Workshop – Prediction Analysis, Frequency Response Analysis (SOL 111)

AN MSC NASTRAN MACHINE LEARNING WEB APP TUTORIAL

Questions? Email: christian@ the-engineering-lab.com

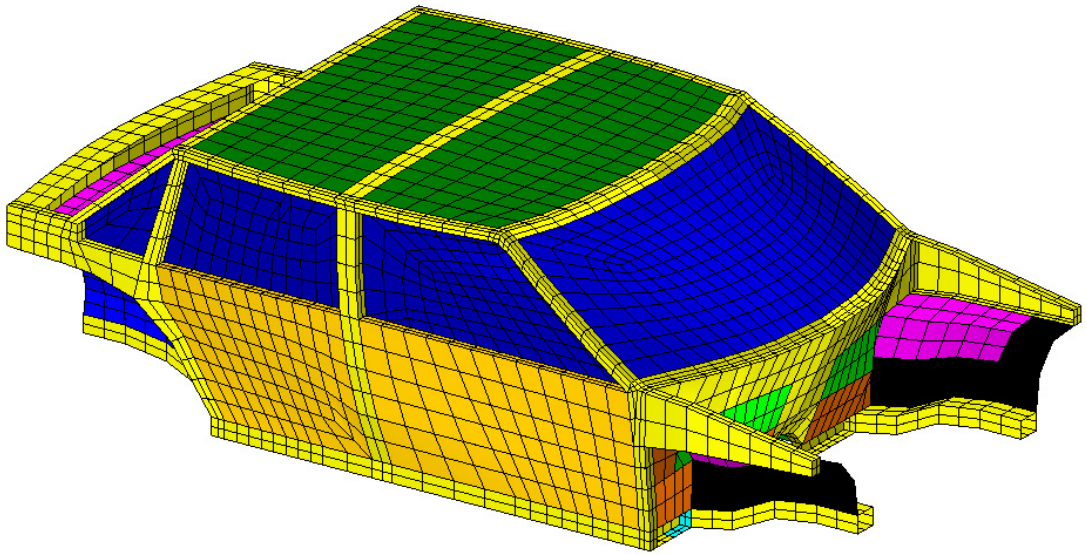
Goal: Prediction Analysis

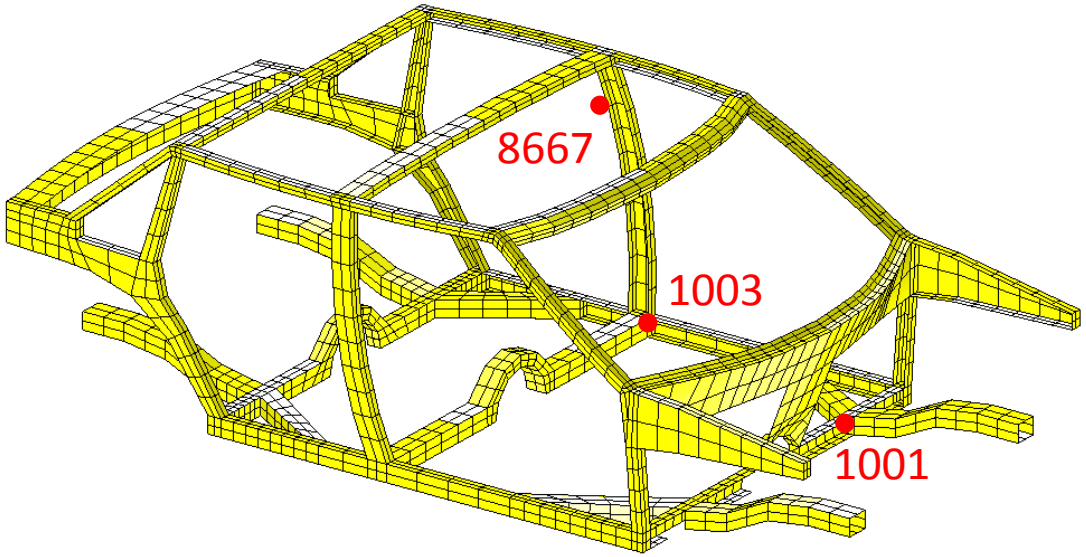
This tutorial consists of multiple parts

1. Configuring The Problem Statement
   - In this tutorial, we configure the parameters and the responses to monitor.
2. Configuring Multiple Batch Runs
   - This section discusses how to configure and execute multiple MSC Nastran runs.
3. Determining Parameter Relevance (Parameter/Variable Screening)
   - This example starts with 11 parameters. Automatic relevance determination (ARD) is used to identify important parameters and reduce the problem to 4 parameters.
4. Performing Predictions
   - Gaussian process (GP) regression is used to train a surrogate model and perform predictions.
5. Creating Response vs. Frequency Plots with the HDF5 Explorer
   - The HDF5 Explorer web app is used to create Response vs. Frequency Plots.

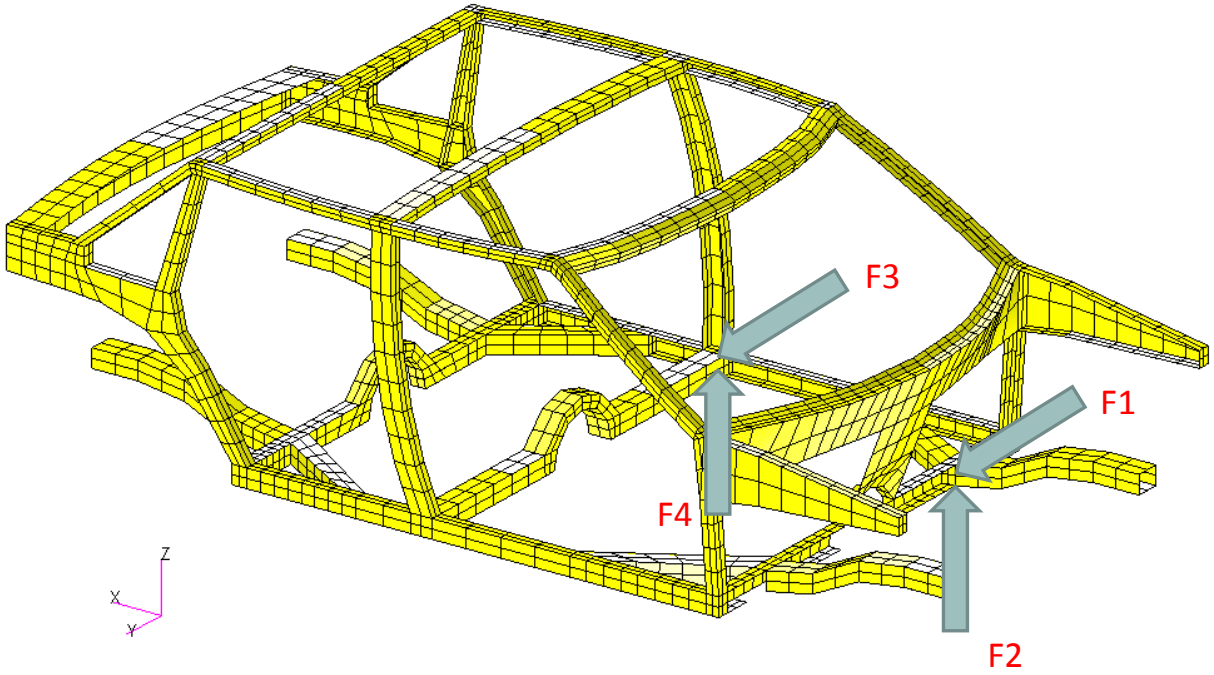
Details of the Structural Model

1. Perform a frequency response analysis for different thickness values
2. Create XYPLOTs for nodes 1001, 1003, and 8667

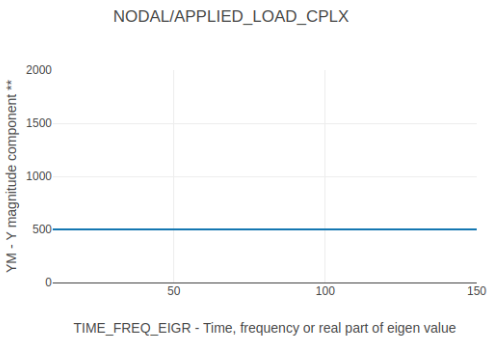




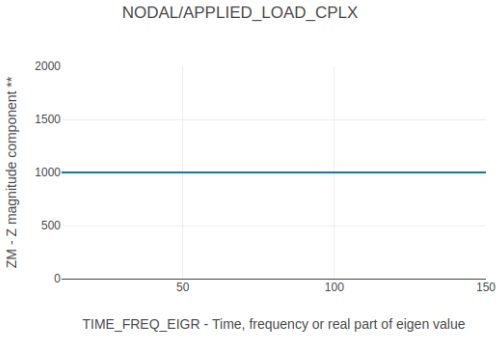
Details of the Structural Model



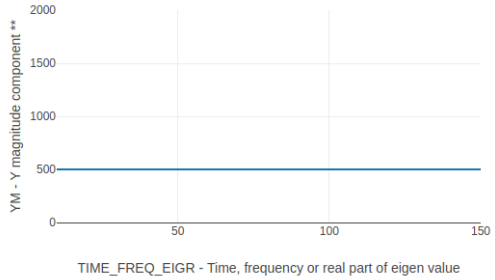
F1 – Load at node 1001, y direction, Subcase 12



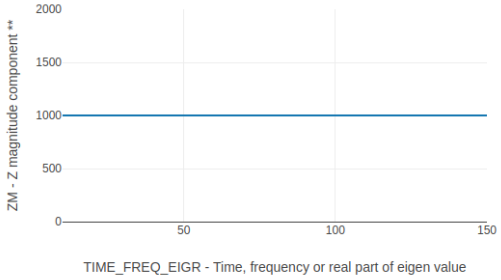
F2 – Load at node 1001, z direction, Subcase 13



F3 – Load at node 1003, y direction, Subcase 32



F4 – Load at node 1003, z direction, Subcase 33



Problem Statement

Design Variables

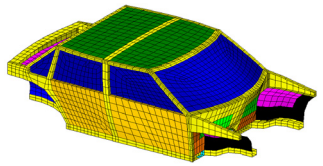
x1: The thickness of PSHELL 1

x2: The thickness of PSHELL 2
...
x11: The thickness of PSHELL 11

1.0 < x1, x2, …, x11, < 6.0

Samples

- Batch set 1 – 55 run LHS Design
- Batch set 2 – 40 run LHS Design
- Batch set 3 – 8 run LHS Design



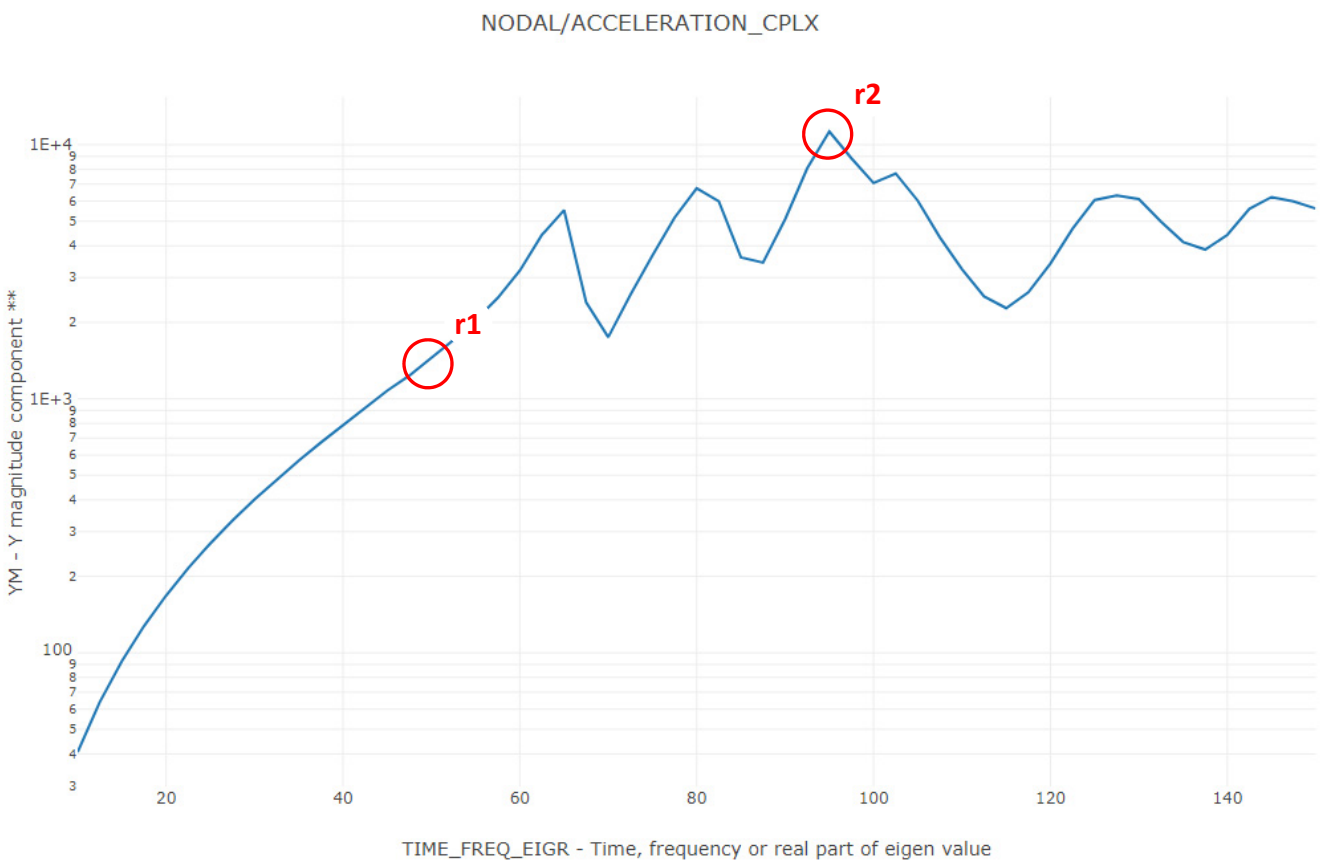
Monitored Responses

Label	Dataset Name	Field	Field Description	Node ID	SUBCASE	Frequency
r1	Acceleration	YM	Y magnitude component	1001	12	50 Hz
r2	Acceleration	YM	Y magnitude component	1001	12	Max Value
r3	Acceleration	ZM	Z magnitude component	1001	13	Max Value
r4	Acceleration	YM	Y magnitude component	1003	32	Max Value
r5	Acceleration	ZM	Z magnitude component	1003	33	Max Value
r6	Pressure	PM	Sound pressure level - magnitude	8667	12	Max Value
r7	Pressure	PM	Sound pressure level - magnitude	8667	13	Max Value
r8	Pressure	PM	Sound pressure level - magnitude	8667	32	Max Value
r9	Pressure	PM	Sound pressure level - magnitude	8667	33	Max Value

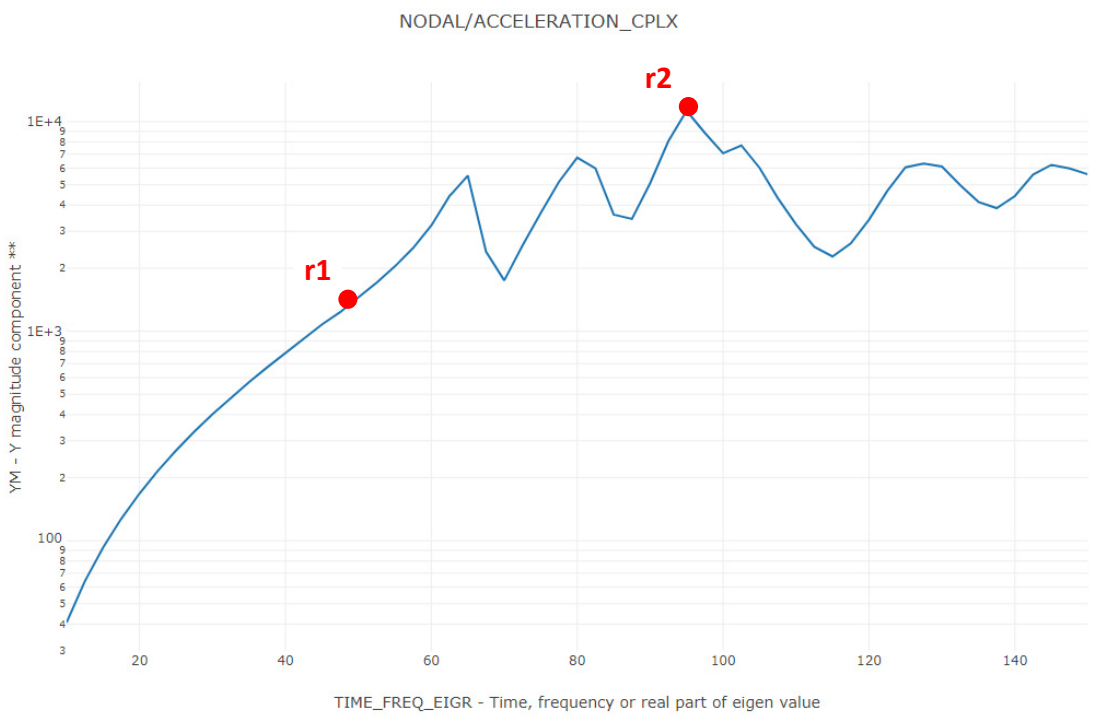
Problem Statement, Continued

The responses defined in this tutorial correspond to points on frequency response plots

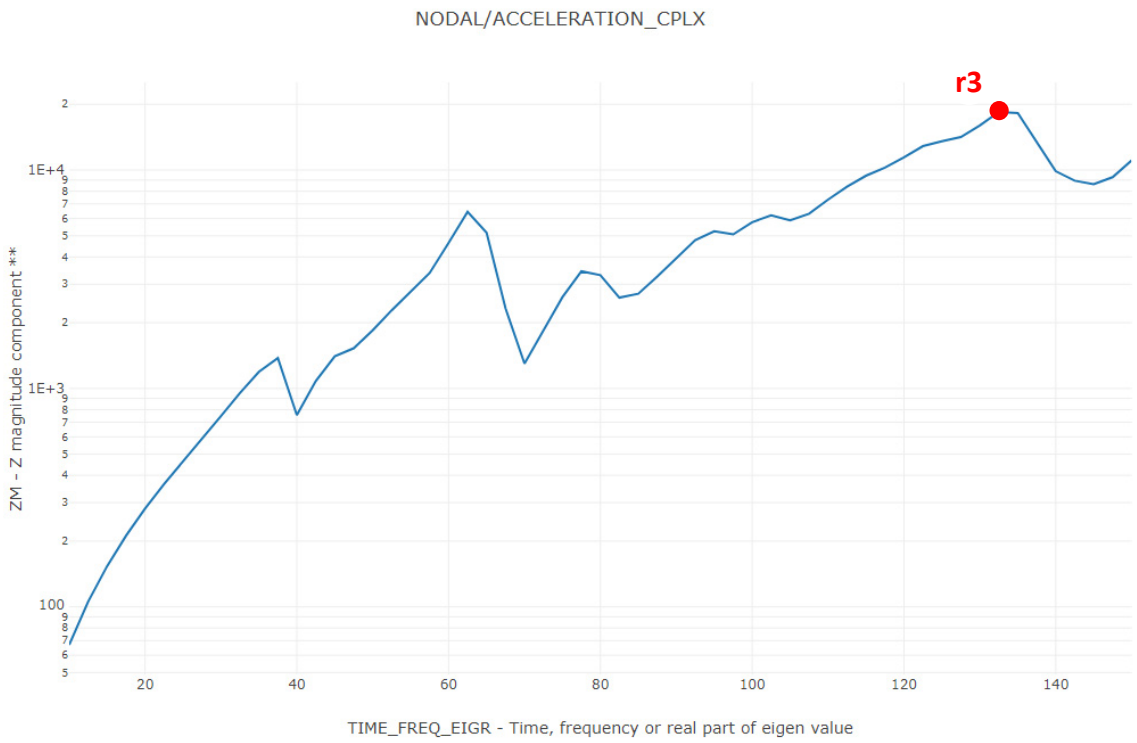
- Response r1 is the acceleration at 50 Hz
- Response r2 is the max acceleration for the forcing frequency range
- Other responses correspond to different node ID, component, subcase number and frequency



