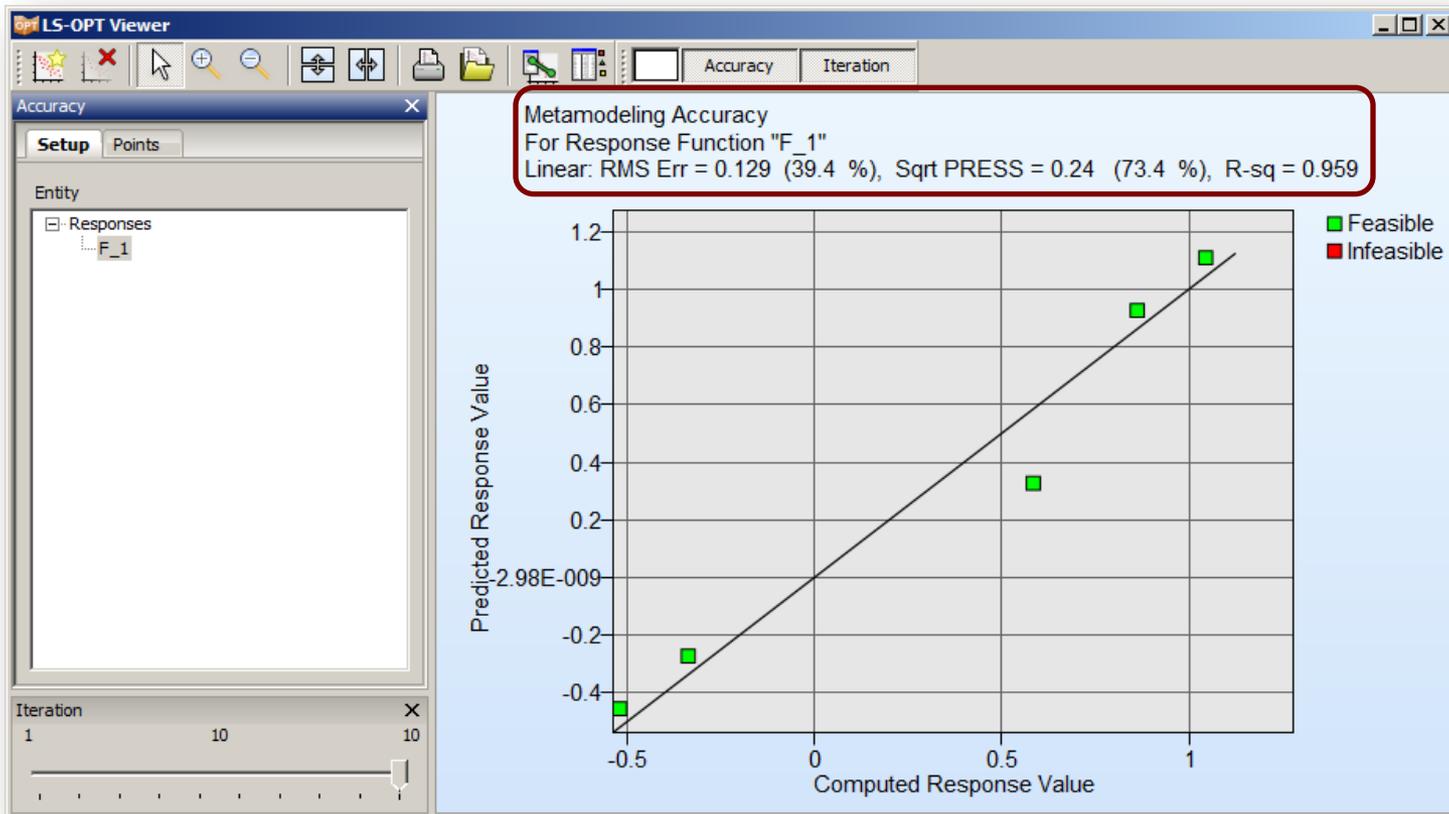


Point selection

Entity	Compu...	Predicted
0.Opt		
1.Opt		
2.Opt		
3.Opt		
4.Opt		
5.Opt		
6.Opt		
7.Opt		
8.Opt		
9.Opt		
10.Opt		
Point		
Variables		
X	-0.82143	-0.82143
Y	-0.619584	-0.619584
Responses		
F_1	1.04499	1.10938
Constraints		
F_1	1.04499	1.10938
Objectives		
F_1	1.04499	1.10938
Multiobjective	1.04499	1.10938
Max Constraint Violation	0	0

