Argonne NATIONAL LABORATORY

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

2.2a – User Defined Function – PERL or OCTAVE

By: Cezary Bojanowski, PhD

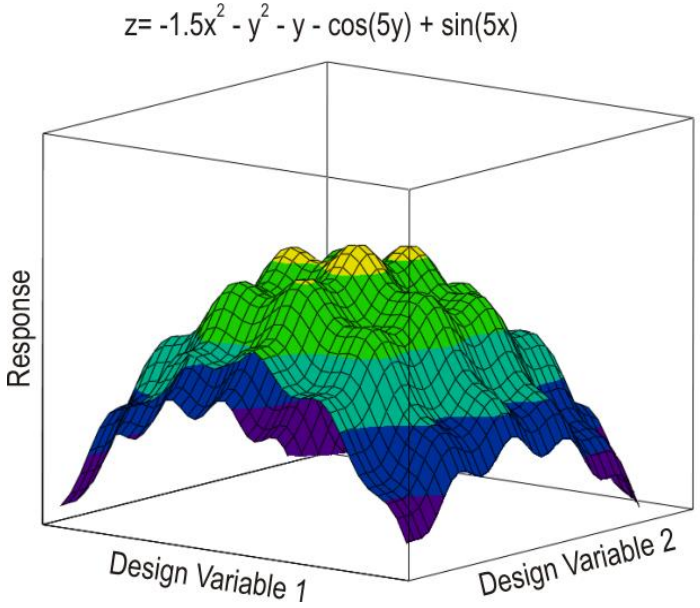
U.S. DEPARTMENT OF ENERGY

Problem Description

- Objective: find global maximum of a function:

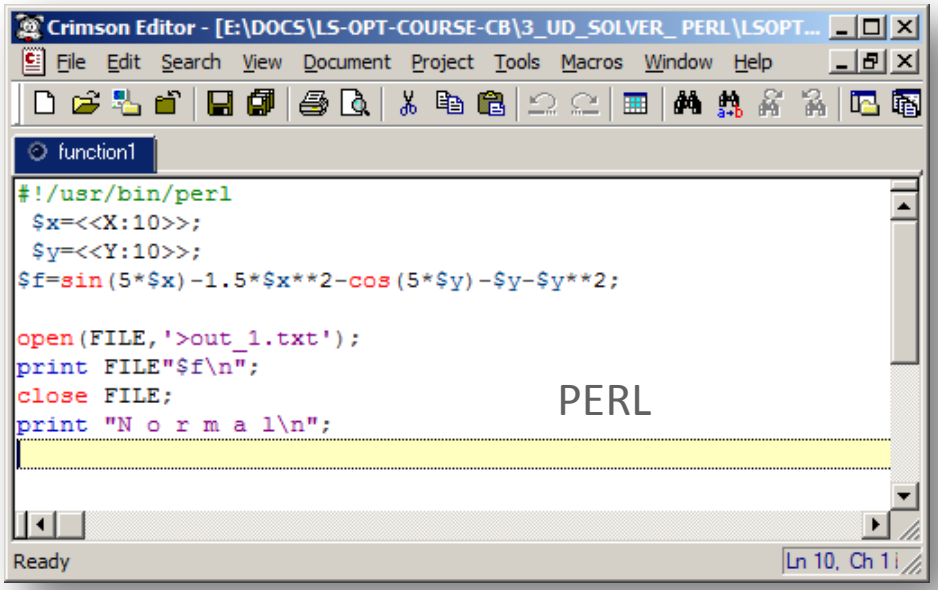
$$z=-1.5x^2-y^2-y-\cos(5y)+\sin(5x)$$

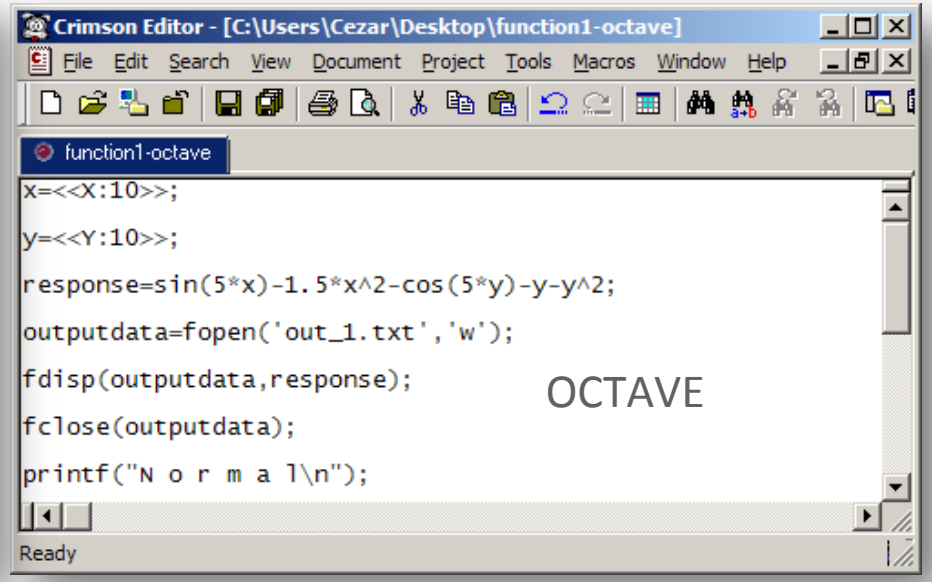
- Two design variables: x and y in the range (-3,3)
- Use Perl (or OCTAVE) as a solver



Perl or OCTAVE script

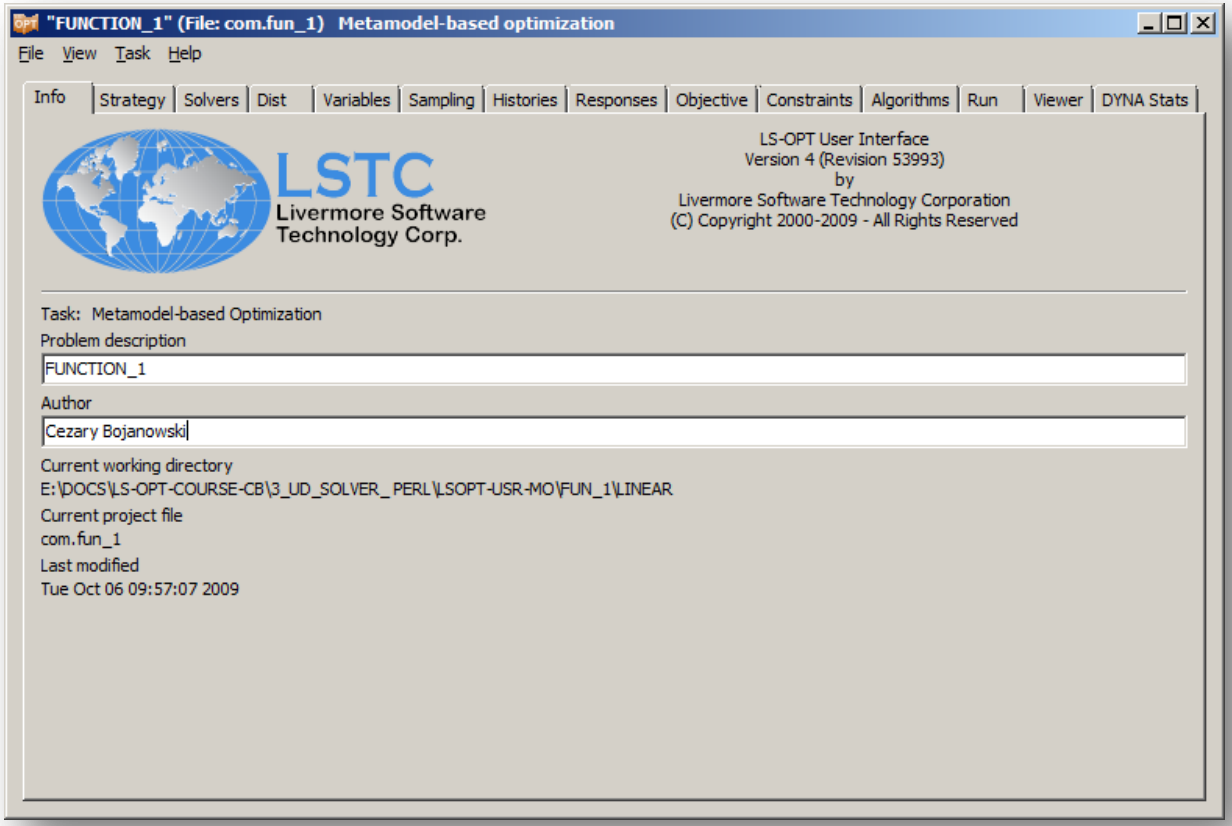
- LS-OPT is ignoring lines starting with "$" – place the space in the front of variable definition in the Perl script
- The values of variables will be fed by LS-OPT® into the places between << >> signs in both codes
- The output will be written to file out_1.txt
- The string "N o r m a l" must be written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