Monitored Responses
r1, r2, r3

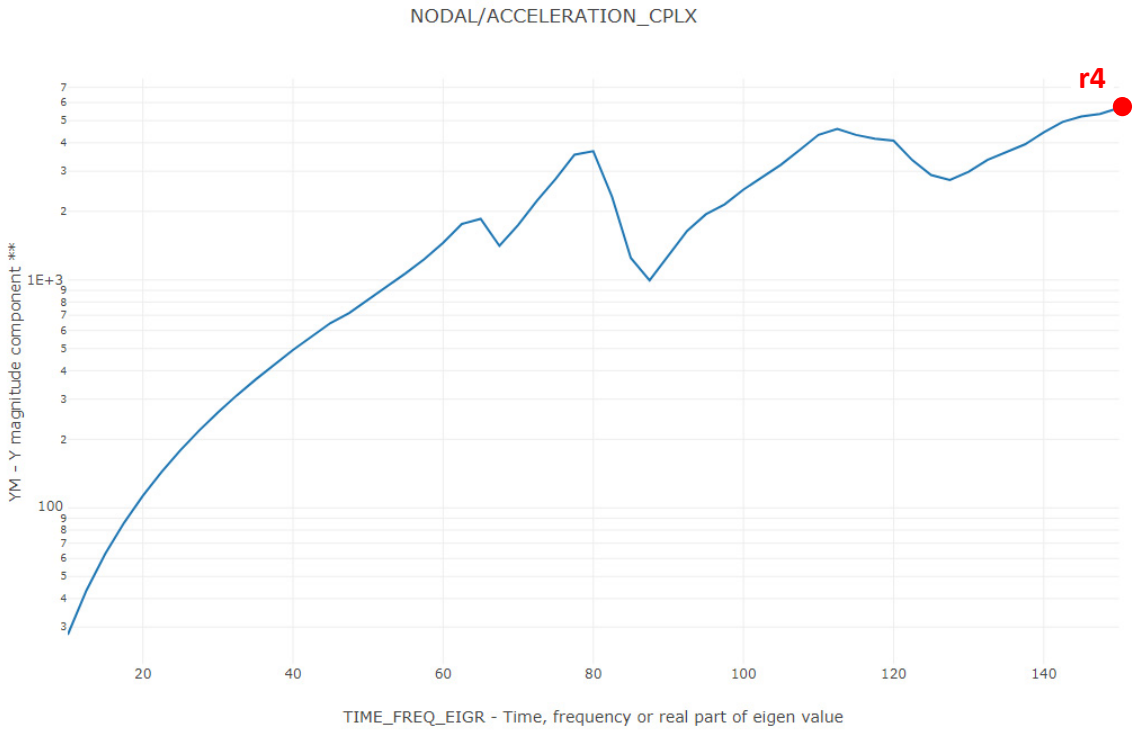


ID: 1001 | SUBCASE: 12 | YM vs. TIME_FREQ_EIGR

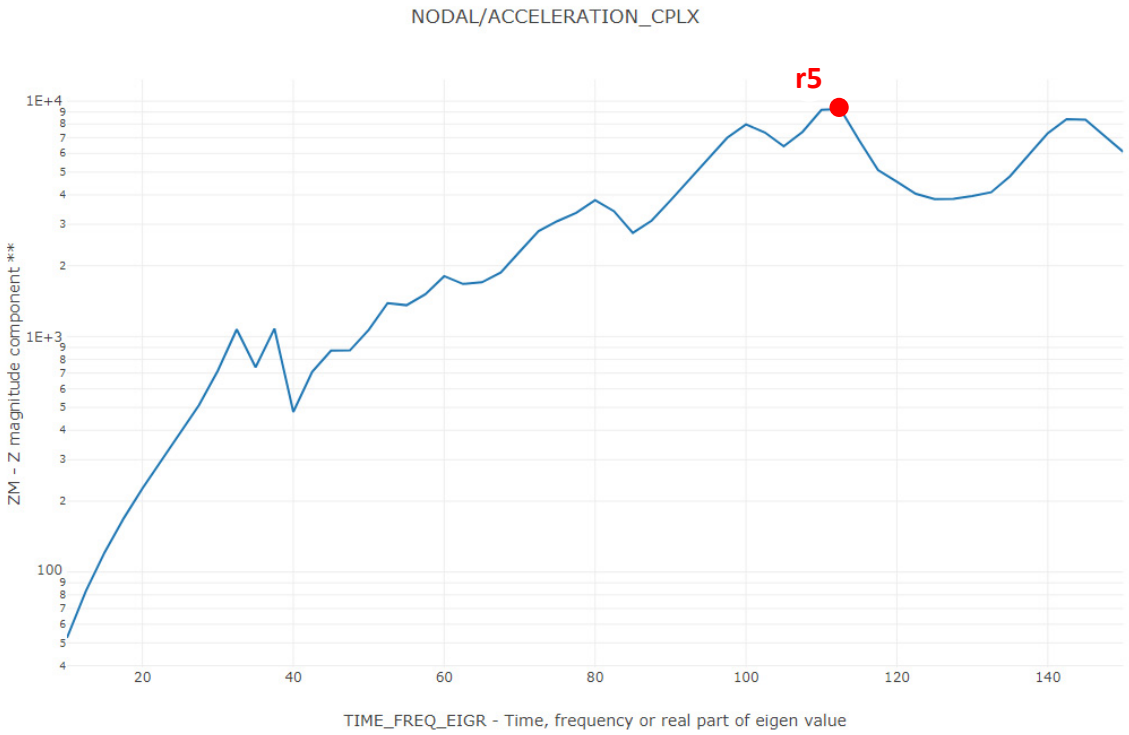


ID: 1001 | SUBCASE: 13 | ZM vs. TIME_FREQ_EIGR

Monitored Responses
r4, r5

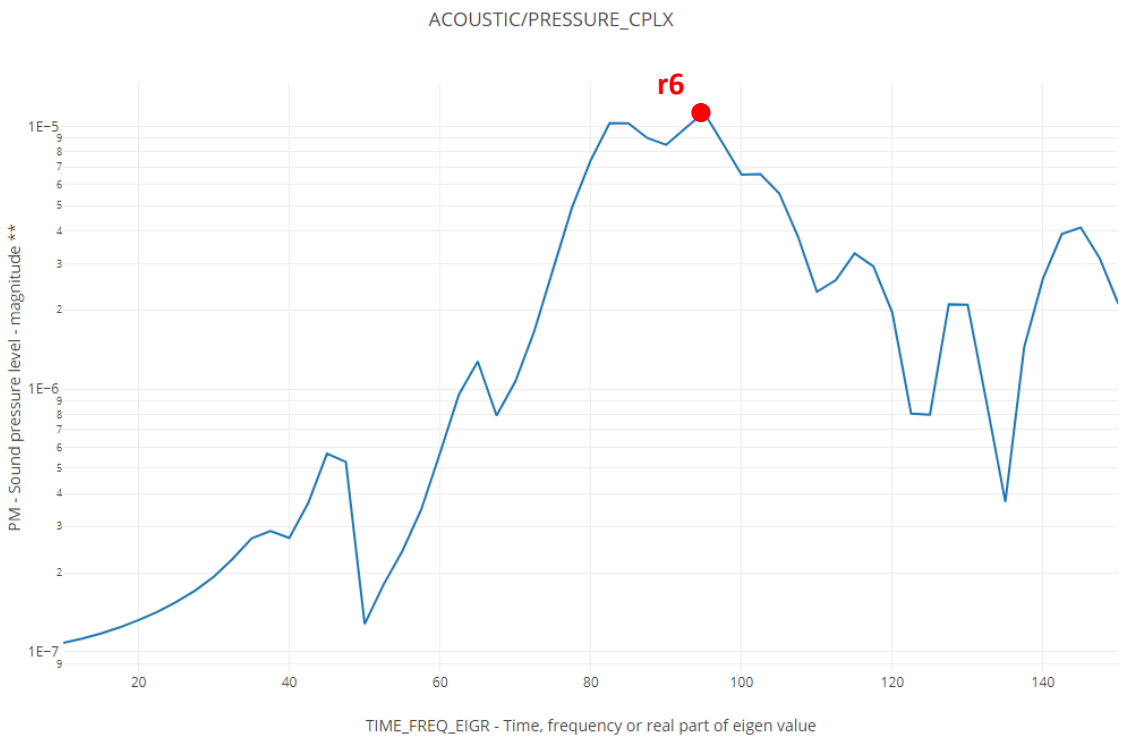


ID: 1003 | SUBCASE: 32 | YM vs. TIME_FREQ_EIGR

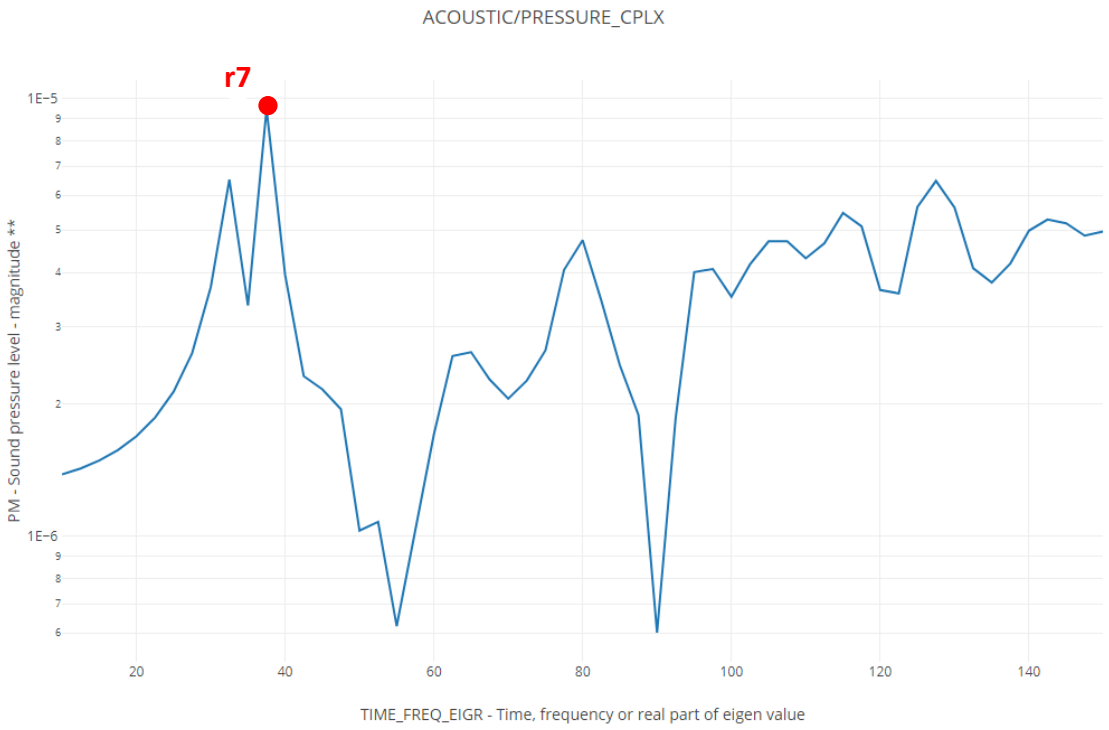


ID: 1003 | SUBCASE: 33 | ZM vs. TIME_FREQ_EIGR

Monitored Responses
r6, r7

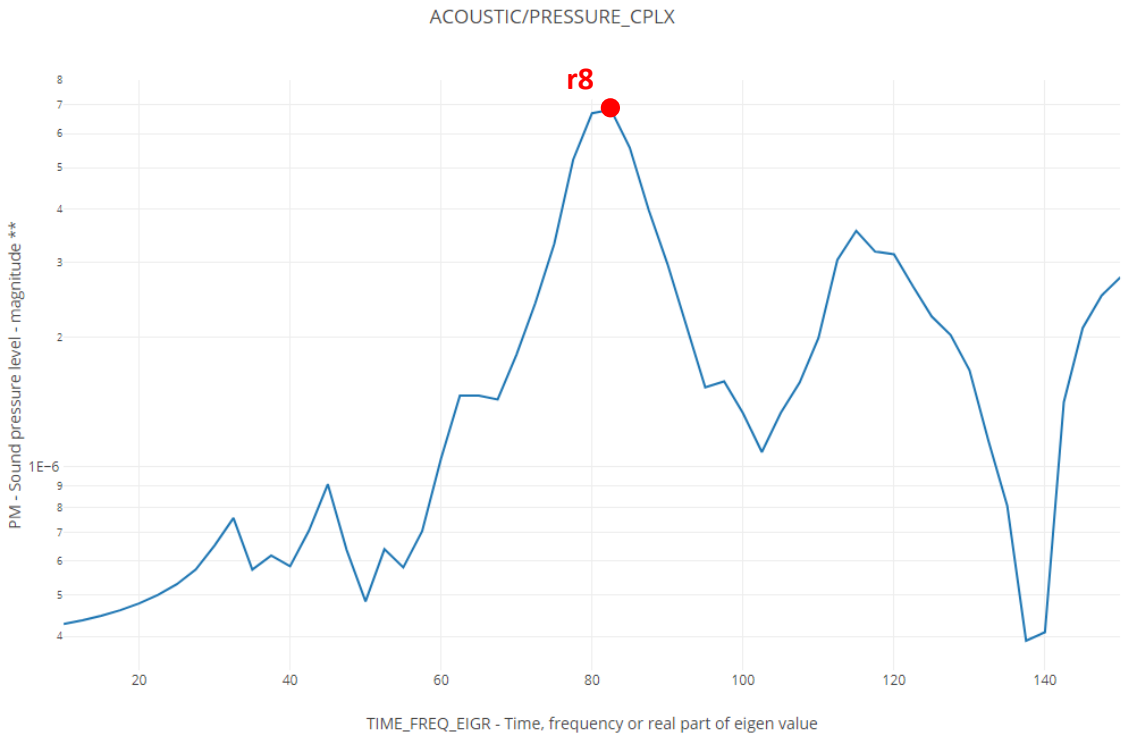


ID: 8667 | SUBCASE: 12 | PM vs. TIME_FREQ_EIGR

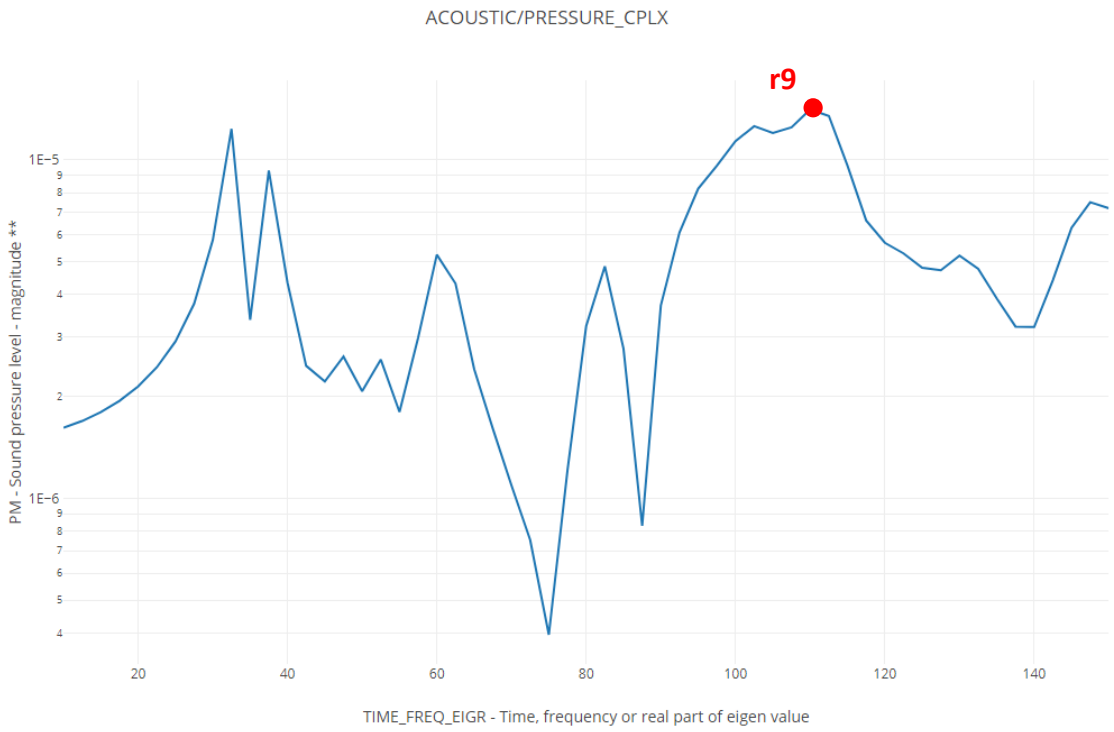


ID: 8667 | SUBCASE: 13 | PM vs. TIME_FREQ_EIGR

Monitored Responses
r8, r9



ID: 8667 | SUBCASE: 32 | PM vs. TIME_FREQ_EIGR

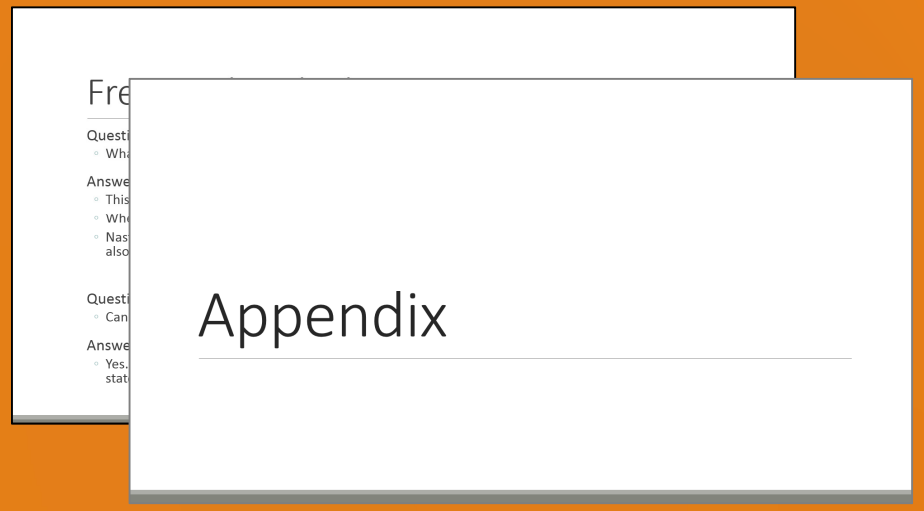


ID: 8667 | SUBCASE: 33 | PM vs. TIME_FREQ_EIGR

More Information Available in the Appendix

The Appendix includes information regarding the following:

- Response Configuration
  - Monitor the maximum or minimum response, whichever has the greatest absolute value: Yes, No or blank
- How to import and edit files
- What is Gaussian Process Regression?



Contact me

- Nastran SOL 200 training
- Nastran SOL 200 questions
- Structural or mechanical optimization questions
- Access to the SOL 200 Web App

christian@ the-engineering-lab.com

Tutorial

Tutorial Overview

1. Start with a .bdf or .dat file
2. Use the Machine Learning web app to:
   1. Configure the problem statement
   2. Configure multiple batch runs
3. Use the Prediction Analysis web app to:
   1. Determine parameter relevance (parameter/variable screening)
   2. Perform predictions
4. Use the HDF5 Explorer to:
   1. Create response vs. frequency plots

Special Topics Covered

Training Data – The training data consists of the parameter inputs and respective output responses for multiple MSC Nastran runs. This tutorial describes how to configure multiple MSC Nastran runs, each with different parameter inputs, and how to monitor each response.

Gaussian process regression – This tutorial describes the procedure to use Gaussian process regression to train a surrogate model and make predictions.

Automatic Response Extraction – Often responses are manually or automatically extracted from the F06 file. This becomes challenging when extracting responses from multiple F06 files. This tutorial highlights the web app's ability to automatically extract responses from multiple H5 files with minimal user effort.

Automatic Plots - Multiple plots must be created. This traditionally involves extracting data from result files, for example the F06 file, and using Excel to create the plots. This tutorial highlights the automatic generation of these plots that require minimal user effort.

SOL 200 Web App Capabilities

The Post-processor Web App and HDF5 Explorer are free to MSC Nastran users.

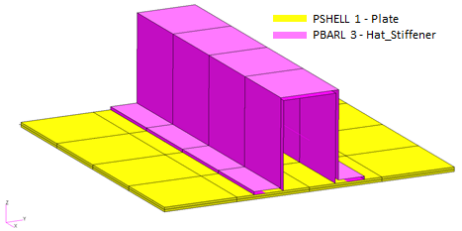
Compatibility

- Google Chrome, Mozilla Firefox or Microsoft Edge
- Windows and Red Hat Linux
- Installable on a company laptop, workstation or server. All data remains within your company.