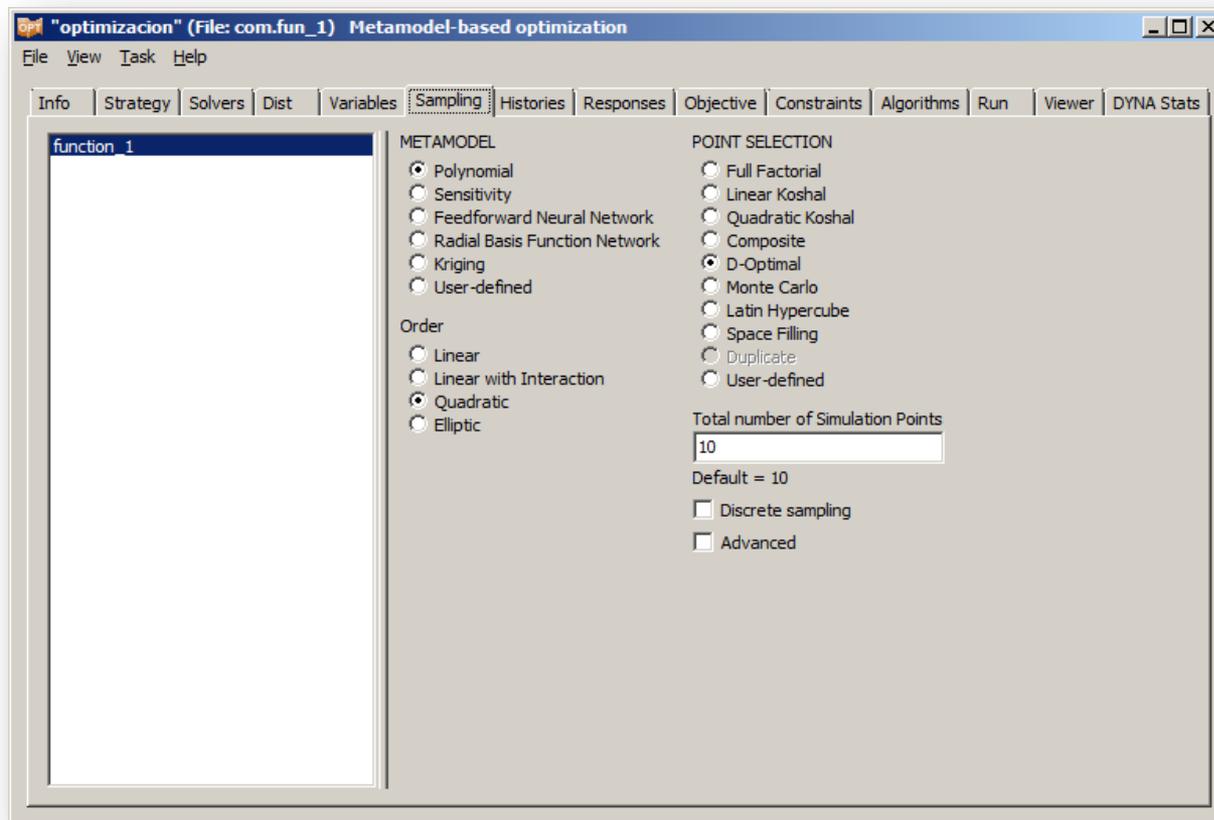
Viewer - Accuracy

- Go to Viewer Panel and Press Restart Viewer
- Select Accuracy from Metamodel menu
- Check RMS and R-sq errors – what they indicate?



Sampling Panel - Quadratic Metamodel

- Make a copy of your **com.** file and **function1** script to other working directory
- Load command file to LS-OPT®
- Browse to the copied **function1** file in the Input File window in Solvers tab
- In Sampling tab change order of polynomial to Quadratic with **10** simulations



Run Panel

- Go to Run panel, press Run button and
- Wait for completion of **81** calculations

The screenshot displays the 'FUNCTION_1' (File: com.fun_1) Metamodel-based optimization software interface. The 'Run' tab is selected, showing a table of job progress, queuing settings, and sequential optimization options.