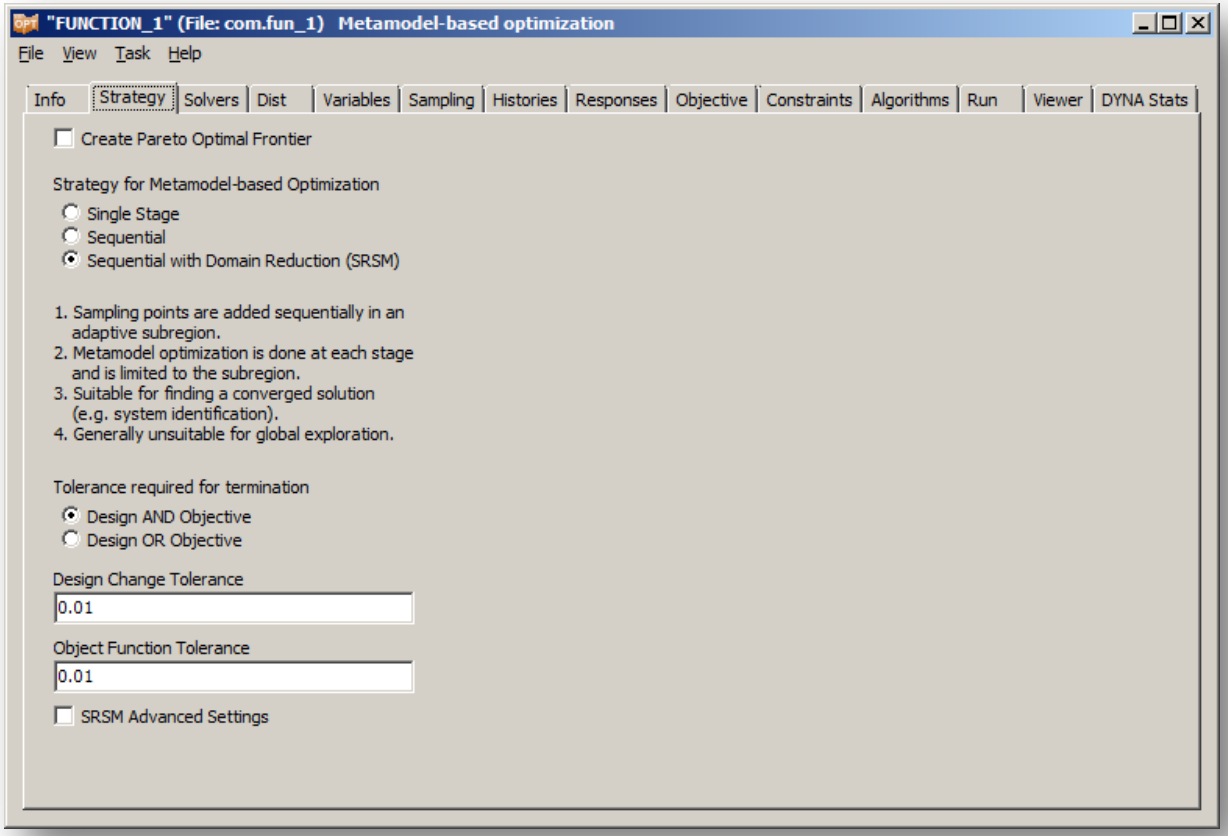
Info Panel

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



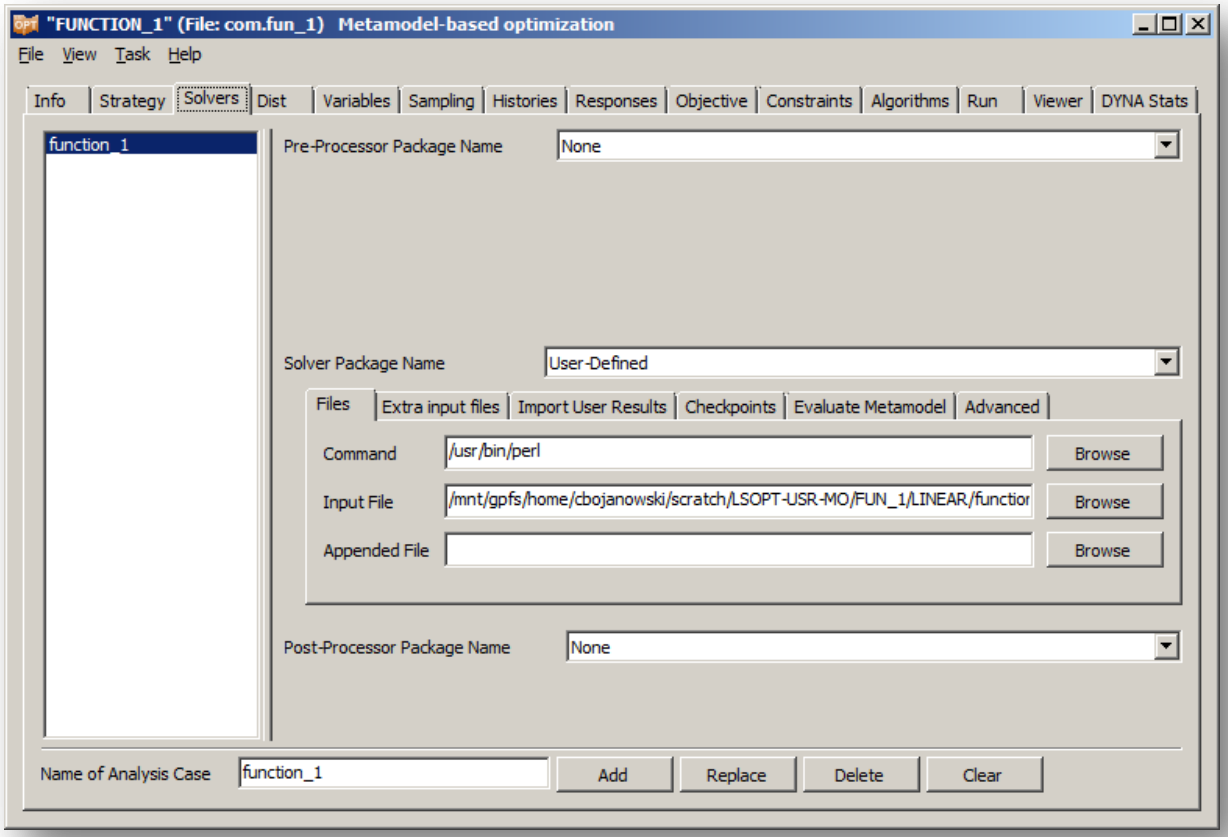
Strategy Panel

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



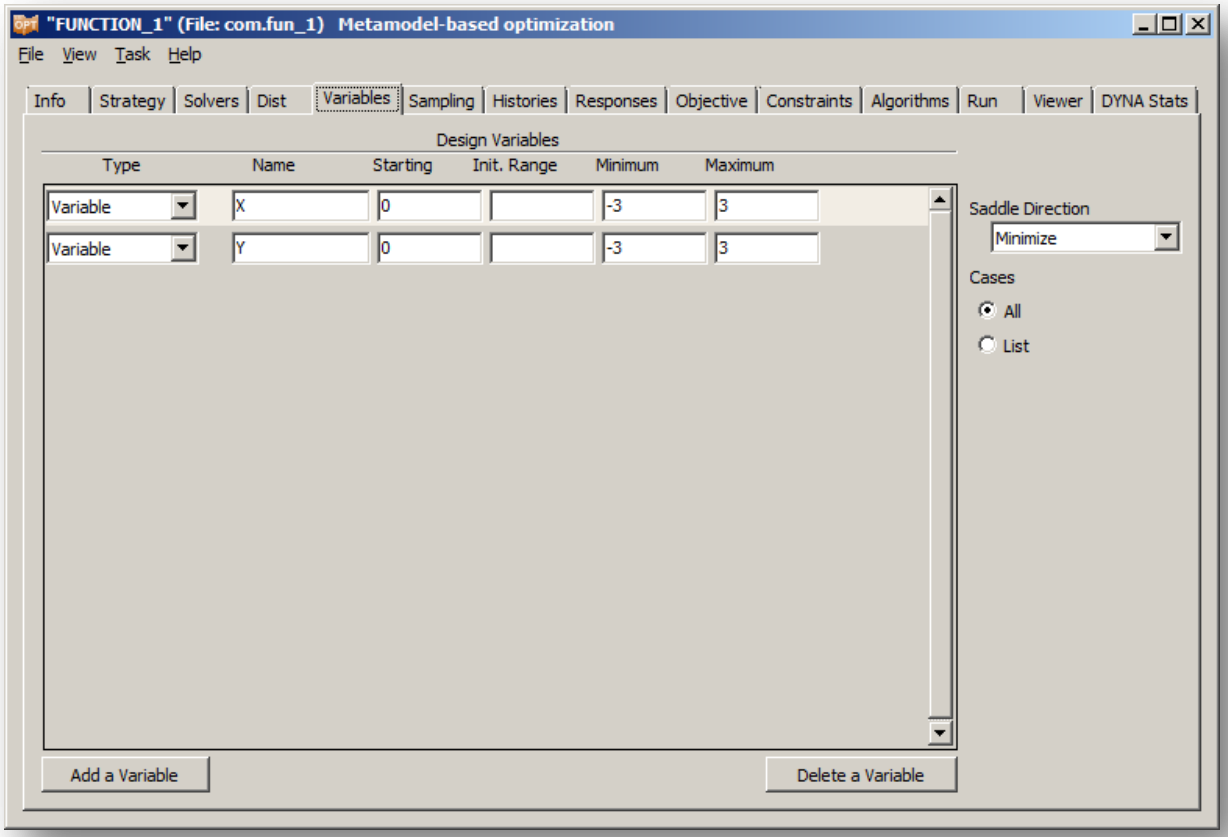
Solvers Panel

- 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