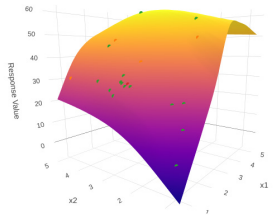
Benefits

- REAL TIME error detection. 200+ error validations.
- REALT TIME creation of bulk data entries.
- Web browser accessible
- Free Post-processor web apps
- +80 tutorials

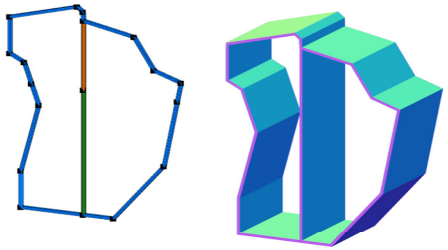
Web Apps



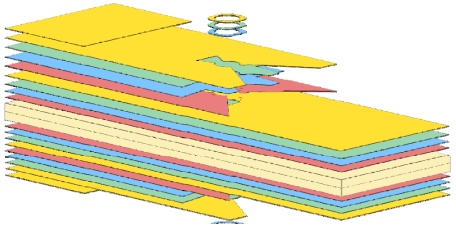
Web Apps for MSC Nastran SOL 200
Pre/post for MSC Nastran SOL 200. Support for size, topology, topometry, topography, multi-model optimization.



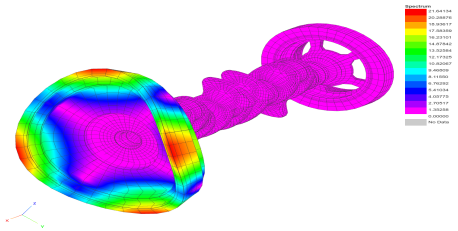
Machine Learning Web App
Bayesian Optimization for nonlinear response optimization (SOL 400)



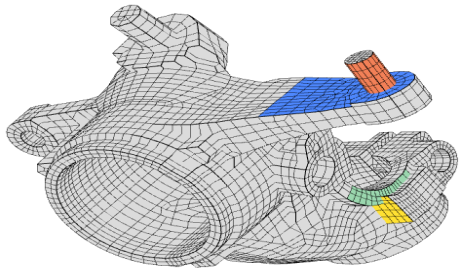
PBMSECT Web App
Generate PBMSECT and PBRSECT entries graphically



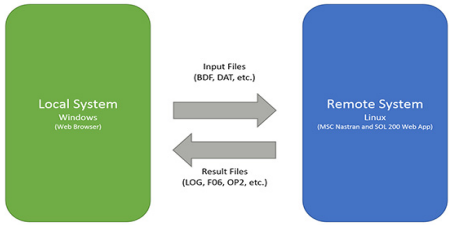
Ply Shape Optimization Web App
Optimize composite ply drop-off locations, and generate new PCOMPG entries



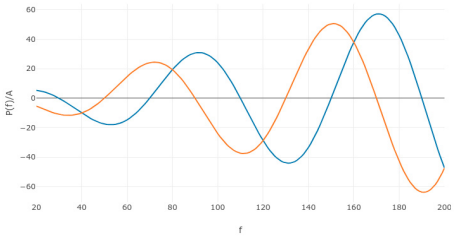
Post-processor Web App
View MSC Nastran results in a web browser on Windows and Linux



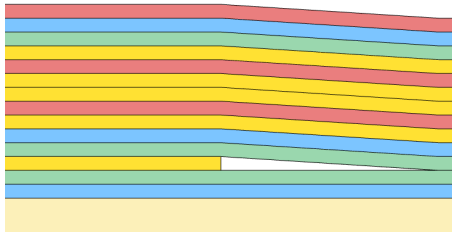
Shape Optimization Web App
Use a web application to configure and perform shape optimization.



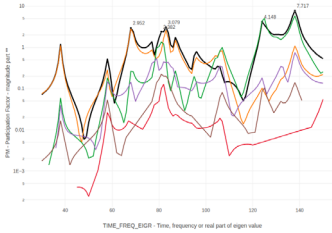
Remote Execution Web App
Run MSC Nastran jobs on remote Linux or Windows systems available on the local network



Dynamic Loads Web App
Generate RLOAD1, RLOAD2 and DLOAD entries graphically



Stacking Sequence Web App
Optimize the stacking sequence of composite laminate plies

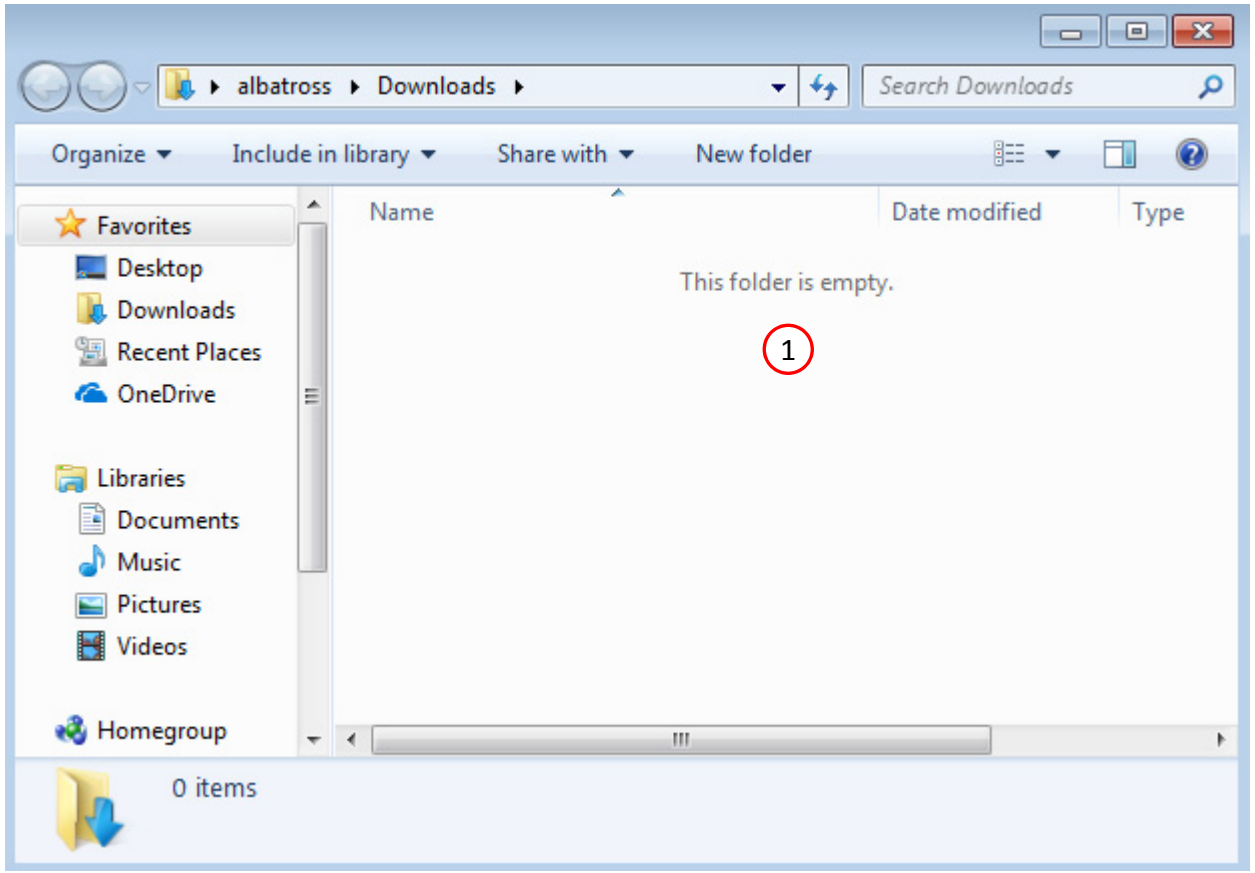


HDF5 Explorer Web App
Create graphs (XY plots) using data from the H5 file

Configuring The Problem Statement

Before Starting

1. Ensure the Downloads directory is empty in order to prevent confusion with other files



- Throughout this workshop, you will be working with multiple file types and directories such as:
  - .bdf/.dat
  - nastran_working_directory
  - .f06, .log, .pch, .h5, etc.
- To minimize confusion with files and folders, it is encouraged to start with a clean directory.

Go to the User's Guide

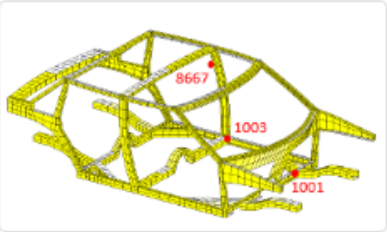
1. Click on the indicated link

- The necessary BDF files for this tutorial are available in the Tutorials section of the User's Guide.

Obtain Starting Files

1. Find the indicated example
2. Click Link
3. The starting file has been downloaded

- When starting the procedure, all the necessary BDF, or DAT, files must be collected and uploaded together. Relevant INCLUDE files must also be collected and uploaded.

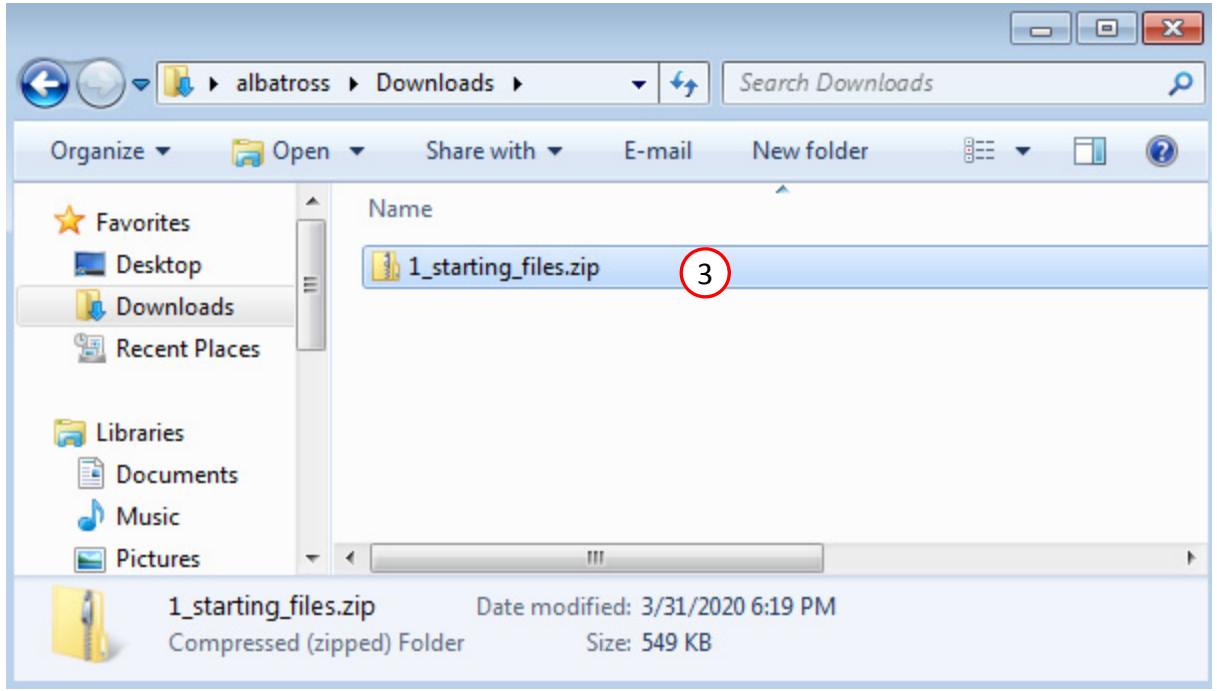


Prediction Analysis, Frequency Response Analysis (SOL 111) 1

Consider a frequency response analysis of a ground vehicle. For different configurations of the ground vehicle, there is a desire to rapidly determine the frequency responses, including accelerations and pressures, while keeping the number of Finite Element (FE) solver runs to a minimum.

This tutorial describes the procedure to use Gaussian progress regression as a surrogate model for computationally expensive Finite Element (FE) based simulations. This tutorial walks users through the process of acquiring training data, fitting the surrogate model, making predictions and quantifying uncertainty. In addition, the process to screen variables/parameters via Automatic relevance determination (ARD) is discussed.

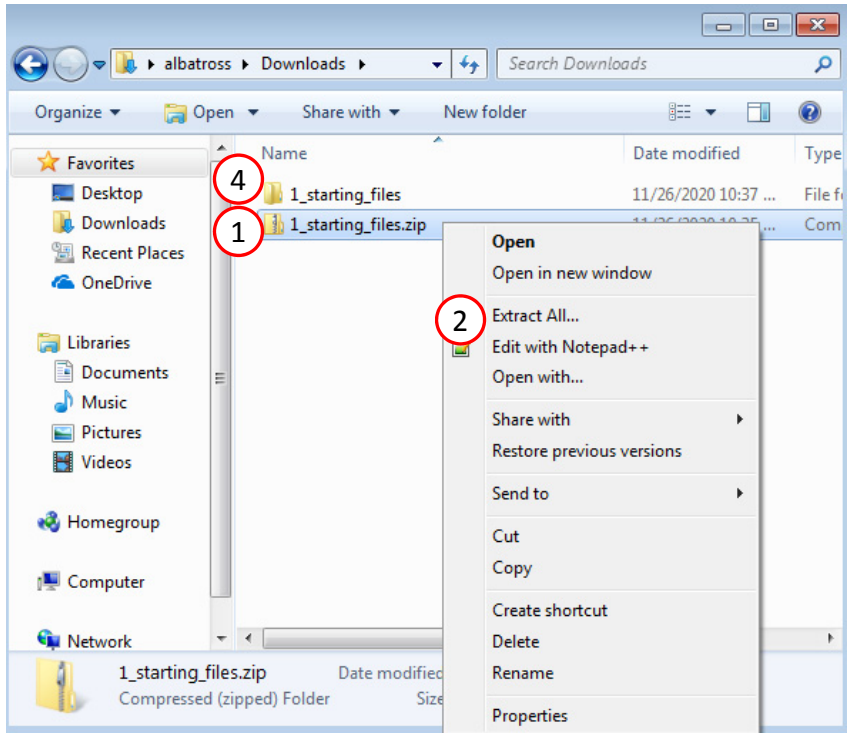
Starting Files: Link 2
Solution BDF Files: Link

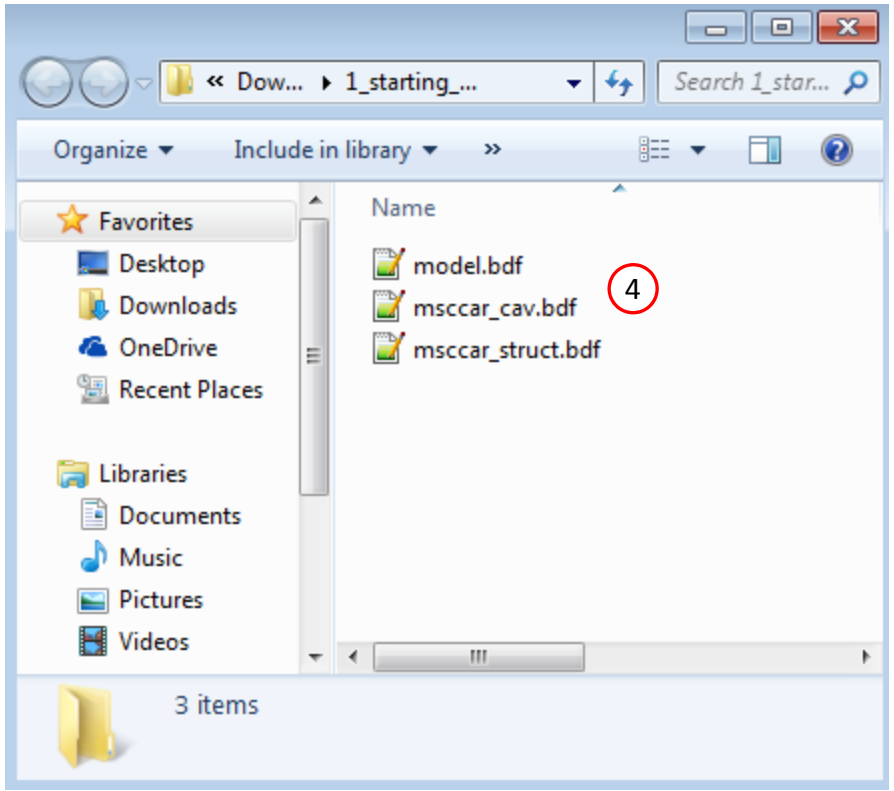


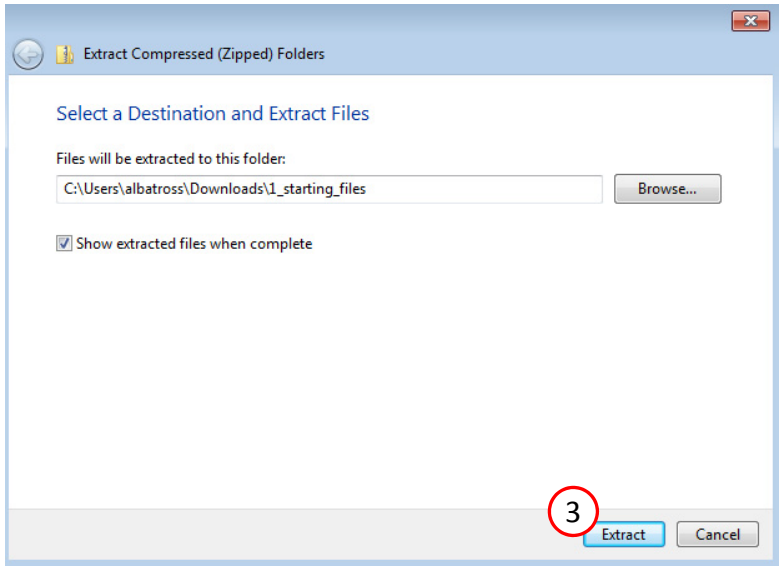
Obtain Starting Files

1. Right click on the zip file
2. Select Extract All…
3. Click Extract
4. The starting files are now available in a folder

- The starting files for this tutorial are contained in a ZIP file and must be extracted as shown.