Job ID	PID	Progress
76	(29762)	Normal Termination
77	(29767)	Normal Termination
78	(29772)	Normal Termination
79	(29779)	Normal Termination
80	(29784)	Normal Termination
81	(29798)	Normal Termination

Time Step
Kinetic Energy
Internal Energy
Total Energy
Energy Ratio
Global X Velocity
Global Y Velocity
Global Z Velocity
Total CPU Time
Time to Completion

QUEUING
None
Concurrent Jobs: 1
Case: function_1

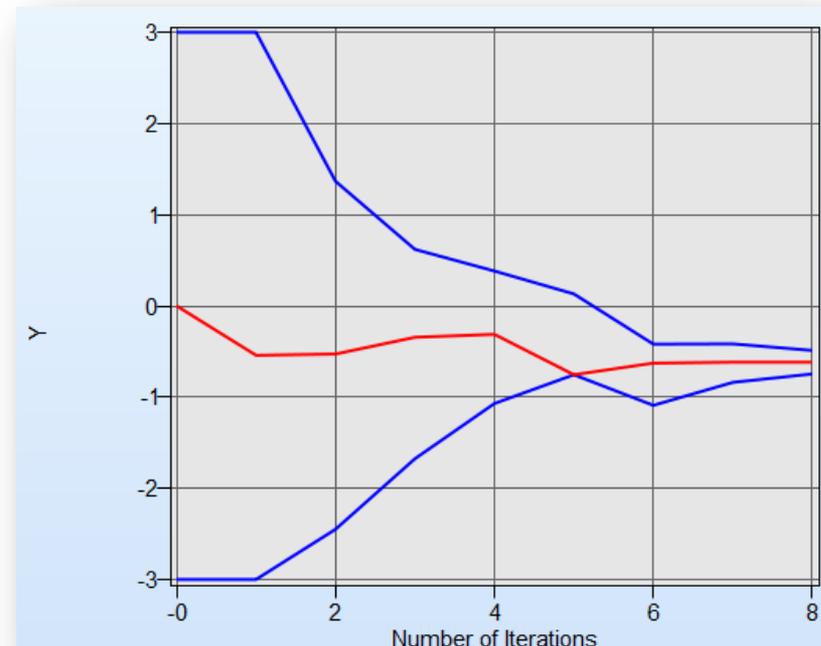
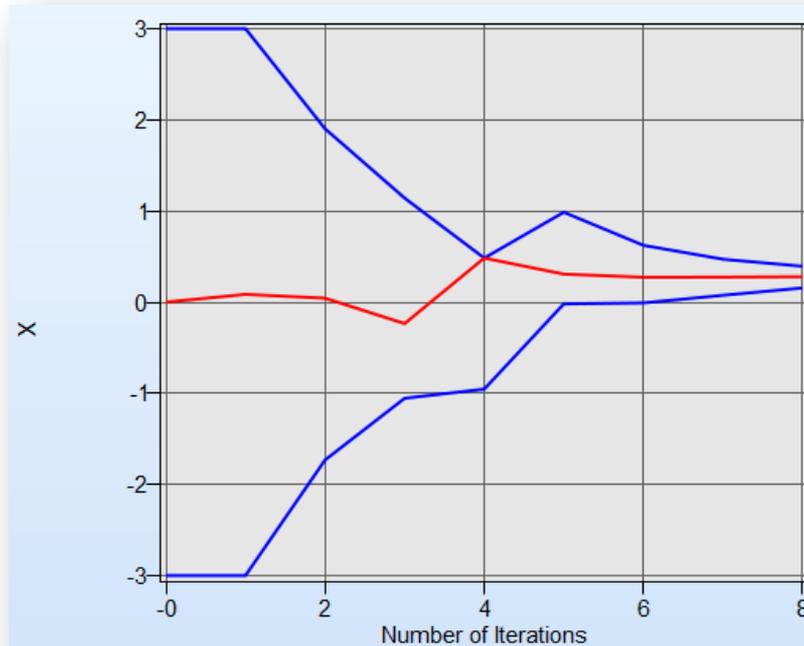
SEQUENTIAL OPTIMIZATION
Number of iterations: 10
 Omit last verification run
 Clean Start from Iteration

Run Stop

No Processes Selected

Viewer - Optimization History

- Go to Viewer panel
- Select Optimization History from Optimization menu
- Select X in Variables list to see the optimization history of that variable
- Point with the cursor on the last iteration to read exact values of the variables and optimal response