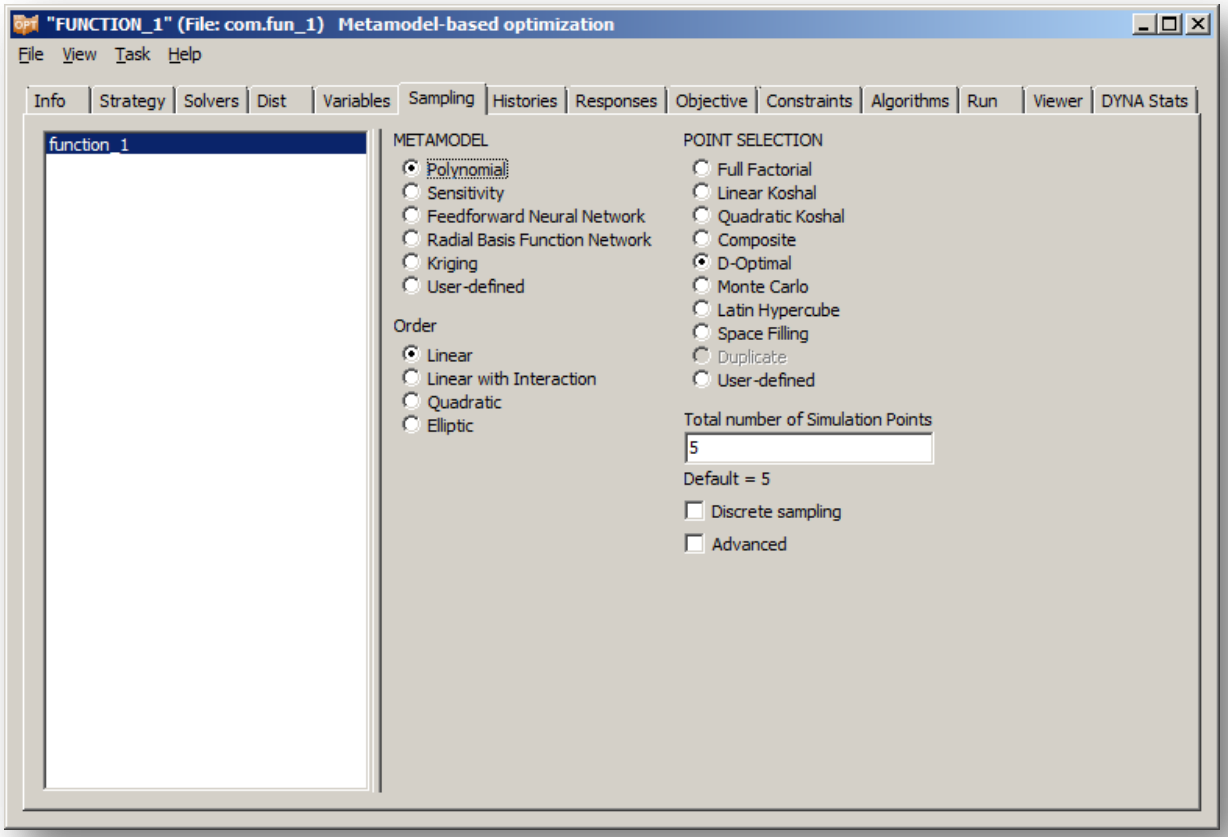
Variables Panel

- 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



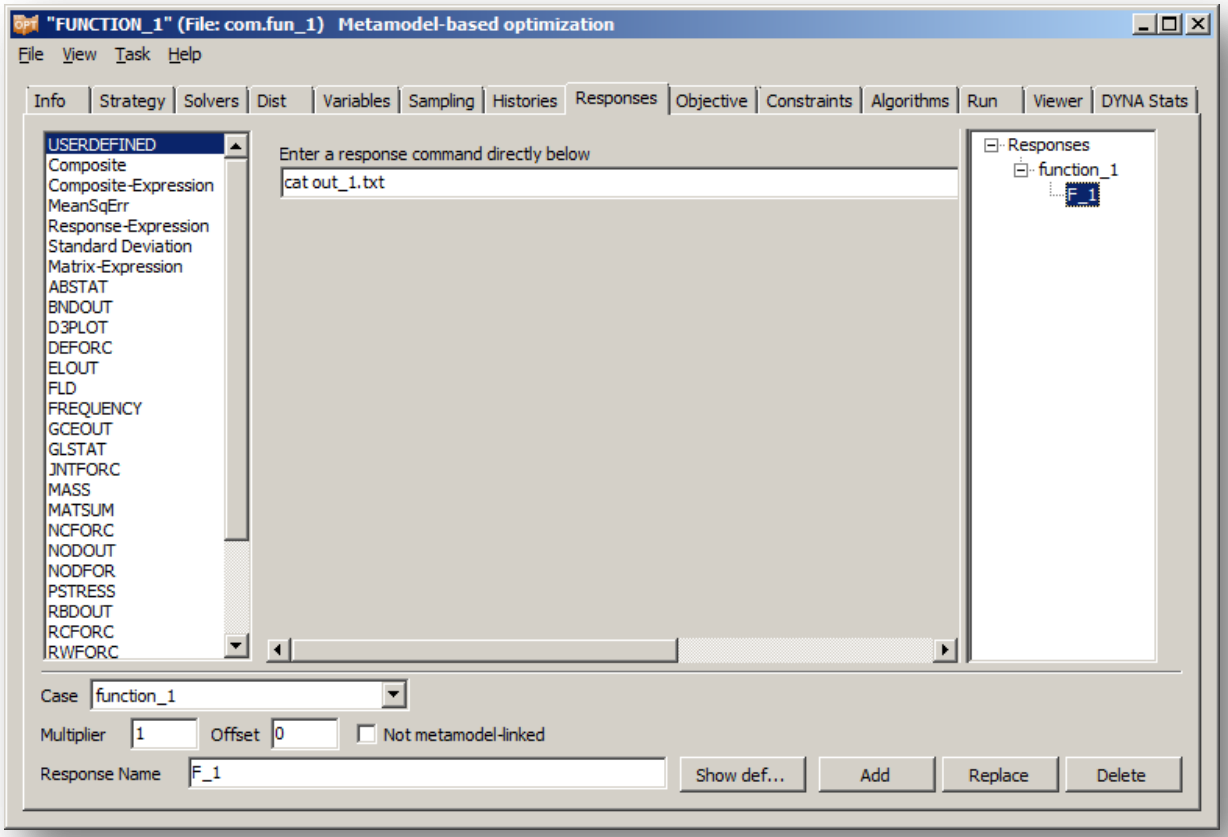
Sampling Panel – Linear Metamodel

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



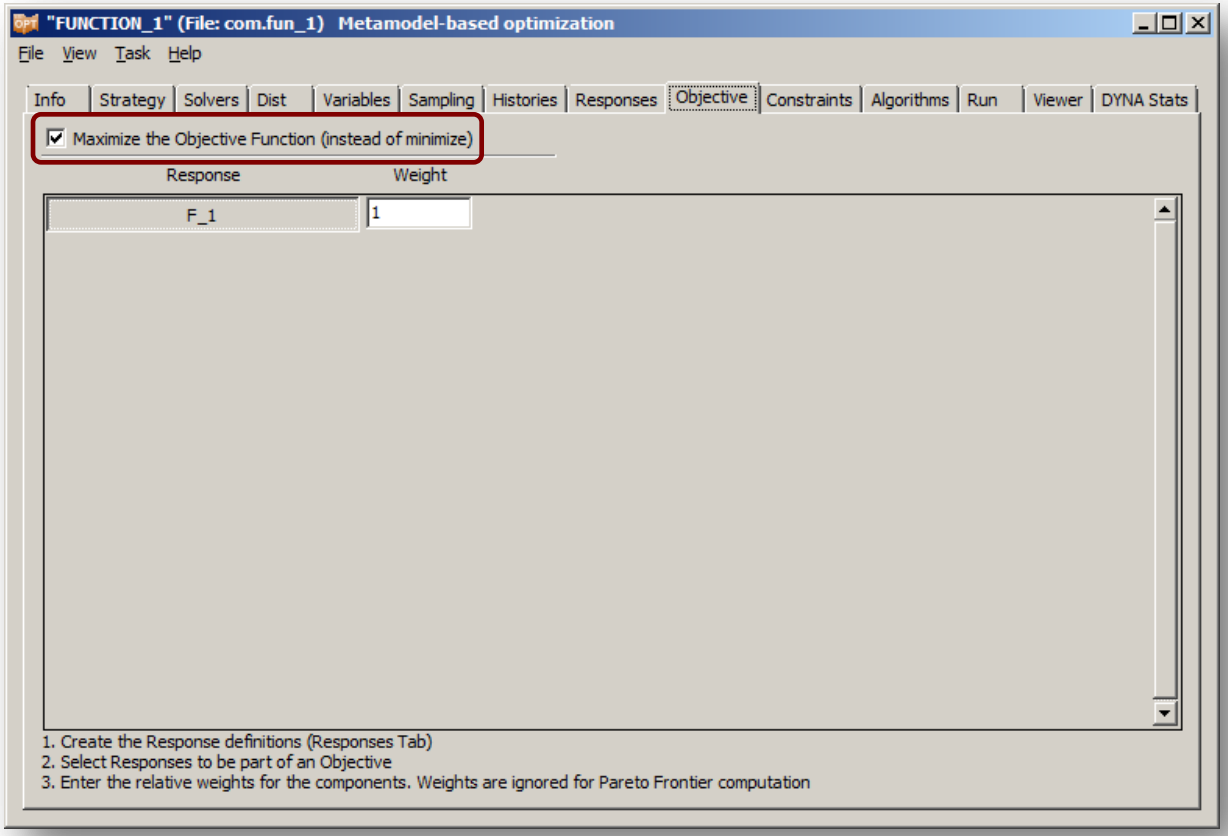
Responses Panel

- 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