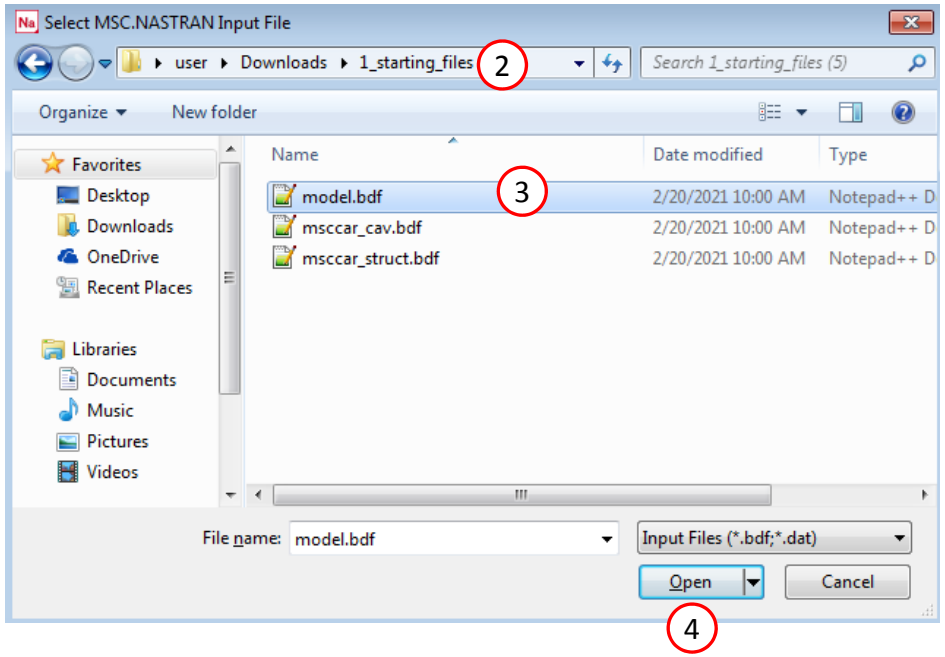


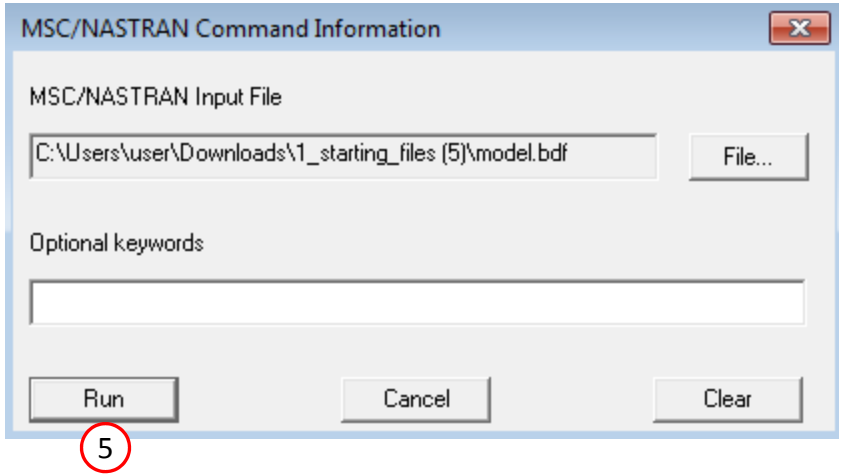


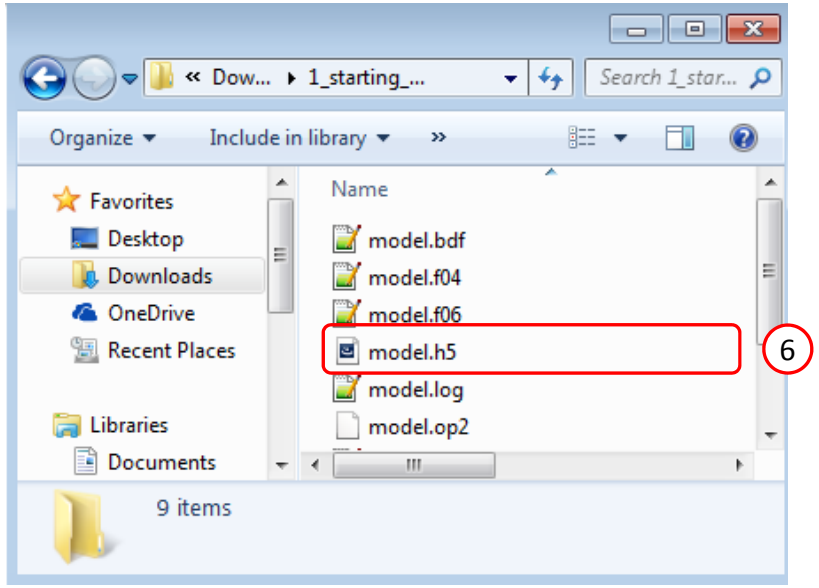
Create the Starting H5 File

A starting H5 file must be created. This H5 file will be used to configure the responses later on.

1. Double click the MSC Nastran desktop shortcut
2. Navigate to the directory named 1_starting_files
3. Select the indicated file
4. Click Open
5. Click Run
6. The starting H5 file is created







Use the same MSC Nastran version throughout this exercise

The following applies if you have multiple versions of MSC Nastran installed.

To ensure compatibility, use the same MSC Nastran version throughout this exercise.
For example, scenario 1 is OK but scenario 2 is NOT OK.

- Scenario 1 - OK
  - MSC Nastran 2021 is used to create the starting H5 file.
  - MSC Nastran 2021 is used for each run during Machine Learning or Parameter study.
- Scenario 2 – NOT OK
  - MSC Nastran 2018.2 is used to create the starting H5 file.
  - MSC Nastran 2021 is used for each run during Machine Learning or Parameter study.

Using the same MSC Nastran version is critical for consistent response extraction from the H5 file. A response configured for Nastran version X may not match in Nastran version Y, which leads to unsuccessful response extraction from the H5 files. The goal is to make sure all H5 files generated are from the same MSC Nastran version.

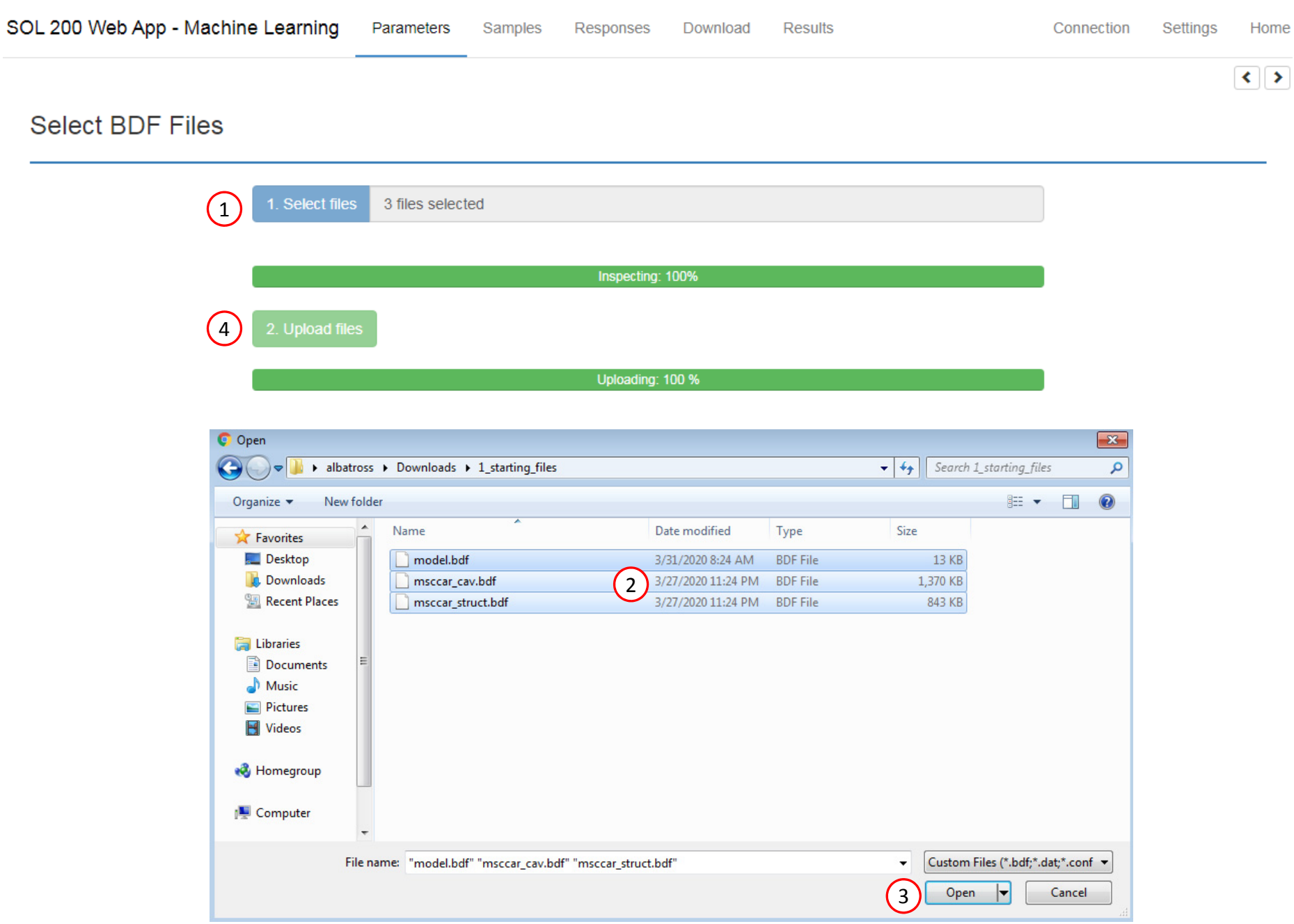
Open the Correct Page

1. Click on the indicated link

- MSC Nastran can perform many optimization types. The SOL 200 Web App includes dedicated web apps for the following:
  - Optimization for SOL 200 (Size, Topology, Topometry, Topography, Local Optimization, Sensitivity Analysis and Global Optimization)
  - Multi Model Optimization
  - Machine Learning
- The web app also features the HDF5 Explorer, a web application to extract results from the H5 file type.

Select BDF Files

1. Click Select files
2. Select the indicated files
3. Click Open
4. Click Upload files



Parameters

1. Set the following fields as parameters
   - x1: The thickness of PSHELL 1
   - x2: The thickness of PSHELL 2
   - …
   - x11: The thickness of PSHELL 11
2. Parameters have been created for the selected fields
3. For each parameter, use the following settings:
   - Low: 1.
   - High: 6.

- Bulk data entries will always be displayed in the small field format.
- Only fields that have real or integer data entries may be selected as parameters. If the field is blank or contains only characters, the field may not be selected.

Select Parameters

```
$__1___||__2___||__3___||__4___||__5___||__6___|

EIGRL   1               225.
EIGRL   2               300.
FORCE   212     1001            500.    0.0
FORCE   213     1001            1000.   0.0
FORCE   232     1003            500.    0.0
FORCE   233     1003            1000.   0.0
FREQ1   5       10.     2.5     56
MAT1    7       210000.0        0.3     7.90E-06
MAT1    8       62000.0         0.24    2.30E-06
MAT10   6               1.23E-12340000.0
PARAM   G       0.06
PARAM   GFL     0.12
PARAM   LFREQ   0.1
PARAM   PREFDB  2.E-11
PARAM   WTMASS  .001
PSHELL  1       7       %x1%    7       1.0
PSHELL  2       7       %x2%    7       1.0
PSHELL  3       7       %x3%    7       1.0
PSHELL  4       7       %x4%    7       1.0
PSHELL  5       7       %x5%    7       1.0
PSHELL  6       7       %x6%    7       1.0
PSHELL  7       7       %x7%    7       1.0
PSHELL  8       7       %x8%    7
PSHELL  9       7       %x9%    7
PSHELL  10      7       %x10%   7
PSHELL  11      8       %x11%   8
RBE3    1501            1001    123456  1.0
        3646    2685    5709    2697    3819
```

1

2

Configure Parameters

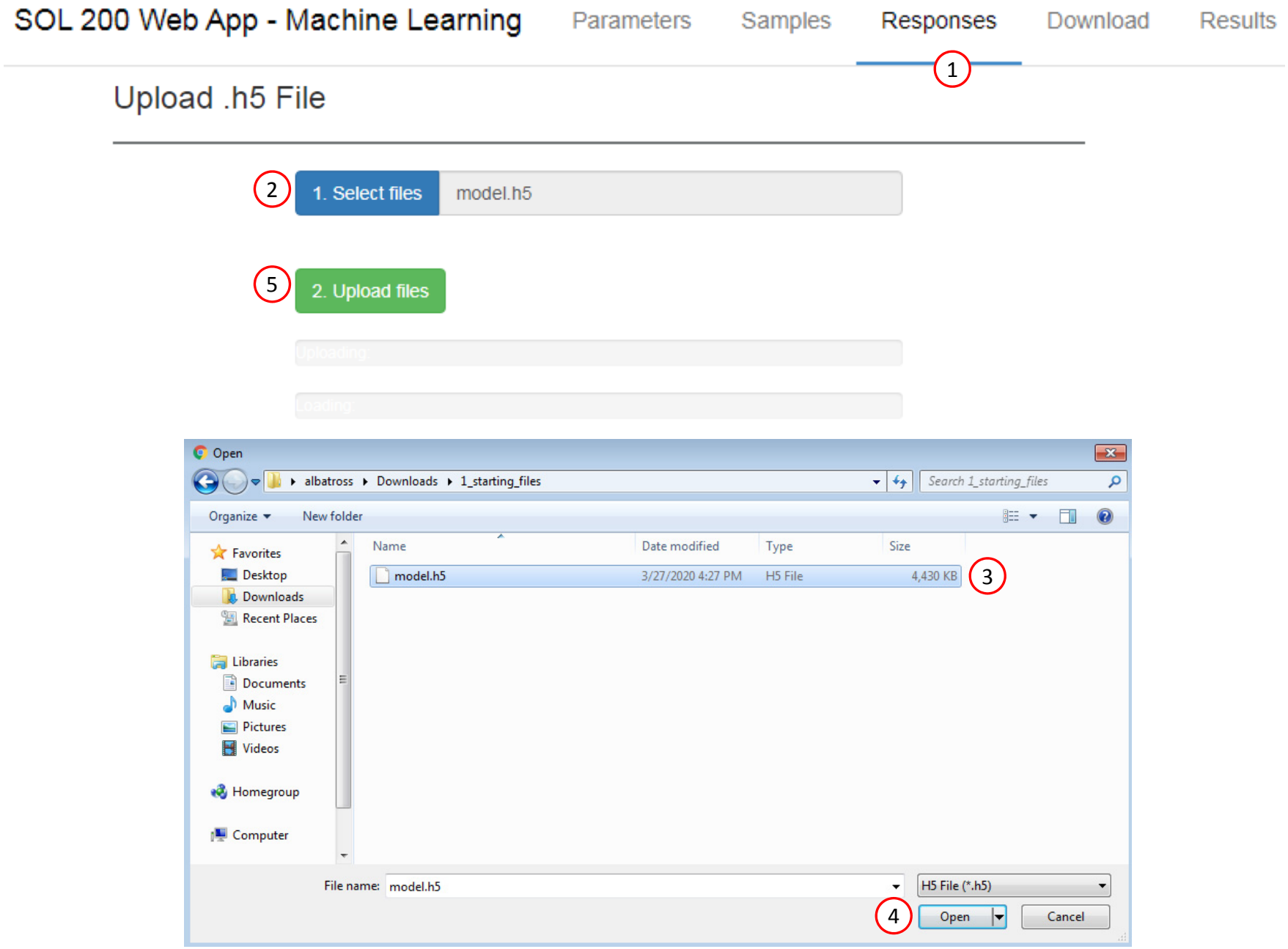
Delete	Parameter	Status	Low	High	Comments
✖	x1	✔	1.	6.	Field 4 of PSHELL
✖	x2	✔	1.	6.	Field 4 of PSHELL
✖	x3	✔	1.	6.	Field 4 of PSHELL
✖	x4	✔	1.	6.	Field 4 of PSHELL
✖	x5	✔	1.	6.	Field 4 of PSHELL
✖	x6	✔	1.	6.	Field 4 of PSHELL
✖	x7	✔	1.	6.	Field 4 of PSHELL
✖	x8	✔	1.	6.	Field 4 of PSHELL
✖	x9	✔	1.	6.	Field 4 of PSHELL
✖	x10	✔	1.	6.	Field 4 of PSHELL
✖	x11	✔	1.	6.	Field 4 of PSHELL

3

Responses

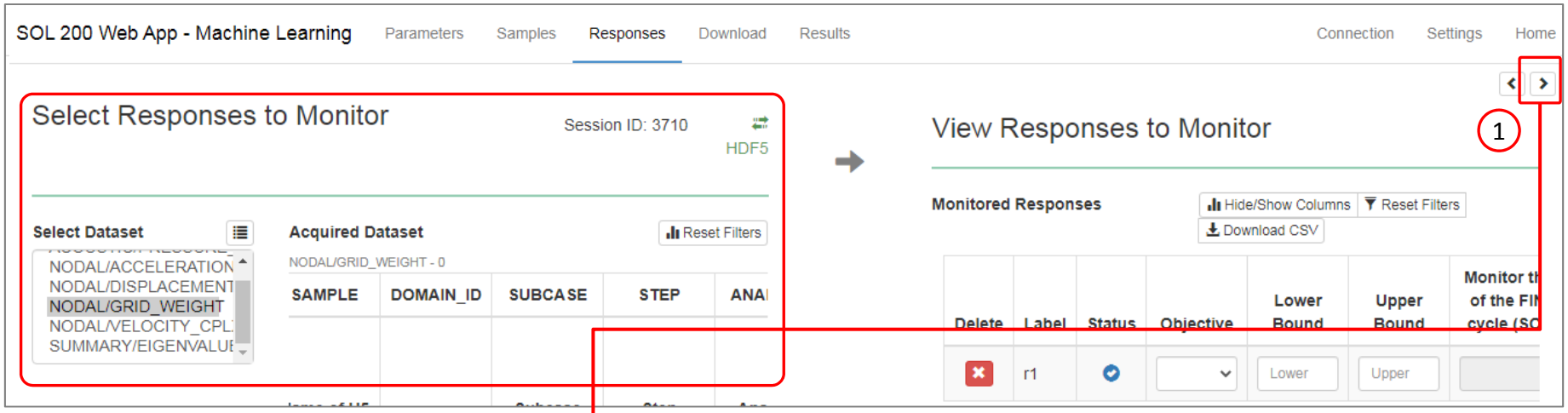
1. Click Responses
2. Click Select files
3. Select the indicated file
4. Click Open
5. Click Upload files

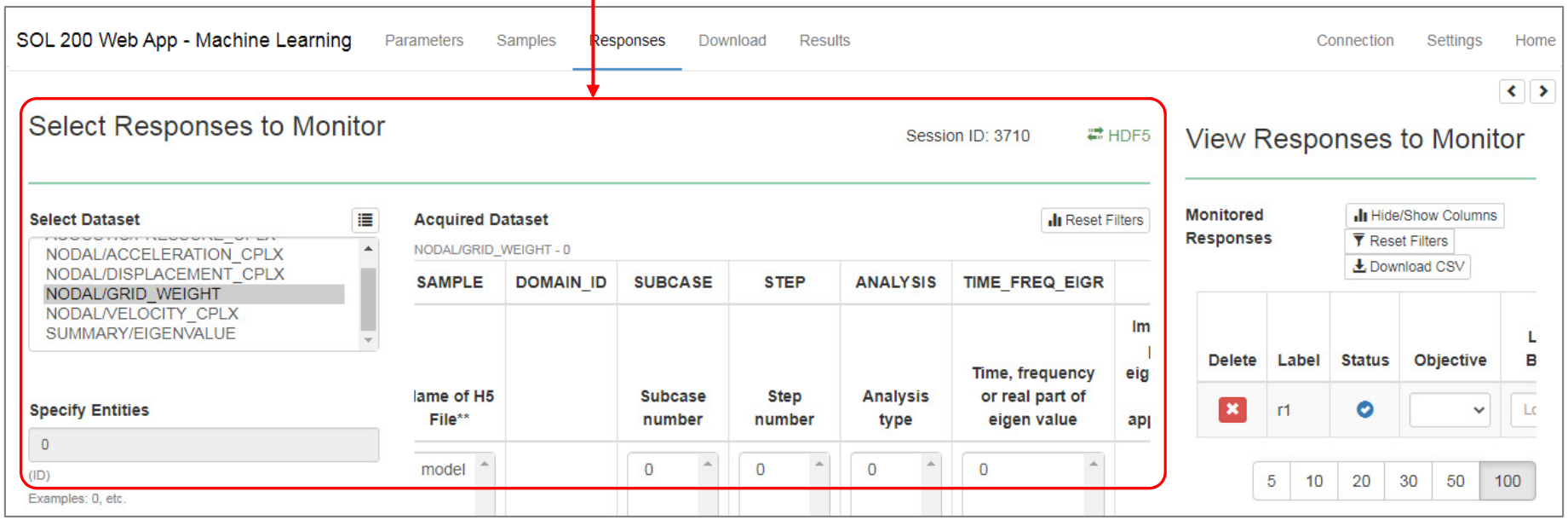
- On this page, the H5 file is uploaded to the web app.