Viewer - Optimization History

- Compare results with the ones from linear metamodeling
- Linear metamodel ended up in one of the local maxima

Linear RS

Entity	Compu...	Predicted
Point		
Variables		
X	-0.82143	-0.82143
Y	-0.619584	-0.619584
Responses		
F_1	1.04499	1.10938
Constraints		
F_1	1.04499	1.10938
Objectives		
F_1	1.04499	1.10938
Multiobjective	1.04499	1.10938
Max Constraint Violation	0	0

Quadratic RS

Entity	Compu...	Predicted
Point		
Variables		
X	0.278325	0.278325
Y	-0.618141	-0.618141
Responses		
F_1	2.10254	2.10214
Constraints		
F_1	2.10254	2.10214
Objectives		
F_1	2.10254	2.10214
Multiobjective	2.10254	2.10214
Max Constraint Violation	0	0

Viewer - Sensitivities

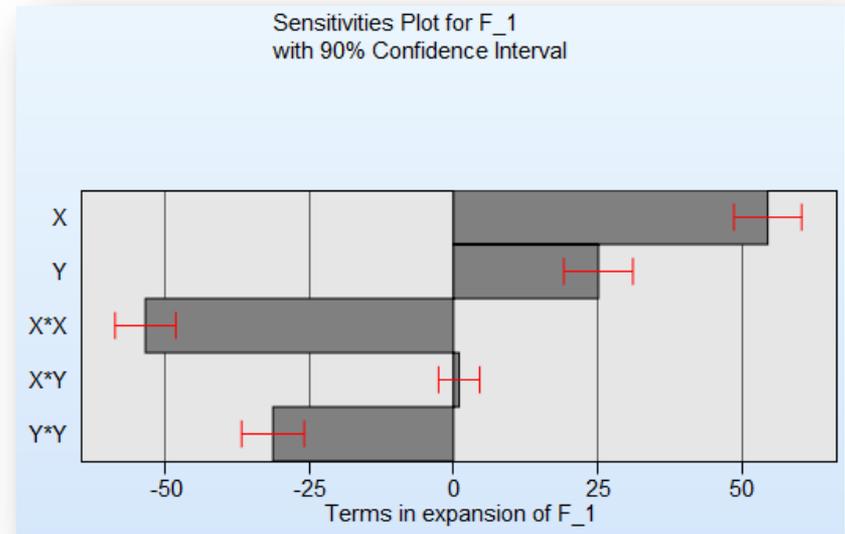
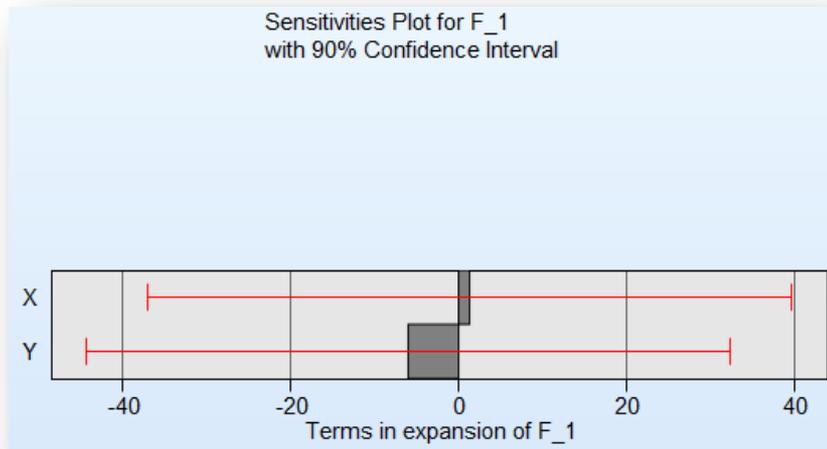
- Go to Viewer panel
- Select Sensitivity from Metamodel menu
- Compare the plots from first iteration for linear and quadratic metamodel

Linear RS

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_{12} x_1 x_2 + \varepsilon$$