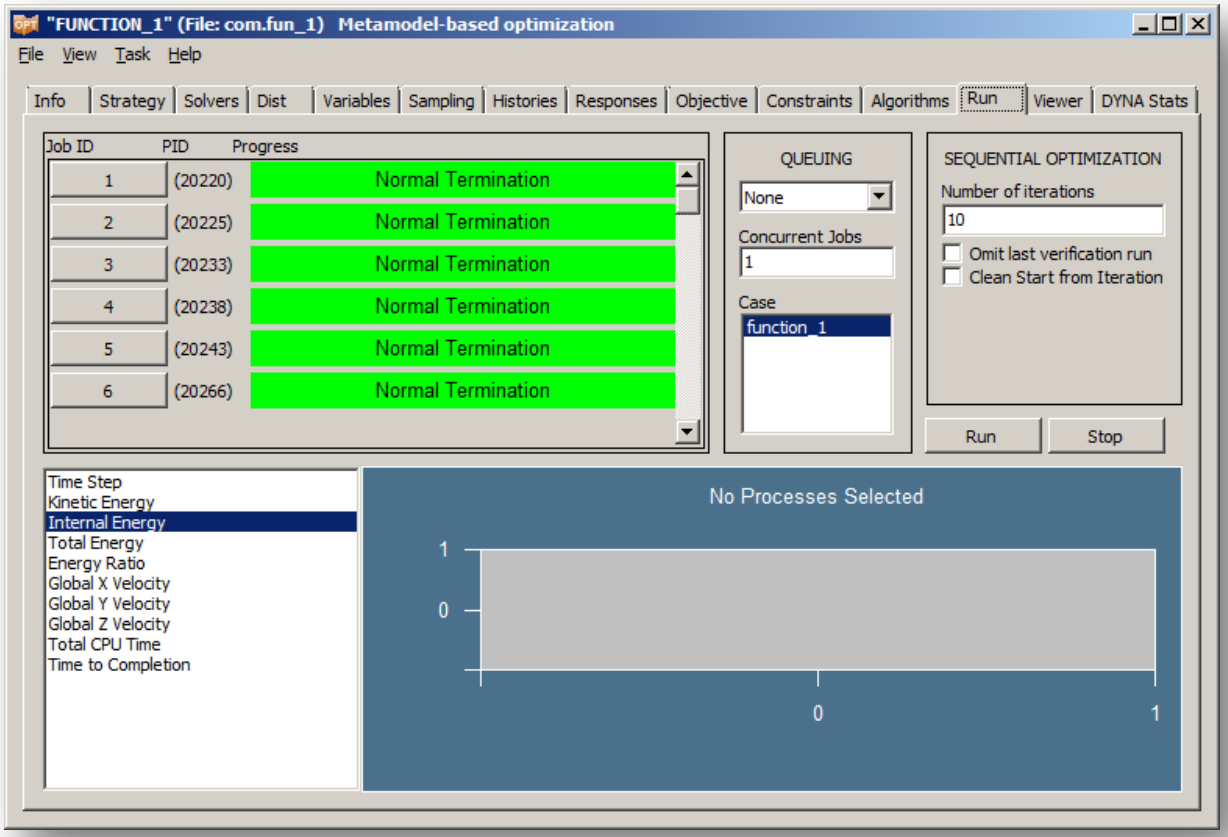
Objective Panel

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



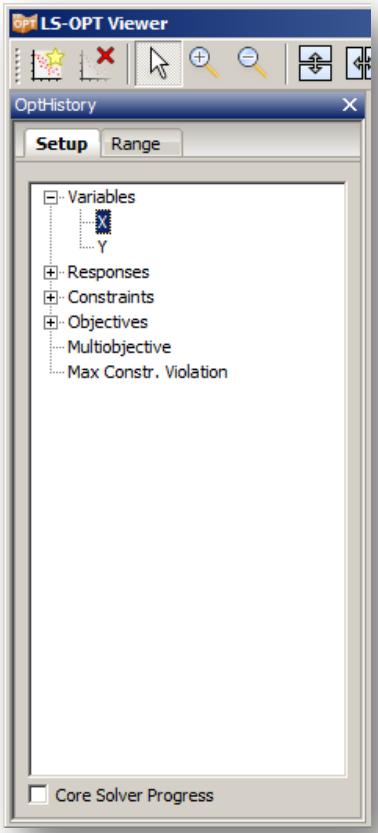
Run Panel

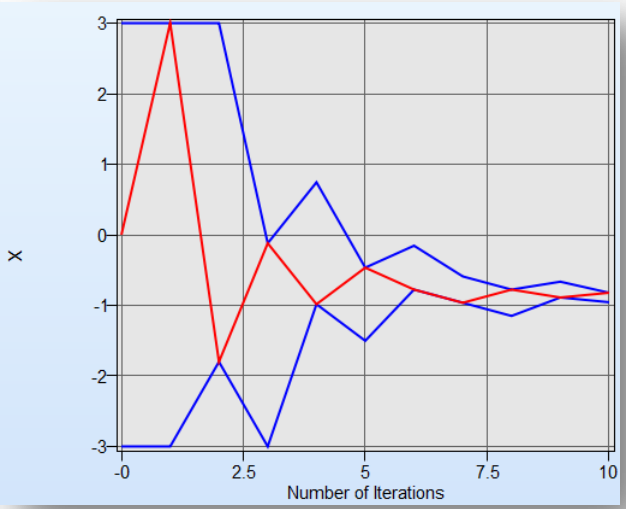
- This time leave None for QUEUING software
- Request 10 iterations
- Leave 1 in Concurrent Jobs window
- Wait for 51 jobs to be finished