Adjust the Column Width

1. Optional - Use at your liking the buttons at the top right hand corner to adjust the width of the left and right columns

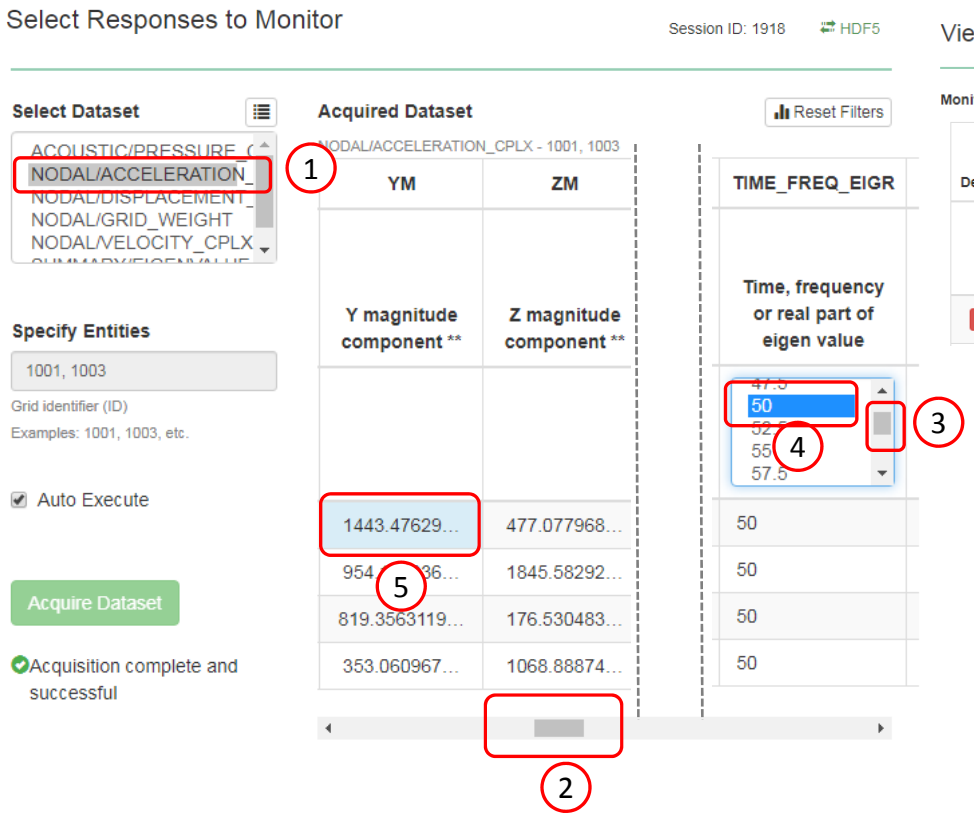


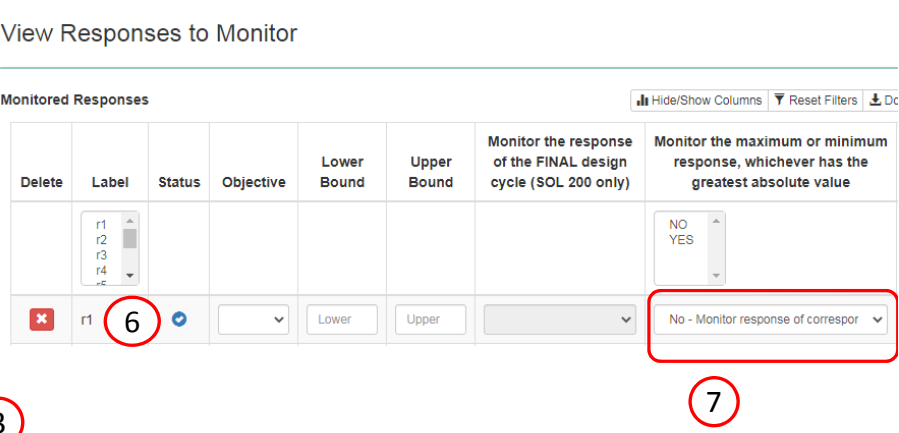


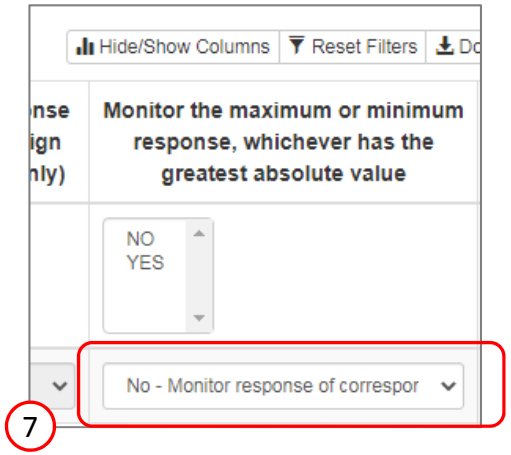
Select Responses

1. Select the following dataset: NODAL/ACCELERATION_CPLX
2. Use the horizontal scroll bar until the column TIME_FREQ_EIGR is visible
3. Use the vertical scroll bar until the value 50 is visible
4. Select the value 50 to only display rows that correspond to 50 Hz
5. Search for the column YM and click the indicated cell
6. A new response r1 is created
7. Set the following option:
   - Monitor the maximum or minimum response, whichever has the greatest absolute value […] response : No

- The responses defined in this tutorial correspond to points on frequency response plots
- Refer to the Appendix for an explanation on the use of the following:
  - Use MAX absolute value of response: Yes, No or blank



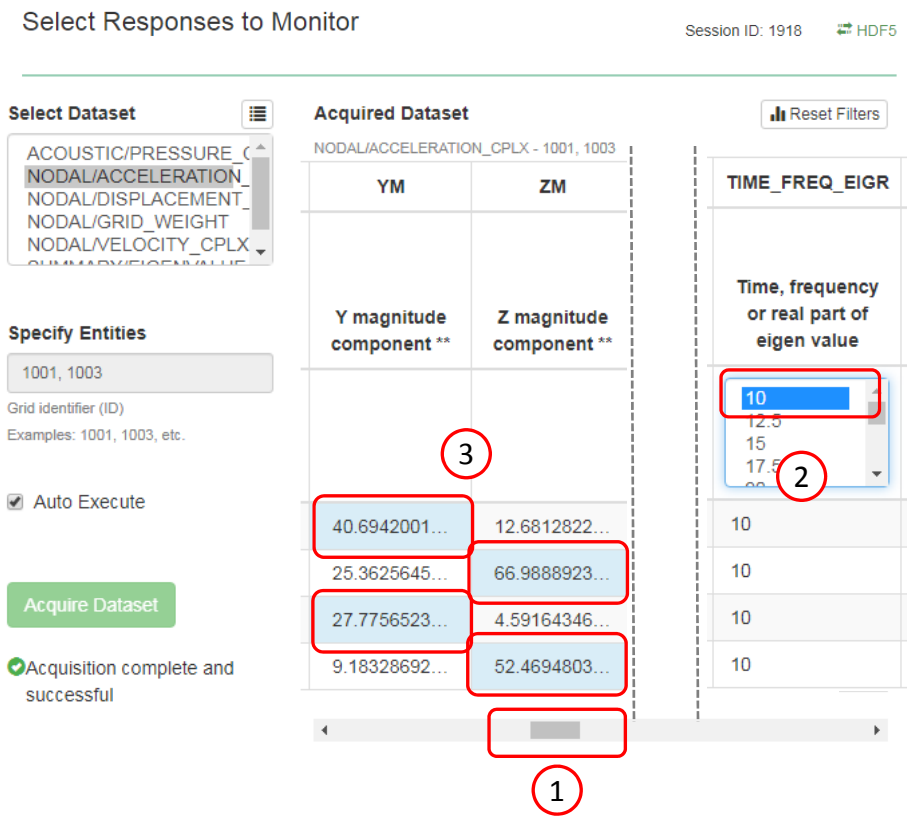


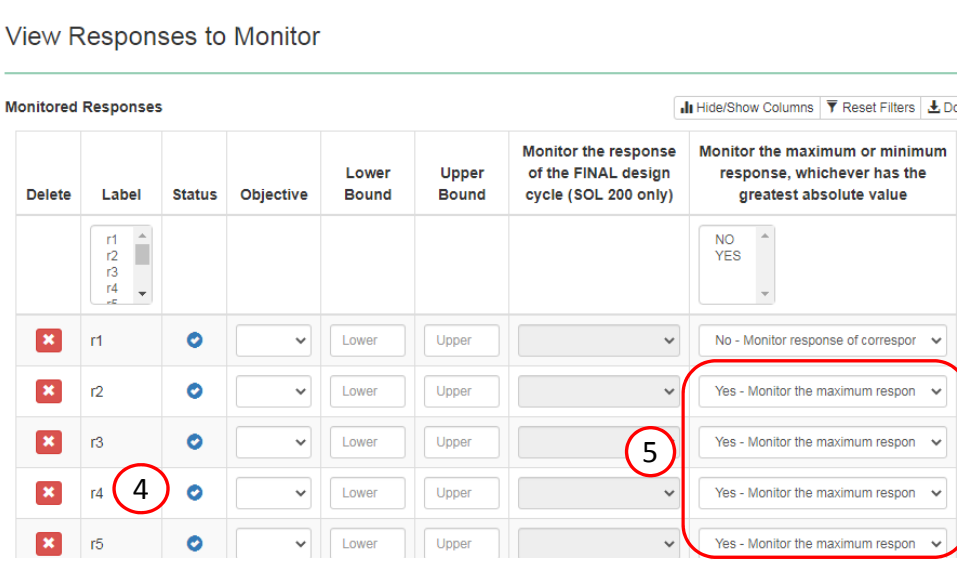


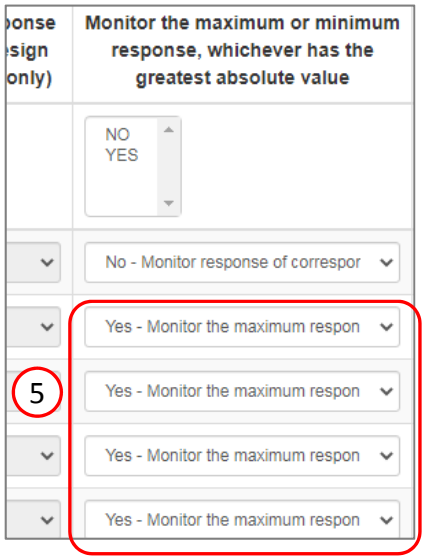
Select Responses

1. Use the horizontal scroll bar until the column TIME_FREQ_EIGR is visible
2. Select the value 10 to only display rows that correspond to 10 Hz
3. Search for the column YM and click the 4 indicated cells
4. Four (4) new response r2, r3, r4 and r5 have been created
5. Set the following option for these 4 new responses:
   - Monitor the maximum or minimum response, whichever has the greatest absolute value […] response : Yes

- The responses defined in this tutorial correspond to points on frequency response plots
- Refer to the Appendix for an explanation on the use of the following:
  - Use MAX absolute value of response: Yes, No or blank



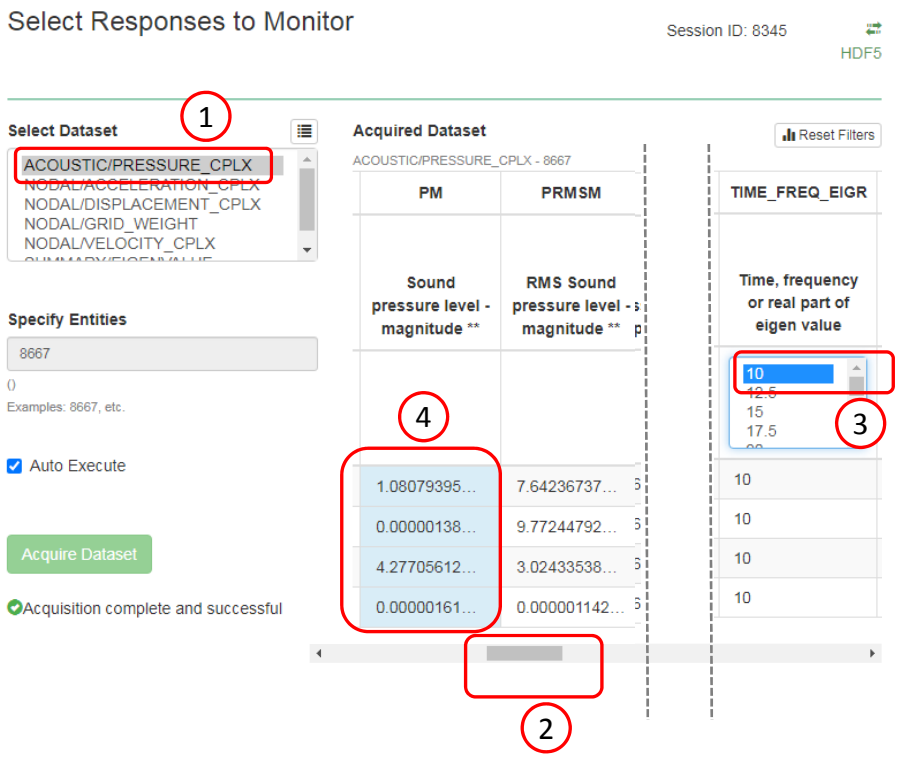


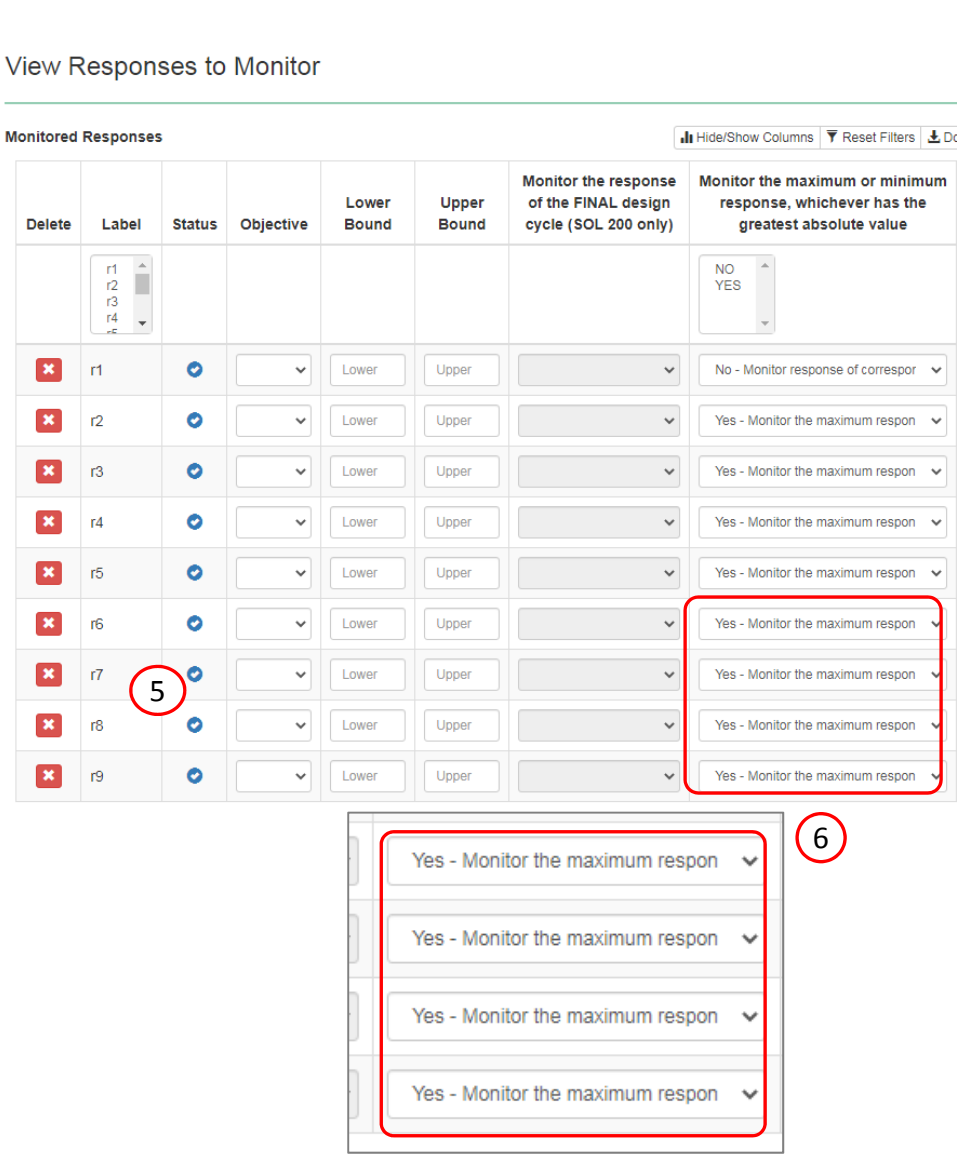


Select Responses

1. Select the following dataset: ACOUSTIC/PRESSURE_CPLX
2. Use the horizontal scroll bar until the column TIME_FREQ_EIGR is visible
3. Select the value 10 to only display rows that correspond to 10 Hz
4. Search for the column PM and click the 4 indicated cells
5. Four (4) new response r6, r7, r8 and r9 have been created
6. Set the following option for these 4 new responses:
   - Monitor the maximum or minimum response, whichever has the greatest absolute value [...] response: Yes

- The responses defined in this tutorial correspond to points on frequency response plots
- Refer to the Appendix for an explanation on the use of the following:
  - Monitor the maximum or minimum response, whichever has the greatest absolute value : Yes, No or blank

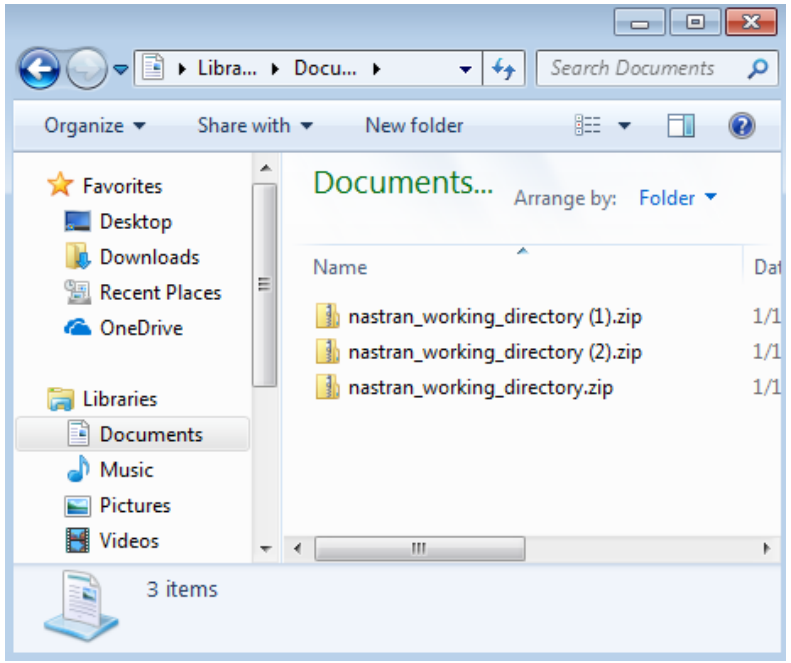




Configuring Multiple Batch Runs

Samples

In the following slides, we will configure 3 batches to run.