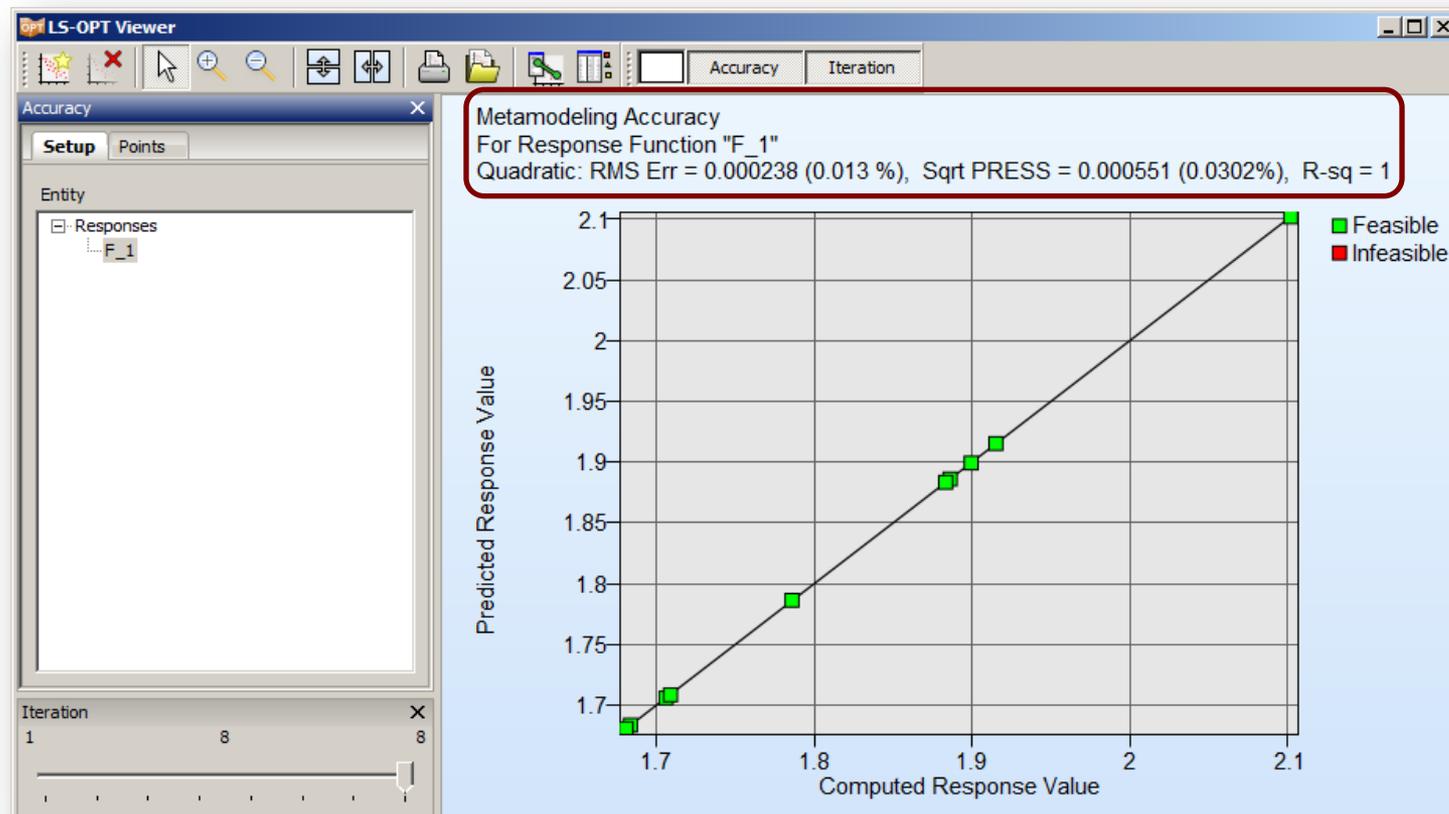
Quadratic RS

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_{11} x_1^2 + \beta_{22} x_2^2 + \beta_{12} x_1 x_2 + \varepsilon$$