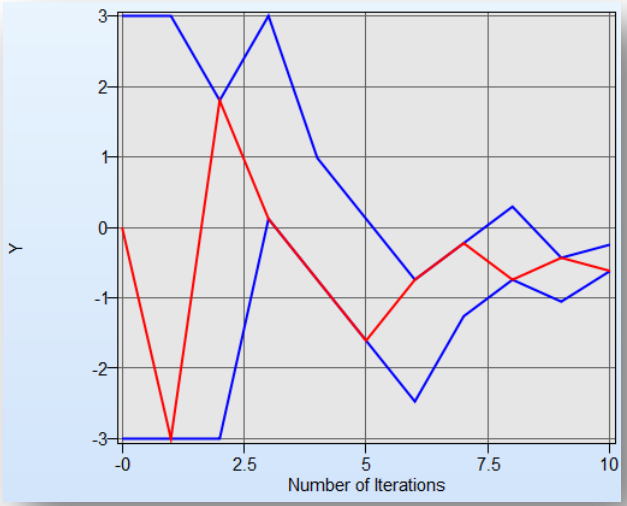


Viewer - Optimization History

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

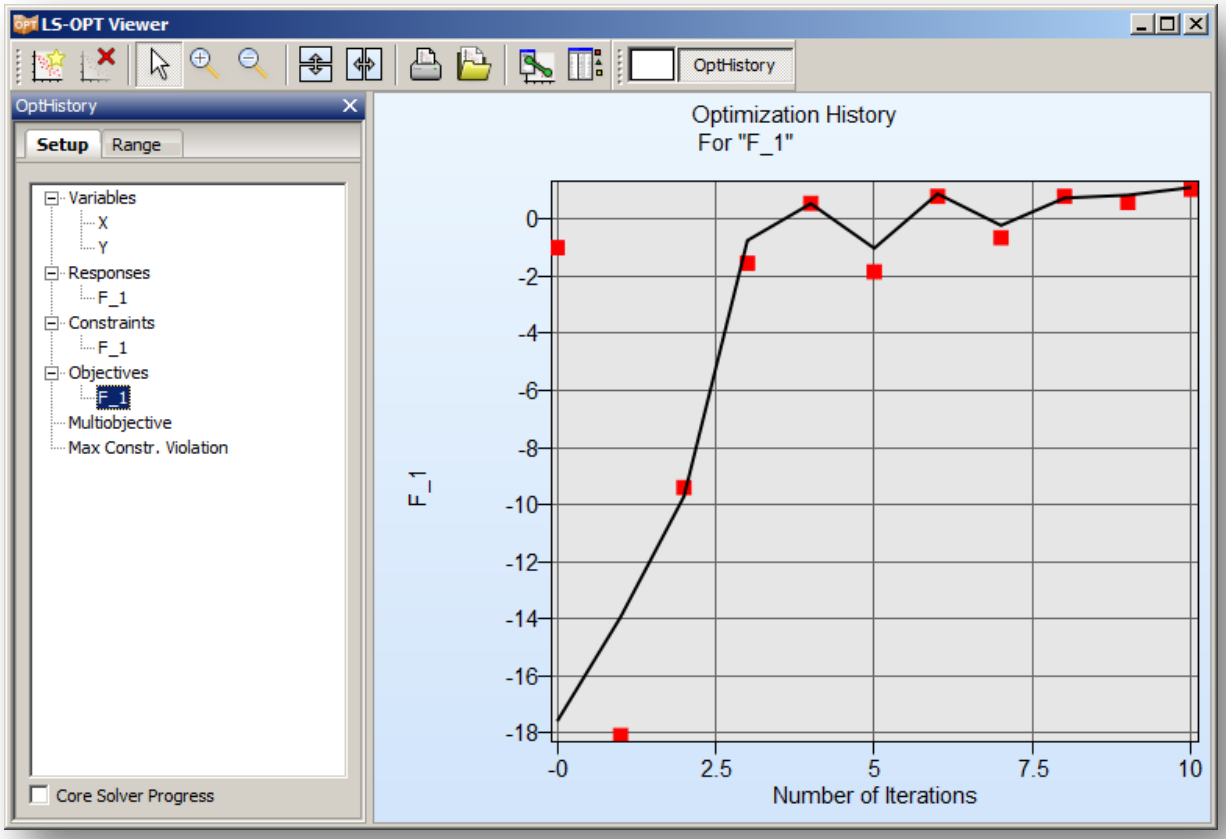


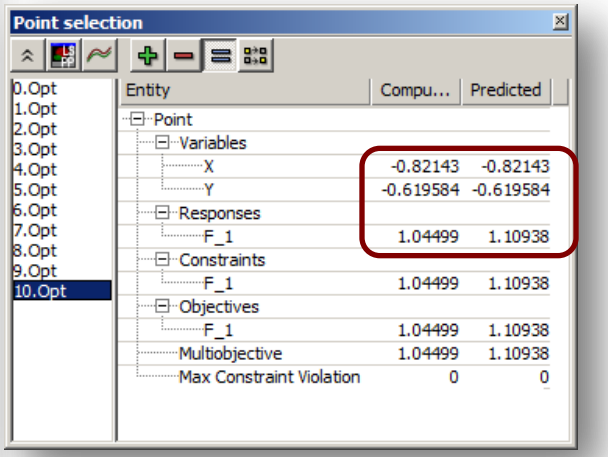




Viewer - Optimization History

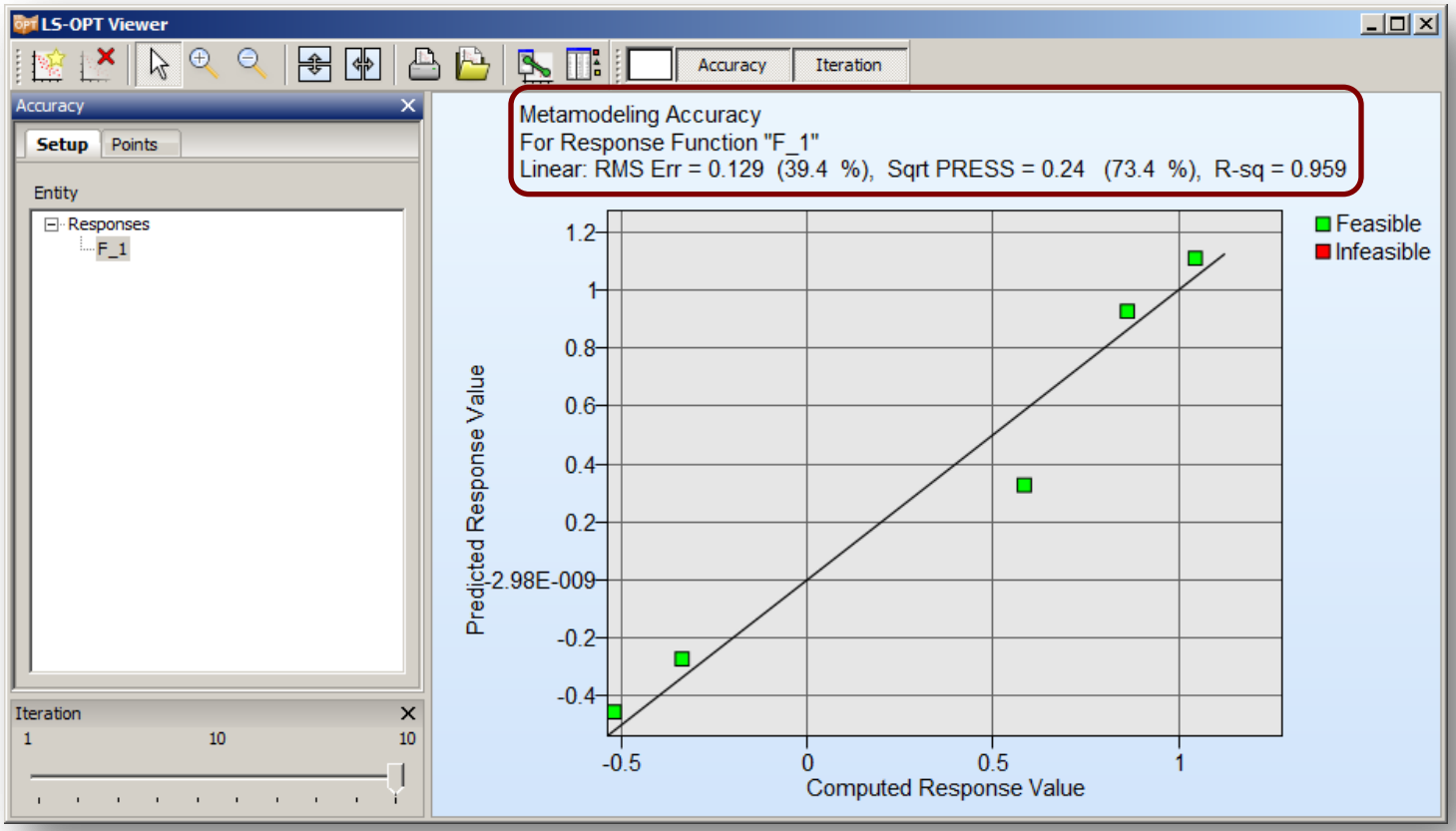
- From the Setup tab in Optimization History window Select F_1 from Objectives
- Indicate with the cursor the last point on the graph
- Read from Point Selection window the values of design variables for the optimal design