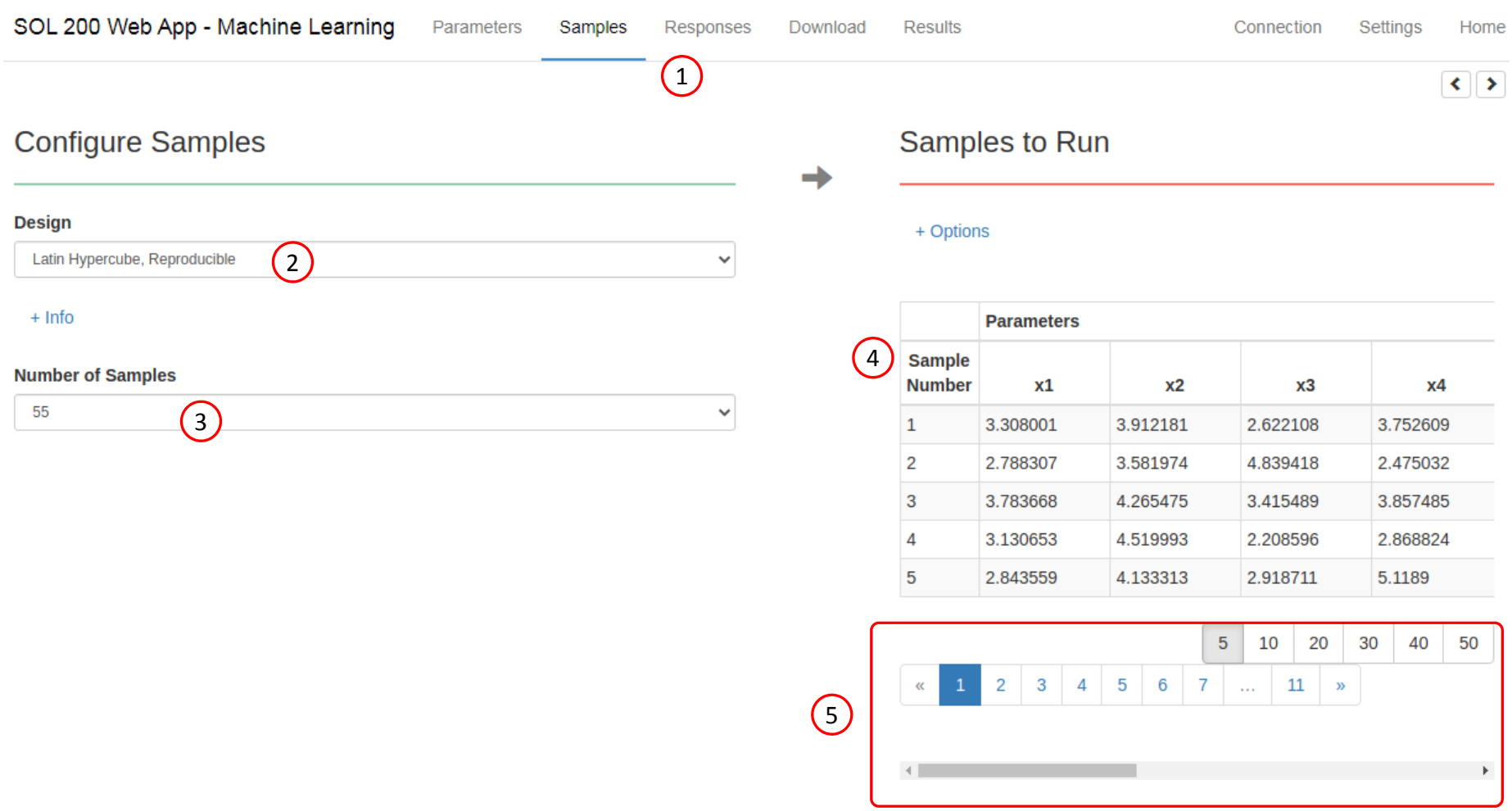


Batch	File Name	Number of Runs	Number of Parameters	Purpose
1	nastran_working_directory.zip	55	11	This configuration includes 11 parameters. The goal is to use the data from the 55 run set to screen parameters and reduce the problem to 4 parameters. Automatic relevance determination (ARD) is used to identify the 4 most relevant parameters.
2	nastran_working_directory (1).zip	40	4	This configuration includes 4 parameters. The goal of this 40 run set is to produce training data to fit the surrogate model and make predictions.
3	nastran_working_directory (2).zip	8	4	This is an 8 run configuration. This set is used to compare the predicted responses with MSC Nastran responses.

Samples

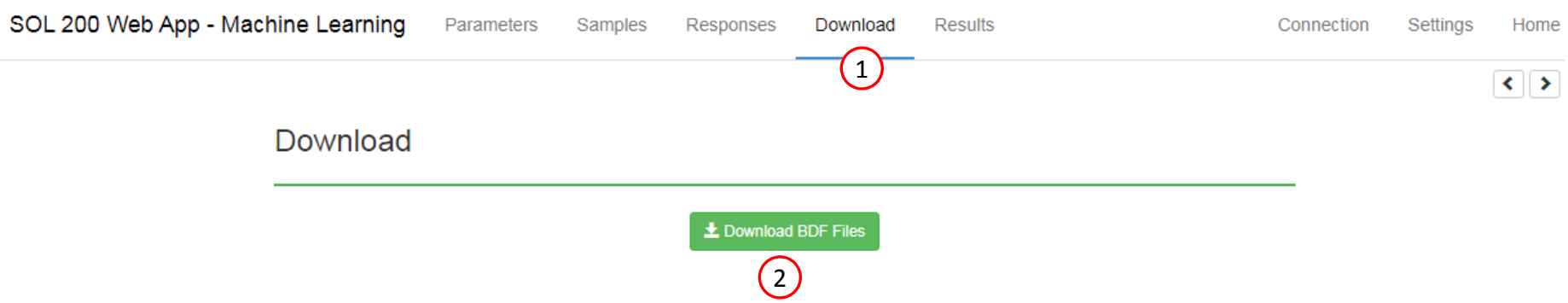
1. Click Samples
2. Ensure the following design is selected: Latin Hypercube, Reproducible
3. Set Number of Samples to 55
4. The samples have been updated, note that samples 1, 2, 3, …, 55 are visible
5. The indicated controls can be used to display the other samples

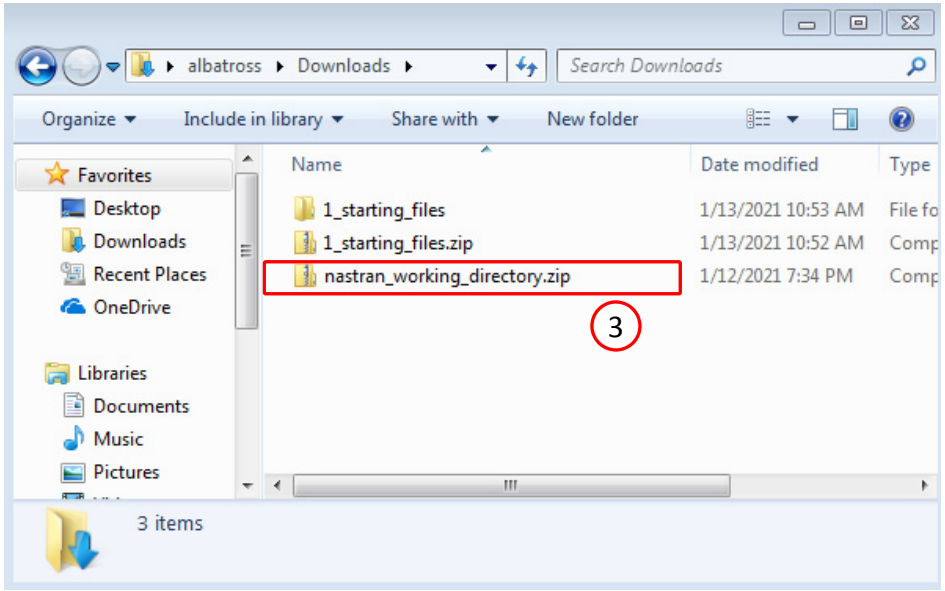
- An initial 55 MSC Nastran runs will be executed to generate training data. The training data will be used for parameter/variable screening, via ARD, to reduce the dimensionality of the problem from 11 to 4 parameters.
- For parameter screening purposes, 5 runs per parameter are used. Since there are 11 parameters configured, a total of 55 MSC Nastran runs have been configured for later execution.
- Later on, when the goal is to fit the surrogate model for prediction purposes, 10 runs per parameter is used.



Download

1. Click Download
2. Click Download BDF Files
3. A new ZIP file has been downloaded





Parameters

1. Click Parameters
2. Deselect the following fields to delete parameters: x3, x4, x5, x6, x7, x9, x10
3. The following 4 parameters should remain: x1, x2, x8, x11

- In a later part of this tutorial, it is described how automatic relevance determination (ARD) is used to reduce the problem from 11 to those 4 parameters.

SOL 200 Web App - Machine Learning | Parameters | Samples | Responses | Download | Results | Connection | Settings | Home

1

Select Parameters

```
$__1___||__2___||__3___||__4___||__5___||__6___||__7___||__8___||__9___||__10__|


EIGRL   1               225.
EIGRL   2               300.
FORCE   212     1001            500.    0.0     1.0     0.0
FORCE   213     1001            1000.   0.0     0.0     1.0
FORCE   232     1003            500.    0.0     1.0     0.0
FORCE   233     1003            1000.   0.0     0.0     1.0
FREQ1   5       10.     2.5     56
MAT1    7       210000.0        0.3     7.90E-06
MAT1    8       62000.0         0.24    2.30E-06
MAT10   6               1.23E-12340000.0
PARAM   G       0.06
PARAM   GFL     0.12
PARAM   LFREQ   0.1
PARAM   PREFDB  2.E-11
PARAM   WTMASS  .001
PSHELL  1       7       %x1%    7       1.0             0.833333
PSHELL  2       7       %x2%    7       1.0             0.833333
PSHELL  3       7       1.905   7       1.0             0.833333
PSHELL  4       7       1.27    7       1.0             0.833333
PSHELL  5       7       6.35    7       1.0             0.833333
PSHELL  6       7       3.81    7       1.0             0.833333
PSHELL  7       7       2.54    7       1.0             0.833333
PSHELL  8       7       %x8%    7               7
PSHELL  9       7       3.0     7               7
PSHELL  10      7       5.0     7               7
PSHELL  11      8       %x11%   8               8
RBE3    1501            1001    123456  1.0     123     7047    263
```

2

Configure Parameters

3

Delete	Parameter	Status	Low	High	Comments
✖	x1	✔	1.	6.	Field 4 of PSHEL
✖	x2	✔	1.	6.	Field 4 of PSHEL
✖	x8	✔	1.	6.	Field 4 of PSHEL
✖	x11	✔	1.	6.	Field 4 of PSHEL

Samples

1. Click Samples
2. Set the Design as Latin Hypercube, Reproducible
3. Set the Number of Samples as 40
4. The table now has 40 samples

SOL 200 Web App - Machine Learning | Parameters | Samples | Responses | Download | Results | Connection | Settings | Home

1

Configure Samples

Design

Latin Hypercube, Reproducible 2

+ Info

Number of Samples

40 3

Samples to Run

+ Options

4

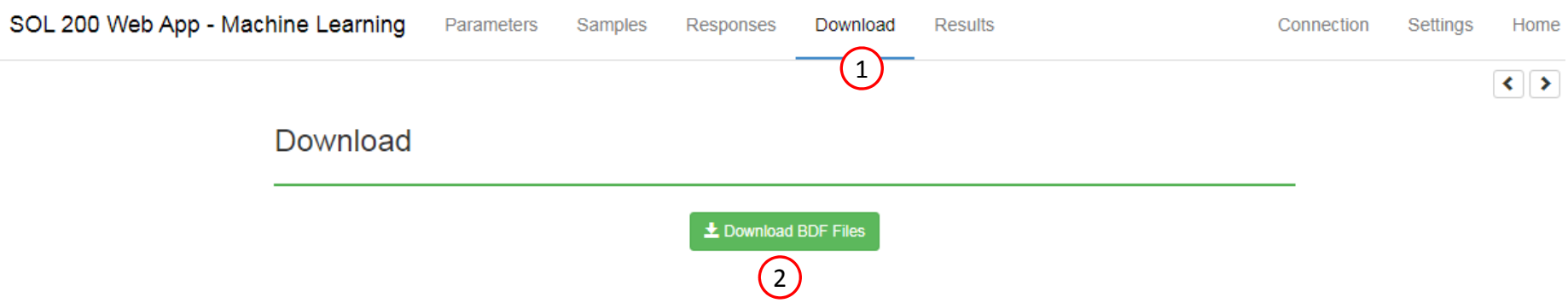
	Parameters			
Sample Number	**x1**	**x2**	**x8**	**x11**
1	1.	4.333333	3.051282	4.717949
2	1.128205	2.538462	3.435897	3.051282
3	1.25641	4.076923	5.102564	1.897436
4	1.384615	5.102564	2.794872	2.282051
5	1.512821	2.025641	3.692308	5.487179

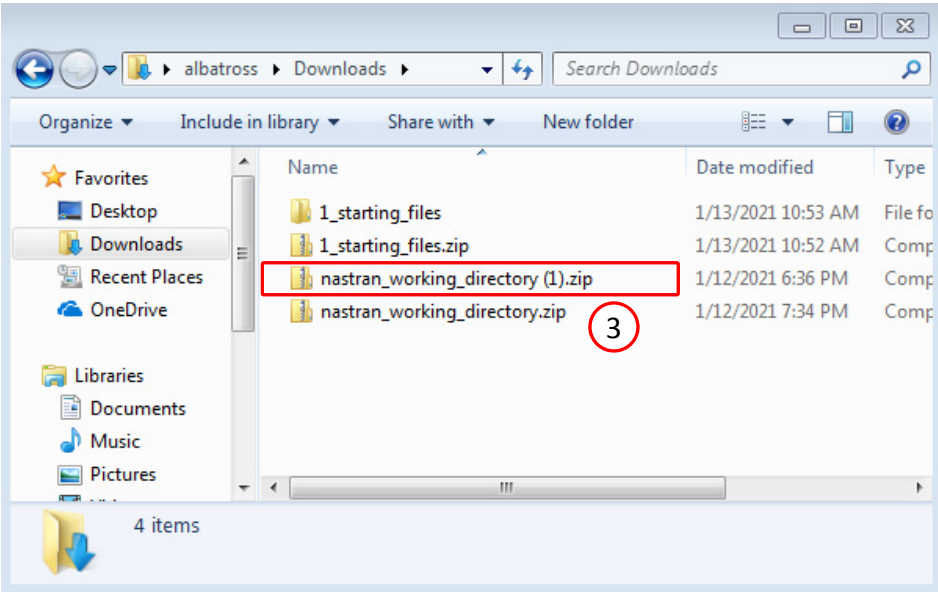
5 10 20 30 40 50

« 1 2 3 4 5 6 7 8 »

Download

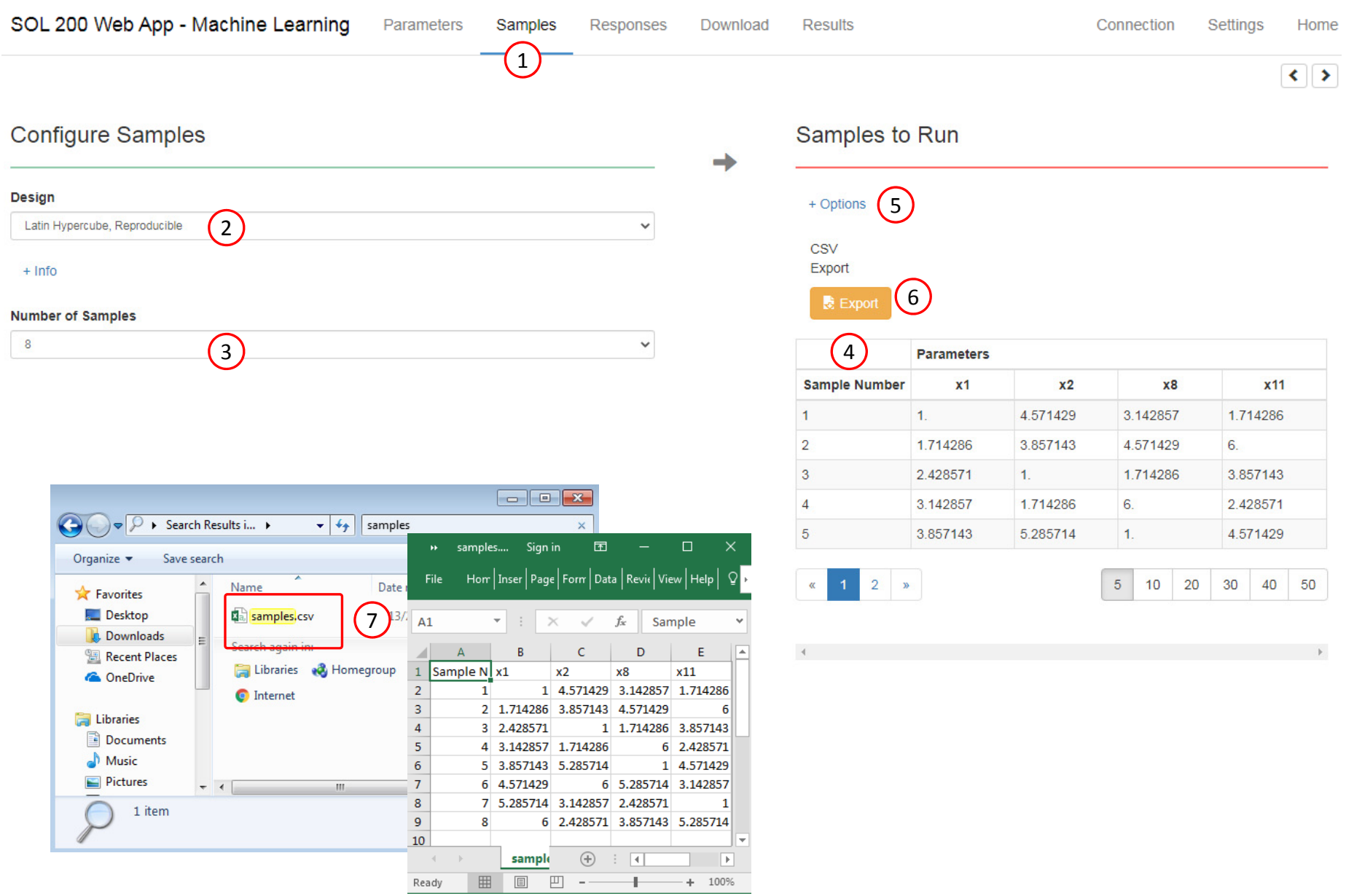
1. Click Download
2. Click Download BDF Files
3. A new ZIP file has been downloaded





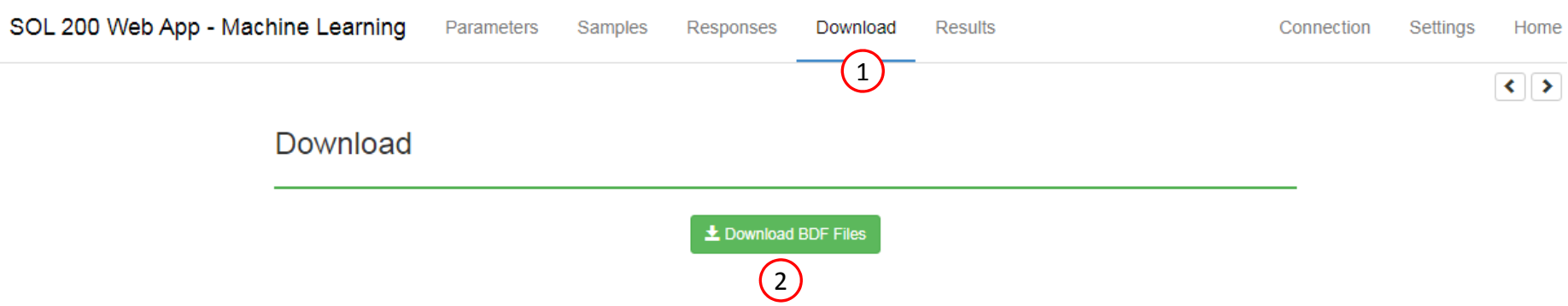
Samples

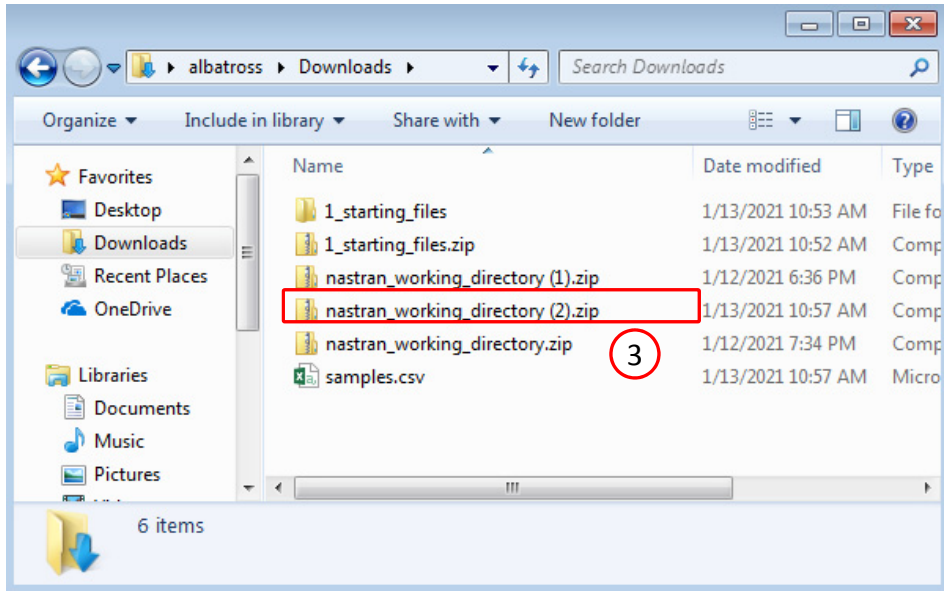
1. Click Samples
2. Set the Design as Latin Hypercube, Reproducible
3. Set the Number of Samples as 8
4. The table now has 8 samples
5. Click +Options
6. Click Export
7. A CSV file has been downloaded and contains the values from the table with 8 samples