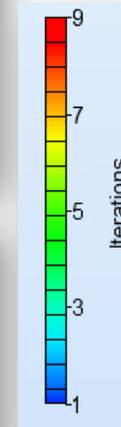
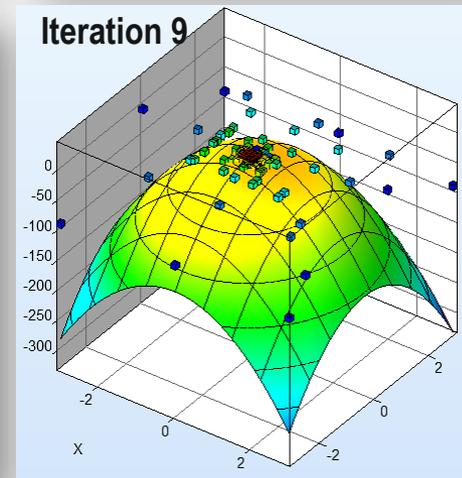
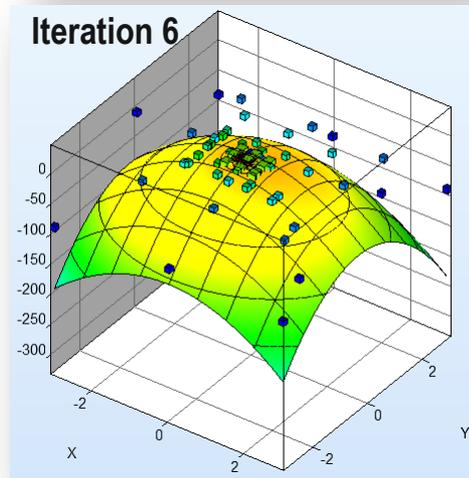
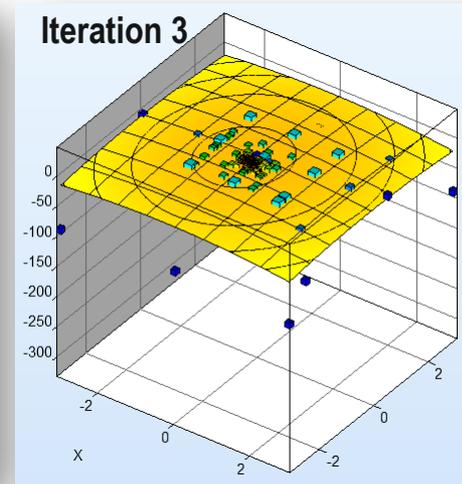
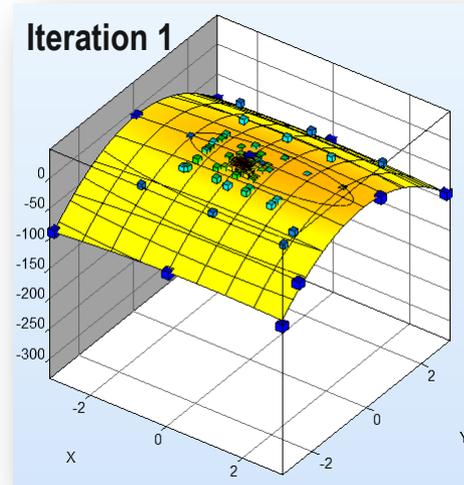


Viewer - Accuracy of the Quadratic Metamodel

- Go to Viewer tab and Restart the viewer
- Select Accuracy from Metamodel menu
- Read values of metamodeling errors and compare them to previous ones from linear metamodel

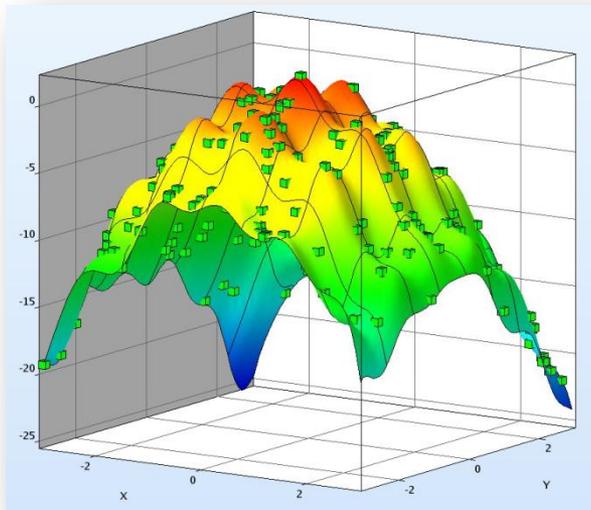


SRSM with Domain Reduction - Quadratic Surface



Radial Basis Function Network

- Additional analysis was performed using RBFN as an metamodel type
- 200 points were selected using LH sampling
- (150 points did not give the shape of the function)
- Gaussian transfer functions were selected under advanced options
- Single stage strategy was selected for optimization
- The optimum was found to be 2.09361
- RBFN is an universal approximation technique if enough training points are provided and enough center points is selected



$$z = -1.5x^2 - y^2 - y - \cos(5y) + \sin(5x)$$