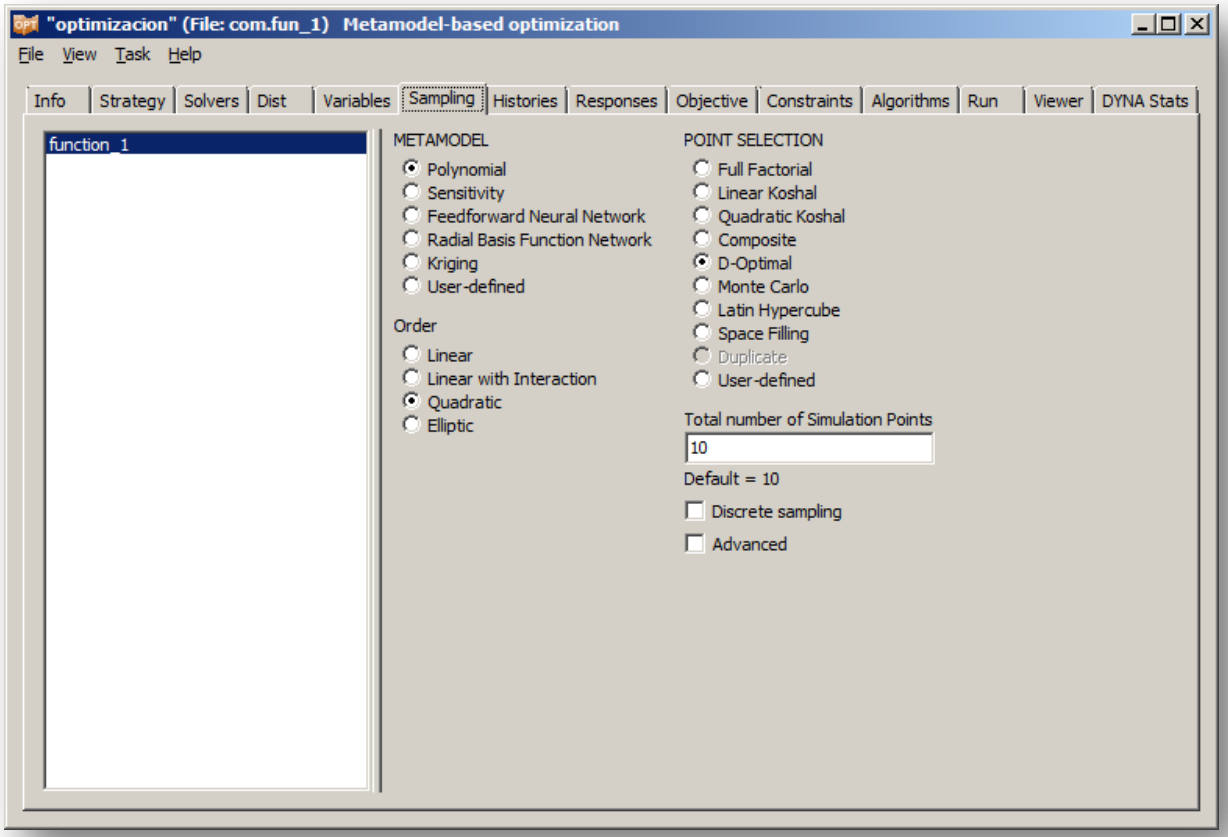
Viewer - Accuracy

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



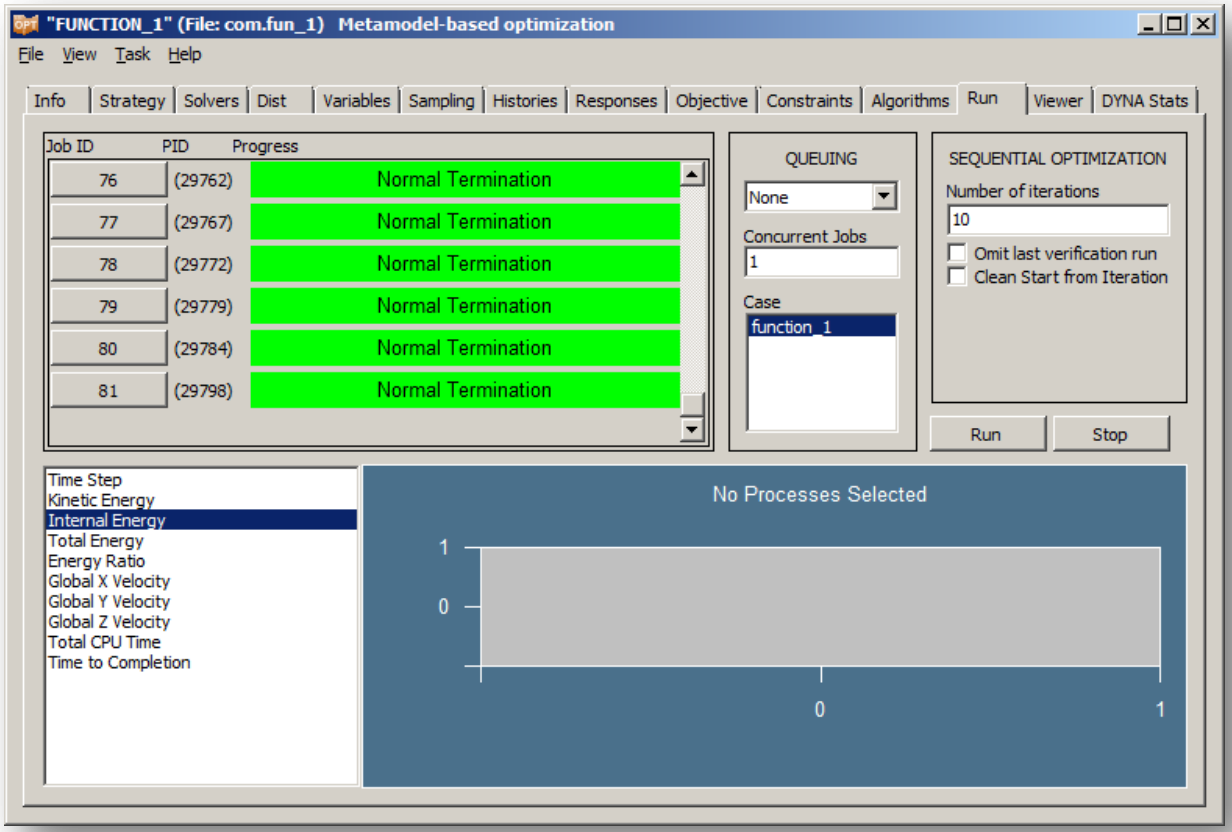
Sampling Panel – Quadratic Metamodel

- 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



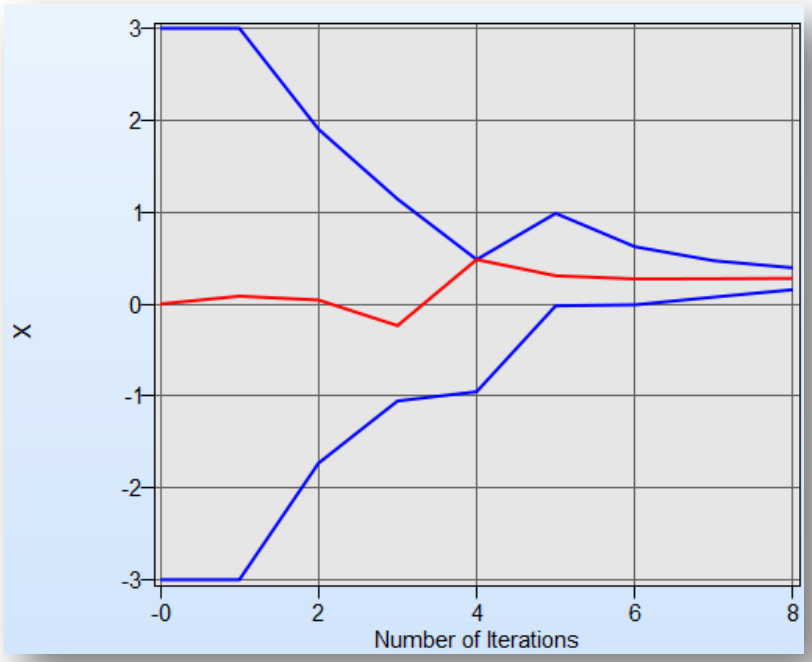
Run Panel

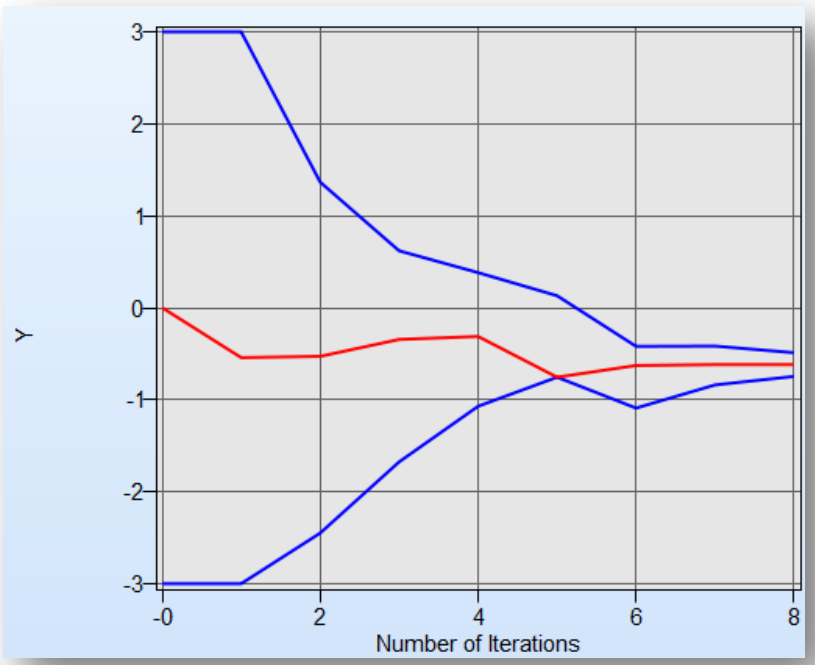
- Go to Run panel, press Run button and
- Wait for completion of 81 calculations