Download

1. Click Download
2. Click Download BDF Files
3. A new ZIP file has been downloaded

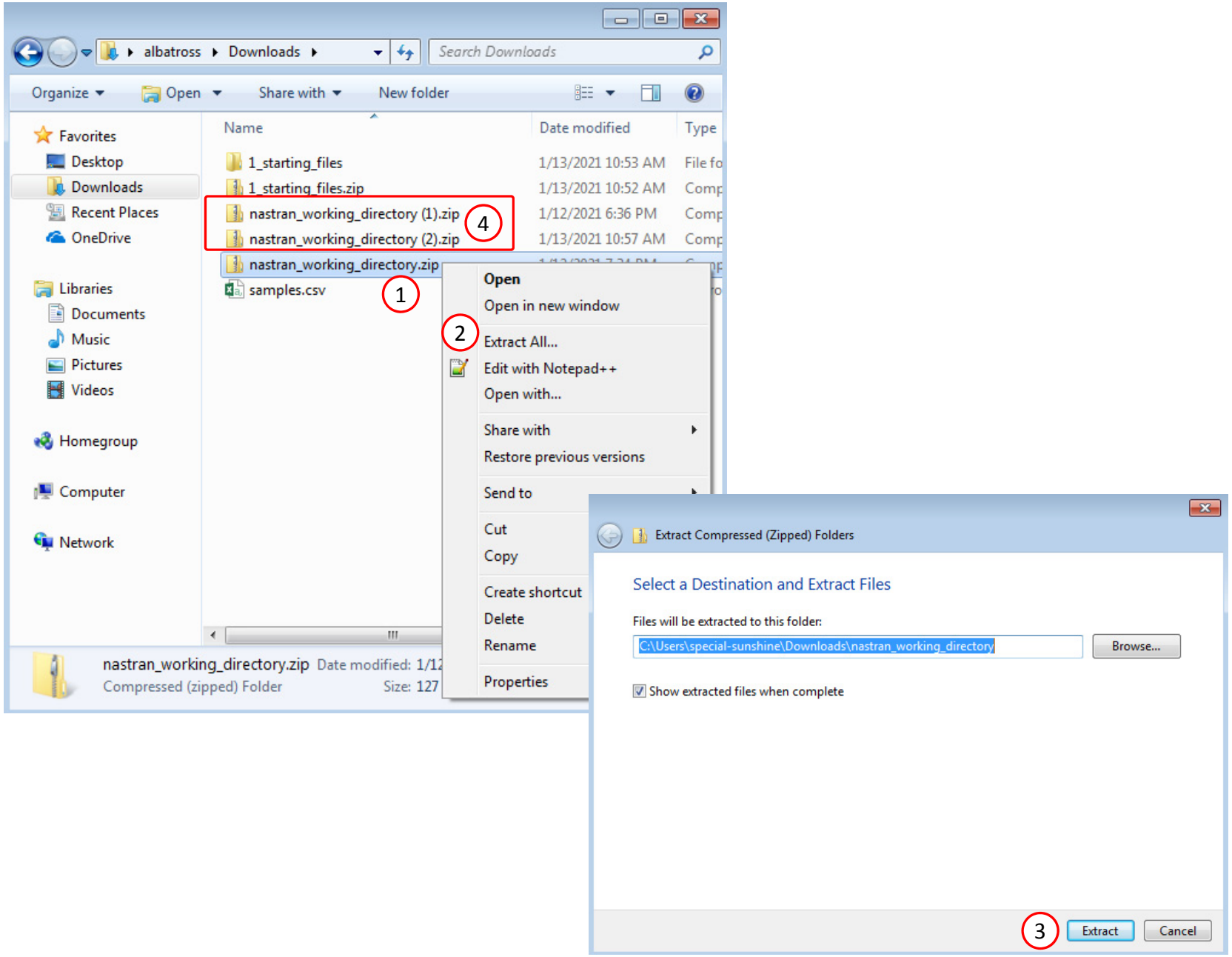




Start Desktop App

1. Right click on the indicated file
2. Click Extract All
3. Click Extract on the following window
4. Repeat steps 1-3 for the indicated files

- Always extract the contents of the ZIP file to a new, empty folder.



Start Desktop App

1. Open this folder: nastran_working_directory
2. Inside of the new folder, double click on Start Desktop App
3. Click Open, Run or Allow Access on any subsequent windows
4. MSC Nastran will now start

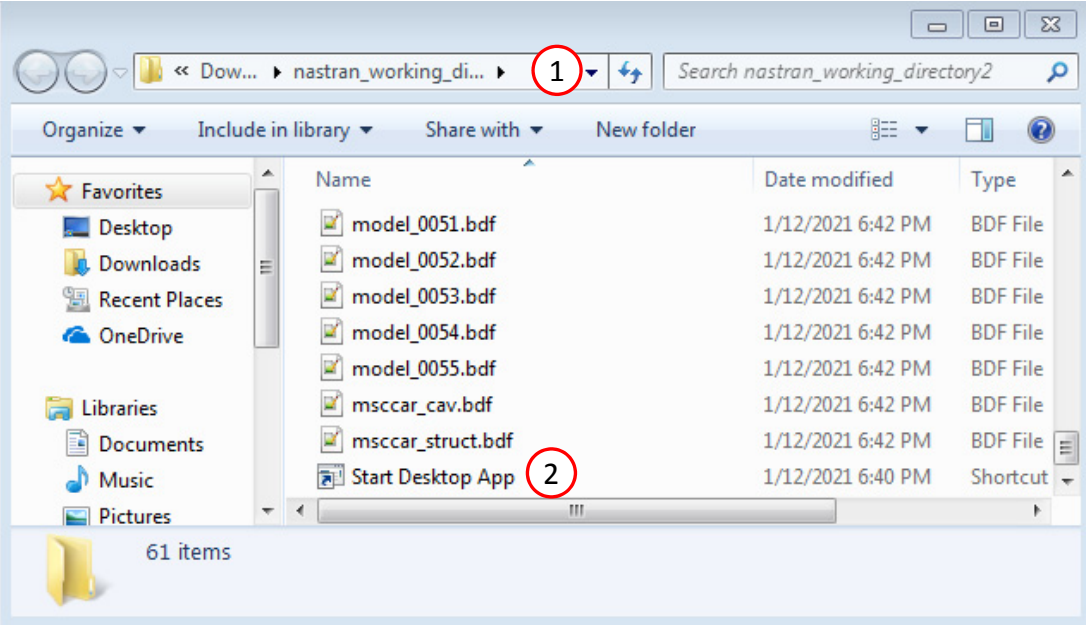
- One can run the Nastran job on a remote machine as follows:
  1) Copy the BDF files and the INCLUDE files to a remote machine. 2) Run the MSC Nastran job on the remote machine. 3) After completion, copy the BDF, F06, LOG, H5 files to the local machine. 4) Click "Start Desktop App" to display the results.

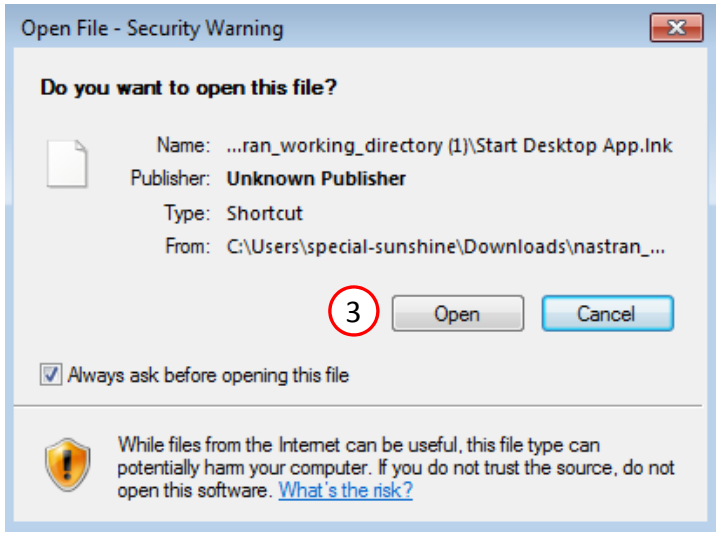
Using Linux?

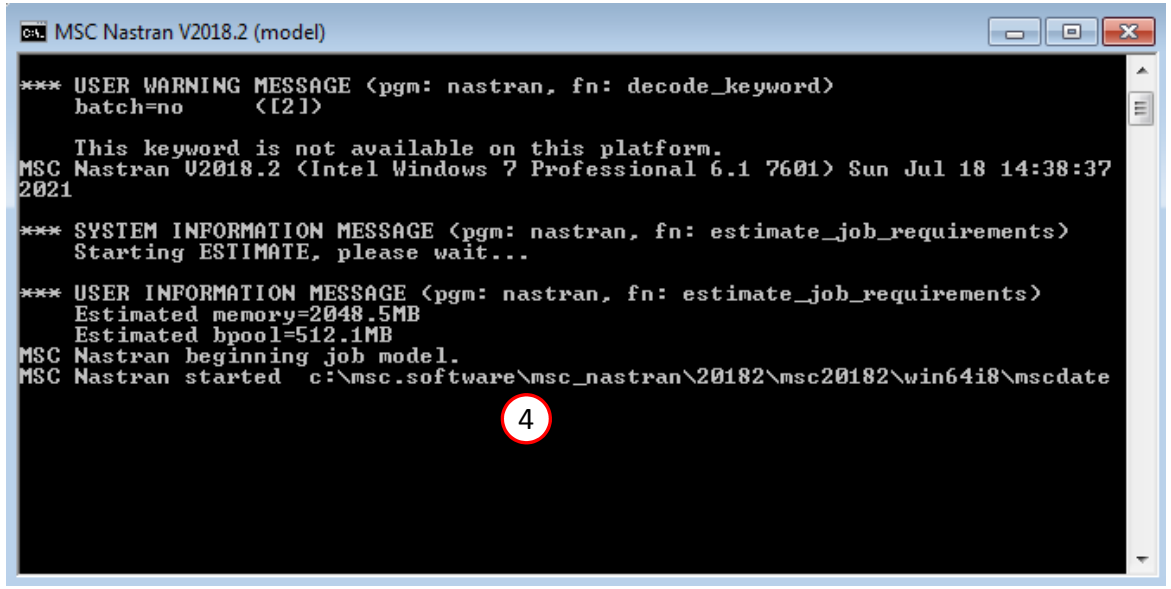
Follow these instructions:
1) Open Terminal
2) Navigate to the nastran_working_directory
   cd ./nastran_working_directory
3) Use this command to start the process
   ./Start_MSC_Nastran.sh

In some instances, execute permission must be granted to the directory. Use this command. This command assumes you are one folder level up.

sudo chmod -R u+x ./nastran_working_directory







Status

- While MSC Nastran is running, a status page will show the current state of MSC Nastran

SOL 200 Web App - Status

Python MSC Nastran

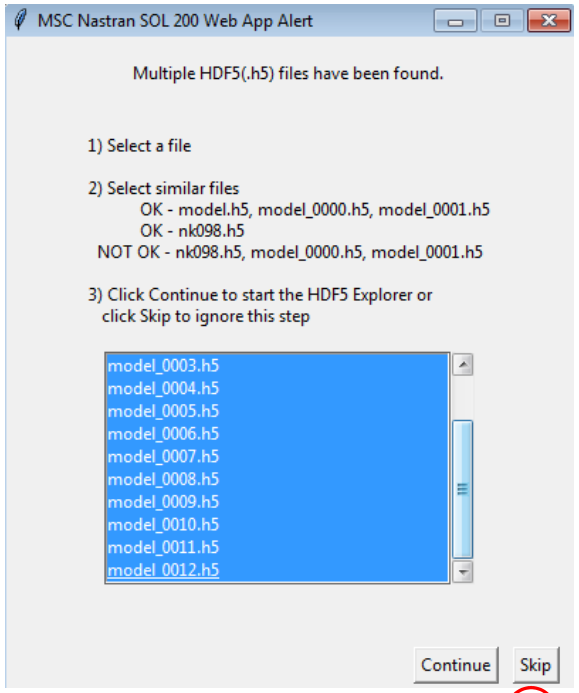
Status

Name	Status of Job	Design Cycle	RUN TERMINATED DUE TO
model.bdf	Running	None	

Review Results

1. A window appears asking to start the HDF5 Explorer
2. Click Skip to not open the HDF5 Explorer

1



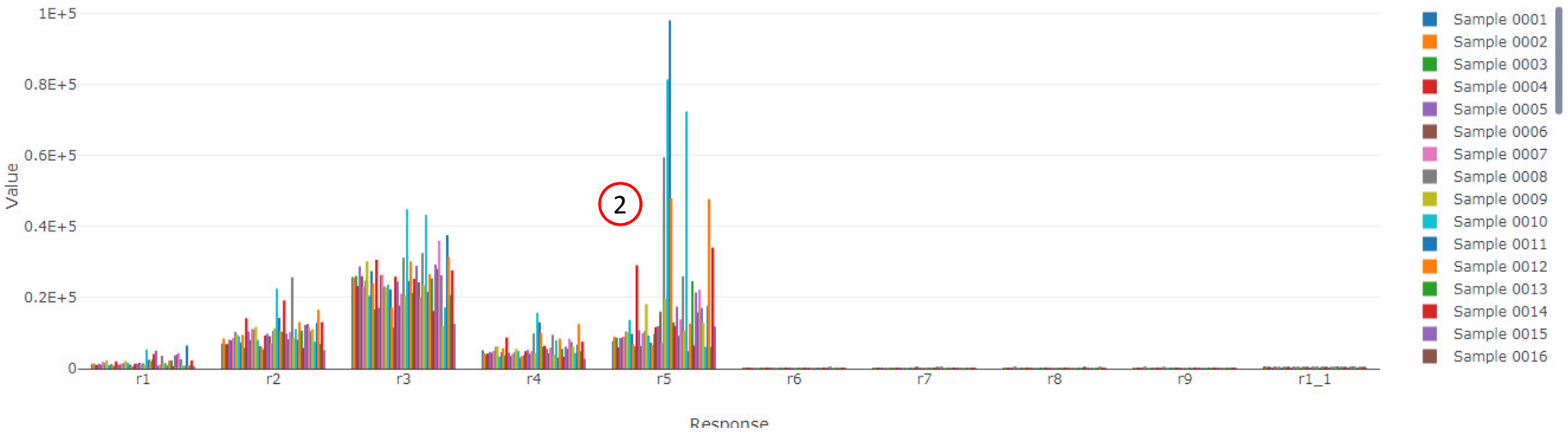
2

Review Results

1. The Monitored Responses web app is opened
2. The value of each response and for each sample is displayed in a bar chart
3. A table lists the values for each response and sample.

A. The table titled Monitored Response can be interacted with. Each column in the table contains filters. Once a filter is modified, the Bar Chart will instantly update.
B. Additional functions include the ability to highlight the MAX and MIN bars, download a CSV file and reset the filters.

SOL 200 Web App - Monitored Responses (1) Home



Monitored Responses (A) (B) Display MAX and MIN | Download CSV | Reset Filters

Label	Dataset Name	Field	Field Description
r1 r1_1 r1_2 r1_3	ACOUSTIC/PRESSURE_CPLX NODAL/ACCELERATION_CPLX	DBM YM ZM	Sound pressure level in dB - magnit Y magnitude component ** Z magnitude component **
r1	NODAL/ACCELERATION_CPLX	YM	Y magnitude component **
r2	NODAL/ACCELERATION_CPLX	YM	Y magnitude component **
r3	NODAL/ACCELERATION_CPLX	ZM	Z magnitude component **
r4	NODAL/ACCELERATION_CPLX	YM	Y magnitude component **
r5	NODAL/ACCELERATION_CPLX	ZM	Z magnitude component **

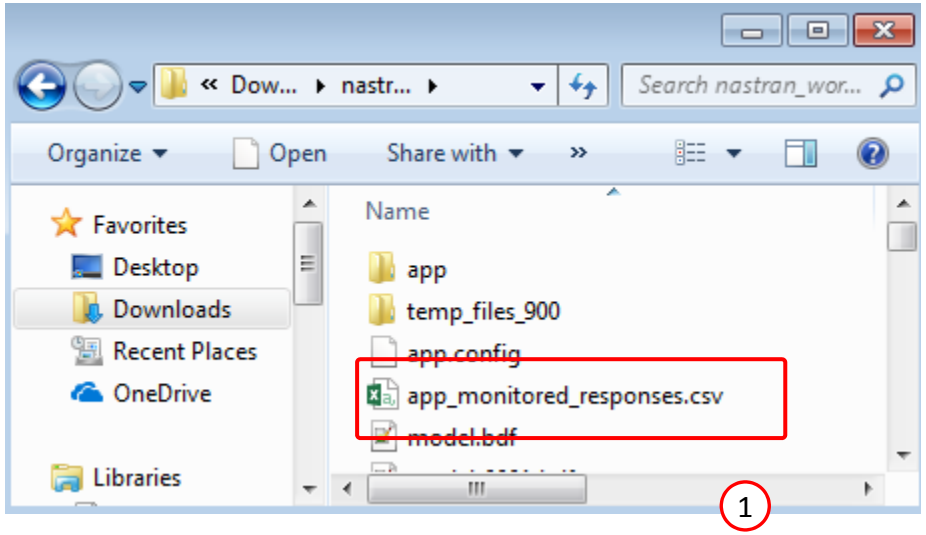
Monitored Responses from Each Sample (3)

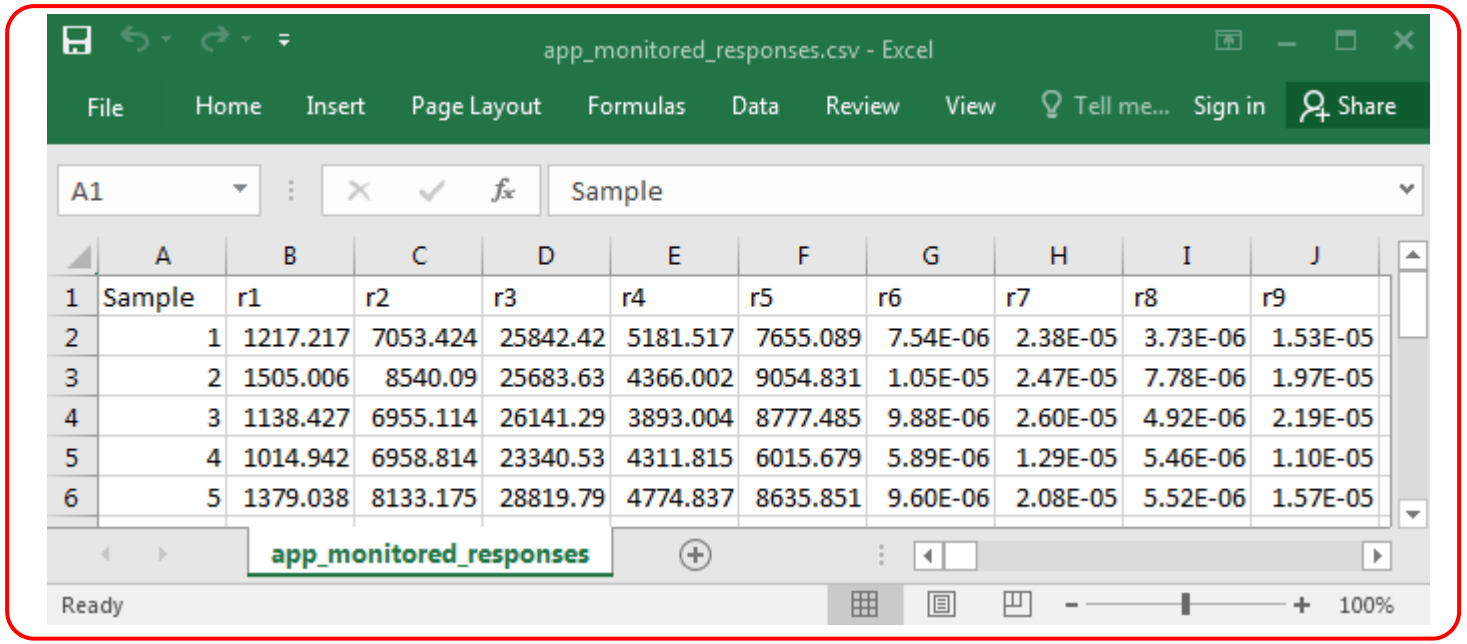
0001	0002	0003	0004	
1217.2174281739094	1505.0063820207042	1138.4266356161363	1014.9415601970021	13
7053.423907396364	8540.089784757196	6955.113624520879	6958.81401718346	81
25842.419807507038	25683.634954437166	26141.29227999461	23340.53010843421	28
5181.517140493611	4366.0019120235875	3893.0039254598646	4311.814597794899	47
7655.088567255526	9054.831254535718	8777.484906180196	6015.679440337792	86

Review Results

1. The monitored responses are contained in the CSV file named app_monitored_responses.csv

The responses in this CSV file will be use to train the surrogate model.