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

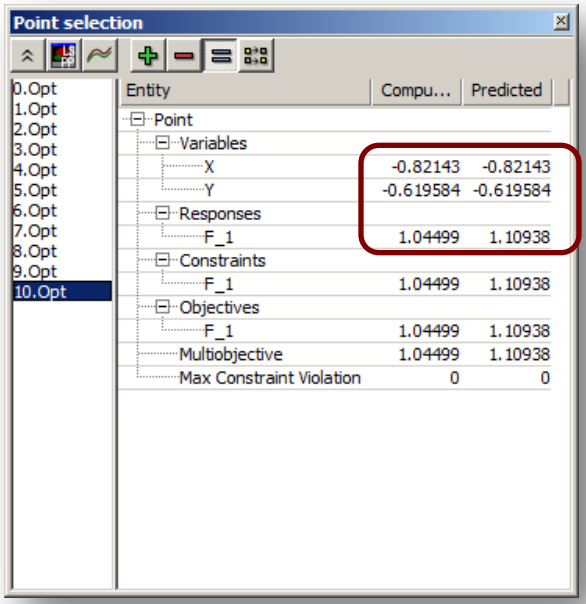




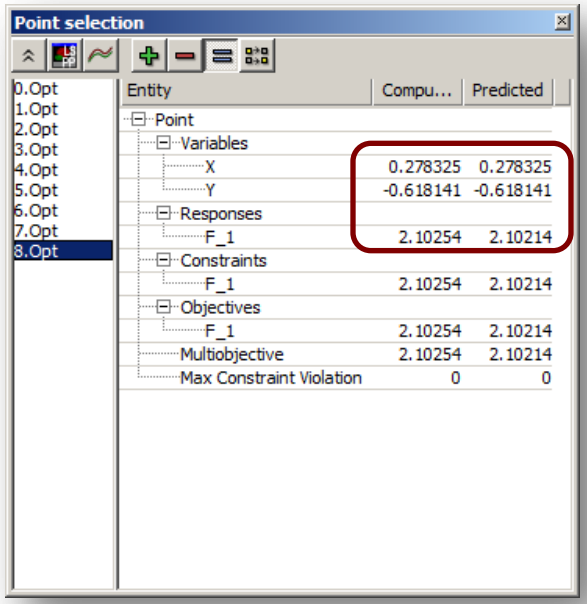
Viewer – Optimization History

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

Linear RS



Quadratic RS



Viewer - Sensitivities

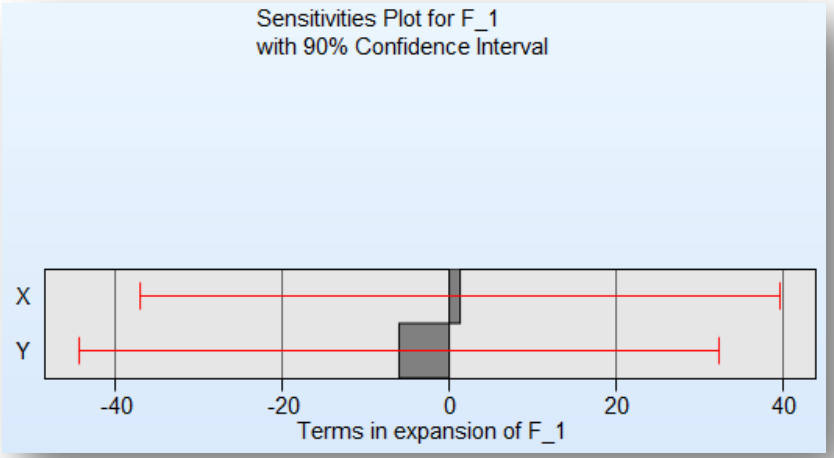
- Go to Viewer panel
- Select Sensitivity from Metamodel menu
- Compare the plots from first iteration for linear and quadratic metamodel

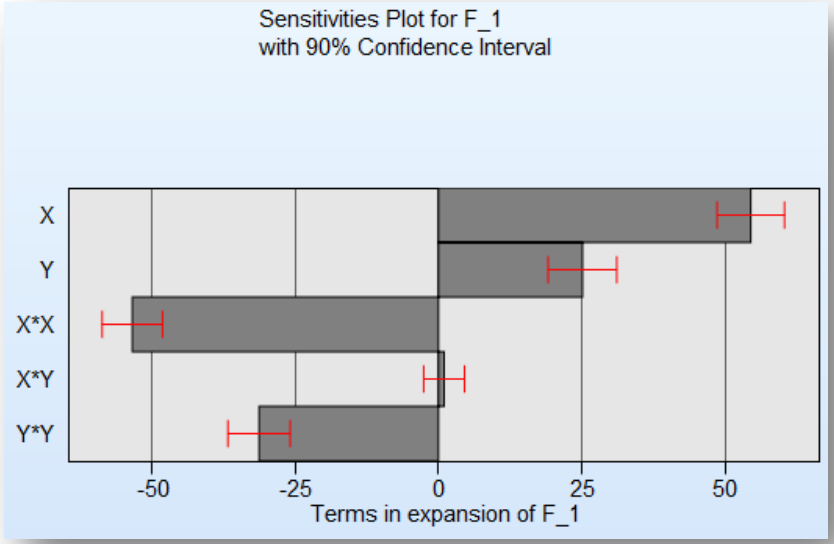
Linear RS

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

Quadratic RS

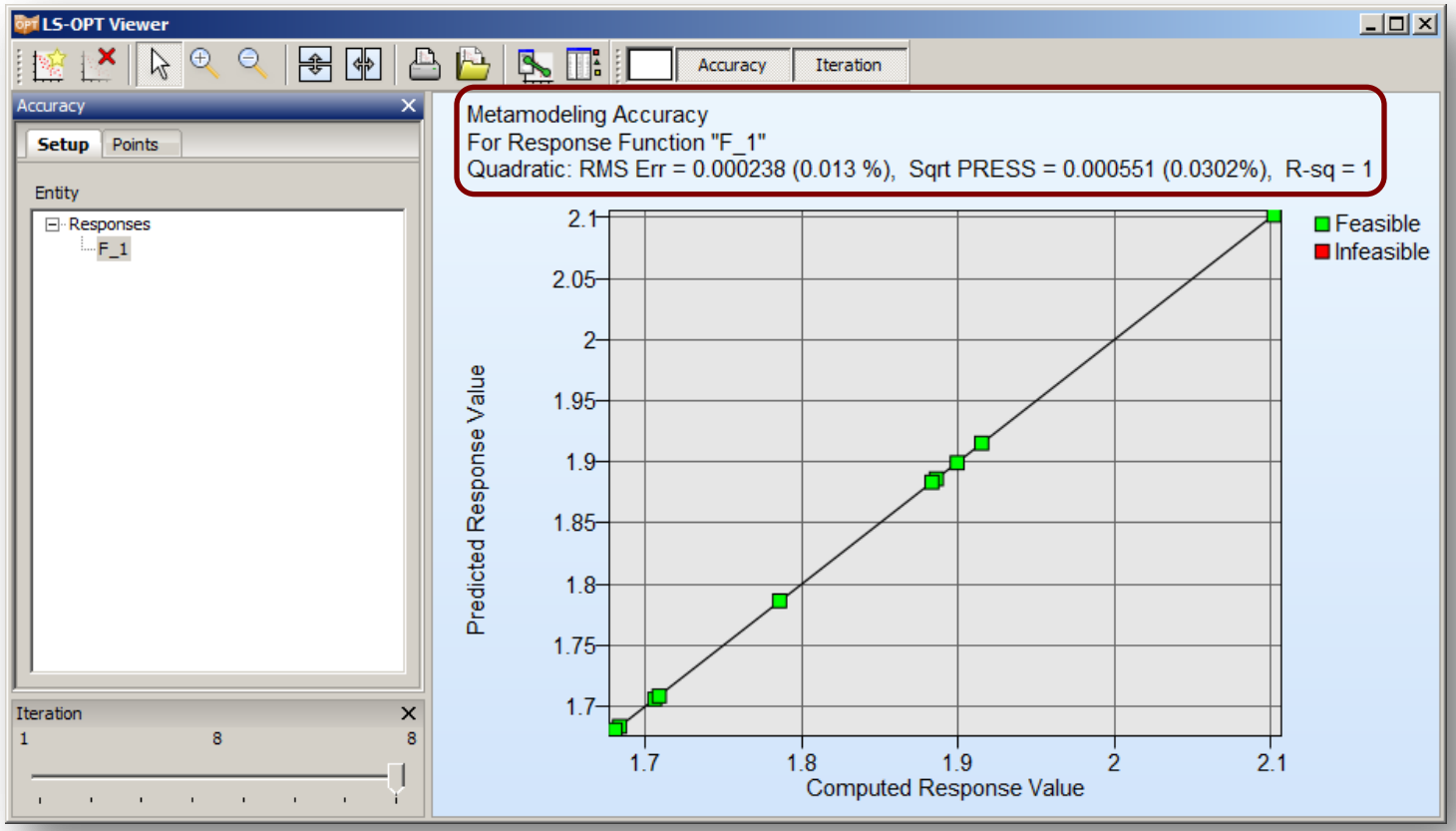
$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_{11} x_1^2 + \beta_{22} x_2^2 + \beta_{12} x_1 x_2 + \varepsilon$$



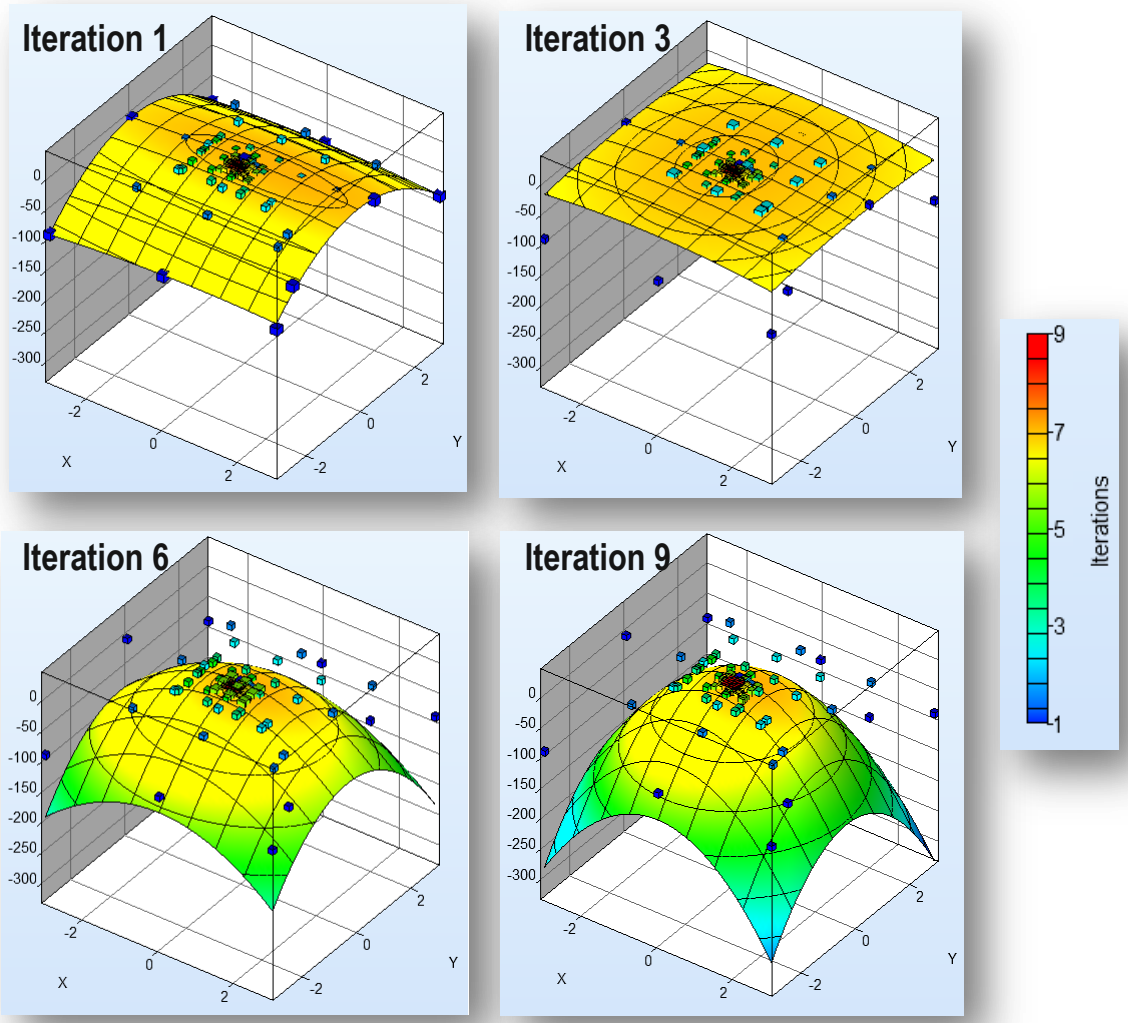


Viewer - Accuracy of the Quadratic Metamodel

- 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