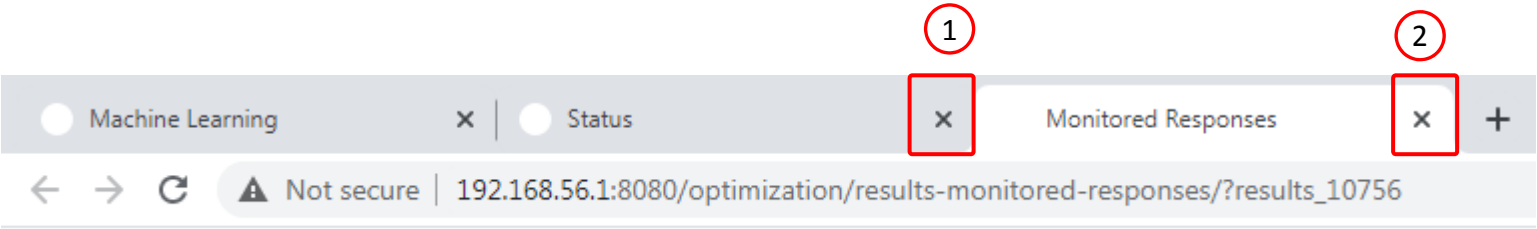




	A	B	C	D	E	F	G	H	I	J
1	Sample	r1	r2	r3	r4	r5	r6	r7	r8	r9
2	1	1217.217	7053.424	25842.42	5181.517	7655.089	7.54E-06	2.38E-05	3.73E-06	1.53E-05
3	2	1505.006	8540.09	25683.63	4366.002	9054.831	1.05E-05	2.47E-05	7.78E-06	1.97E-05
4	3	1138.427	6955.114	26141.29	3893.004	8777.485	9.88E-06	2.60E-05	4.92E-06	2.19E-05
5	4	1014.942	6958.814	23340.53	4311.815	6015.679	5.89E-06	1.29E-05	5.46E-06	1.10E-05
6	5	1379.038	8133.175	28819.79	4774.837	8635.851	9.60E-06	2.08E-05	5.52E-06	1.57E-05

Close Pages

1. The Status page can be closed
2. The Monitored Responses page can be closed



Start Desktop App

1. Open this folder: nastran_working_directory (1)
2. Inside of the new folder, double click on Start Desktop App
3. Click Open, Run or Allow Access on any subsequent windows
4. MSC Nastran will now start

- One can run the Nastran job on a remote machine as follows:
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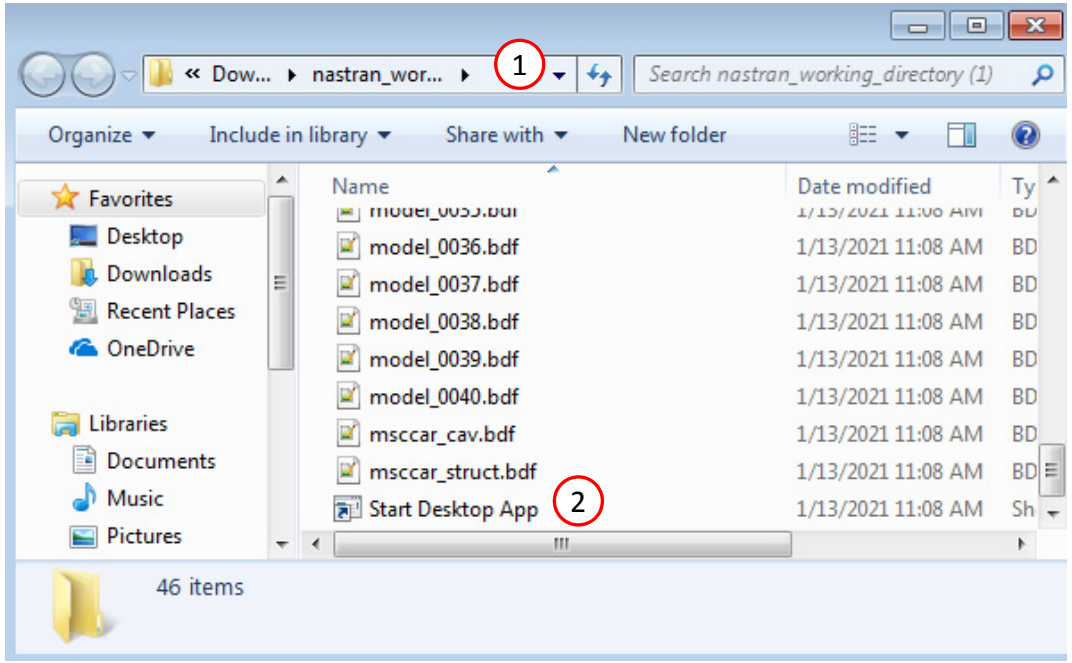
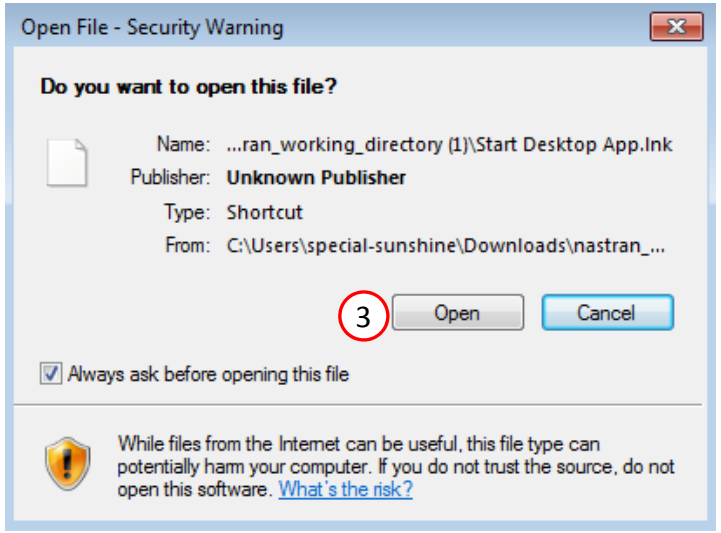
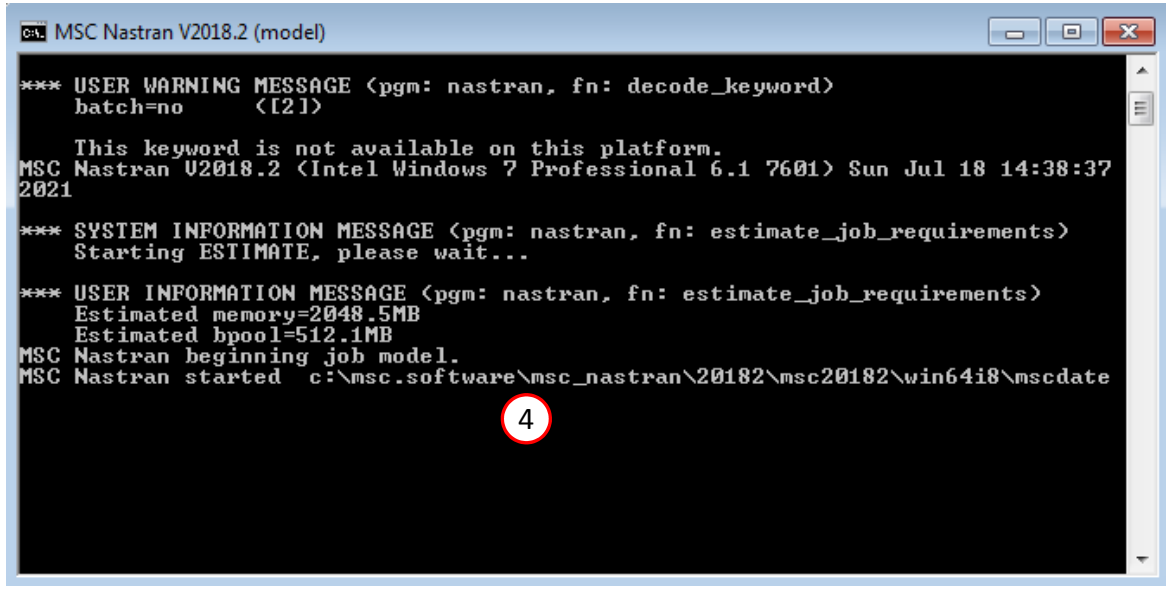
Follow these instructions:
1) Open Terminal
2) Navigate to the nastran_working_directory
   cd ./nastran_working_directory
3) Use this command to start the process
   ./Start_MSC_Nastran.sh

In some instances, execute permission must be granted to the directory. Use this command. This command assumes you are one folder level up.

sudo chmod -R u+x ./nastran_working_directory







Status

- While MSC Nastran is running, a status page will show the current state of MSC Nastran

SOL 200 Web App - Status

Python MSC Nastran

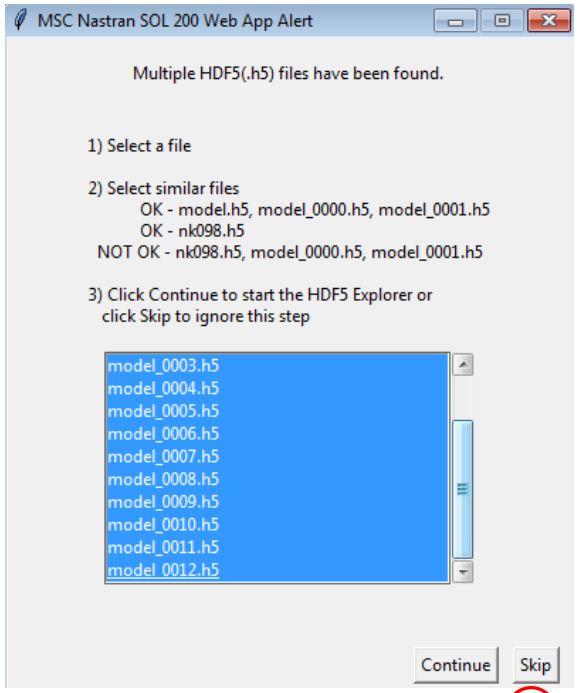
Status

Name	Status of Job	Design Cycle	RUN TERMINATED DUE TO
model.bdf	Running	None	

Review Results

1. A window appears asking to start the HDF5 Explorer
2. Click Skip to not open the HDF5 Explorer

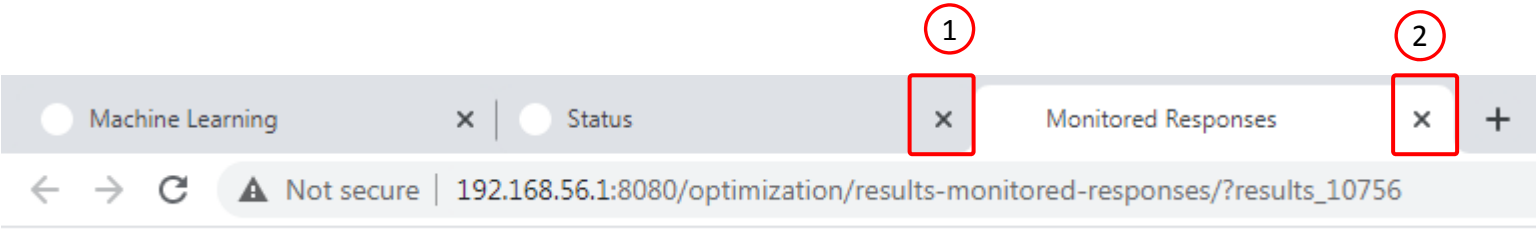
1



2

Close Pages

1. The Status page can be closed
2. The Monitored Responses page can be closed



Start Desktop App

1. Open this folder: nastran_working_directory (2)
2. Inside of the new folder, double click on Start Desktop App
3. Click Open, Run or Allow Access on any subsequent windows
4. MSC Nastran will now start

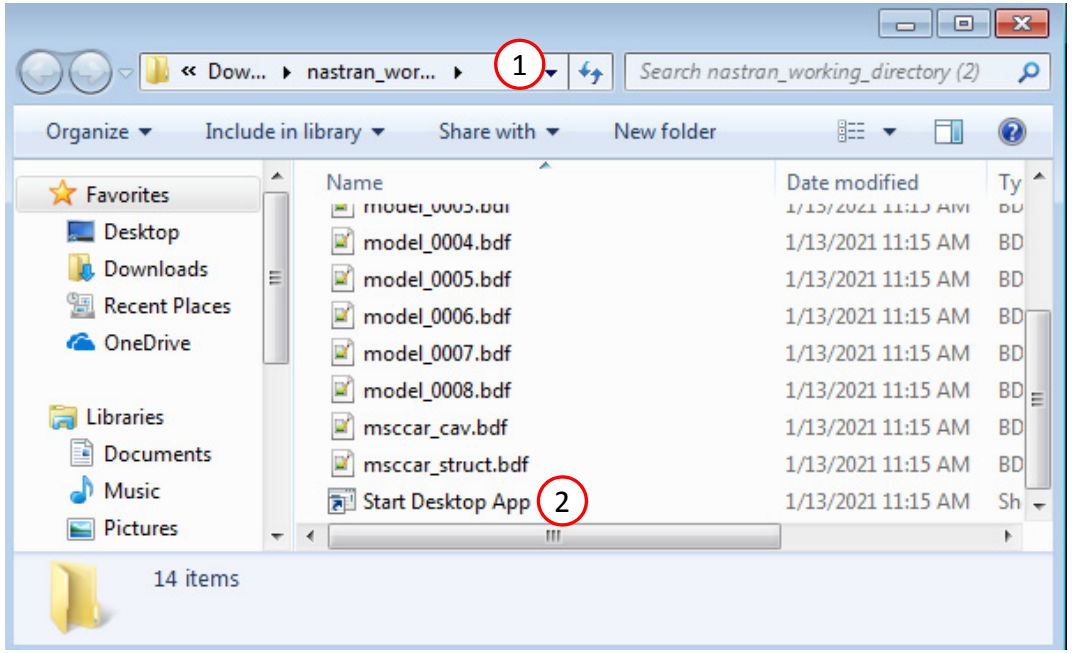
- One can run the Nastran job on a remote machine as follows:
  1) Copy the BDF files and the INCLUDE files to a remote machine. 2) Run the MSC Nastran job on the remote machine. 3) After completion, copy the BDF, F06, LOG, H5 files to the local machine. 4) Click "Start Desktop App" to display the results.

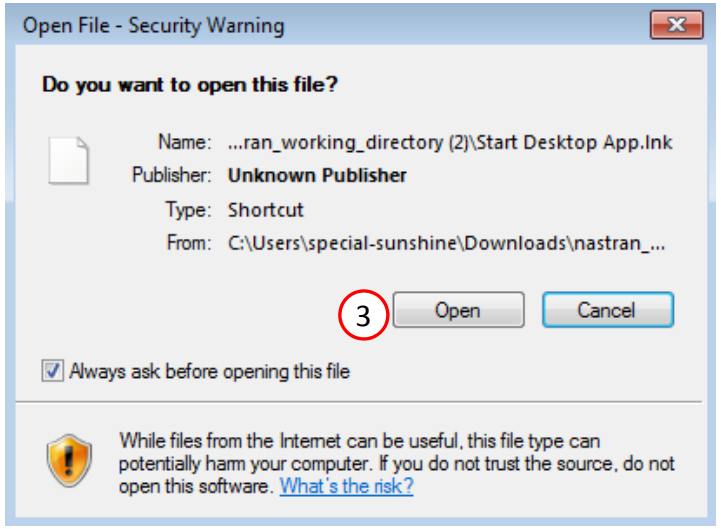
Using Linux?

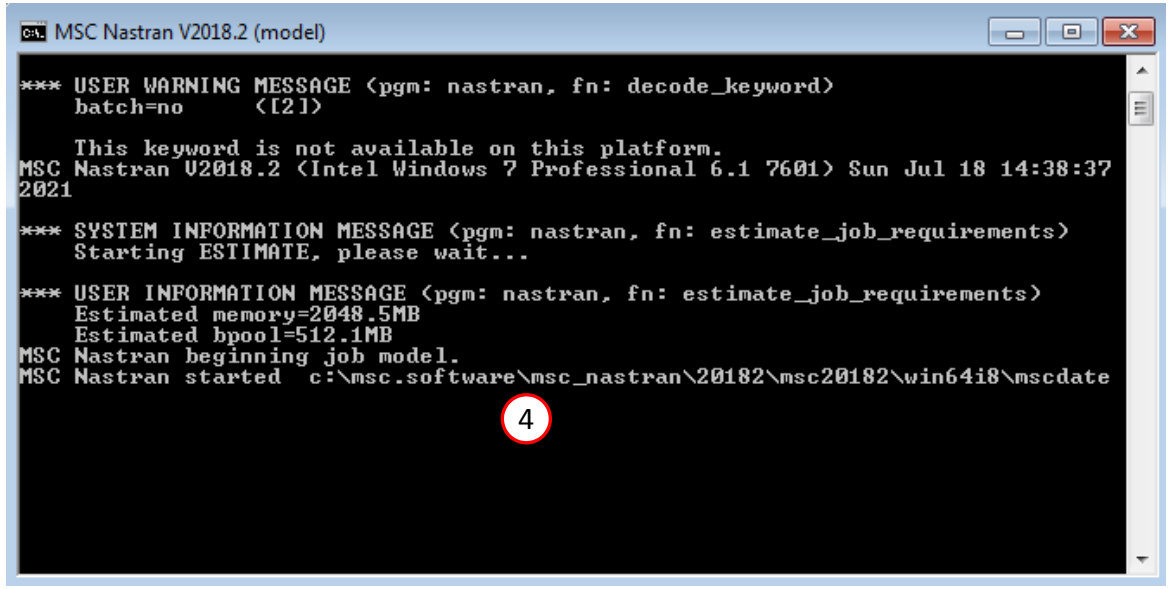
Follow these instructions:
1) Open Terminal
2) Navigate to the nastran_working_directory
   cd ./nastran_working_directory
3) Use this command to start the process
   ./Start_MSC_Nastran.sh

In some instances, execute permission must be granted to the directory. Use this command. This command assumes you are one folder level up.

sudo chmod -R u+x ./nastran_working_directory







Status

- While MSC Nastran is running, a status page will show the current state of MSC Nastran

SOL 200 Web App - Status

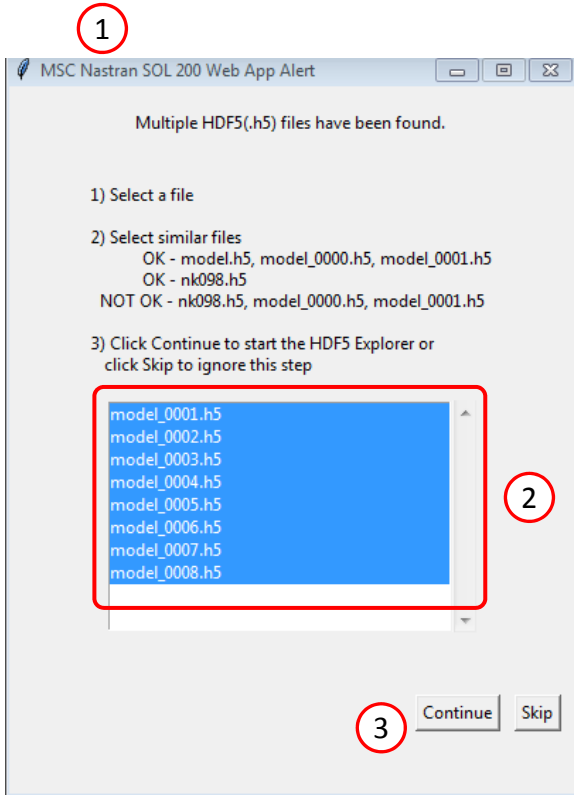
Python MSC Nastran

Status

Name	Status of Job	Design Cycle	RUN TERMINATED DUE TO
model.bdf	Running	None	

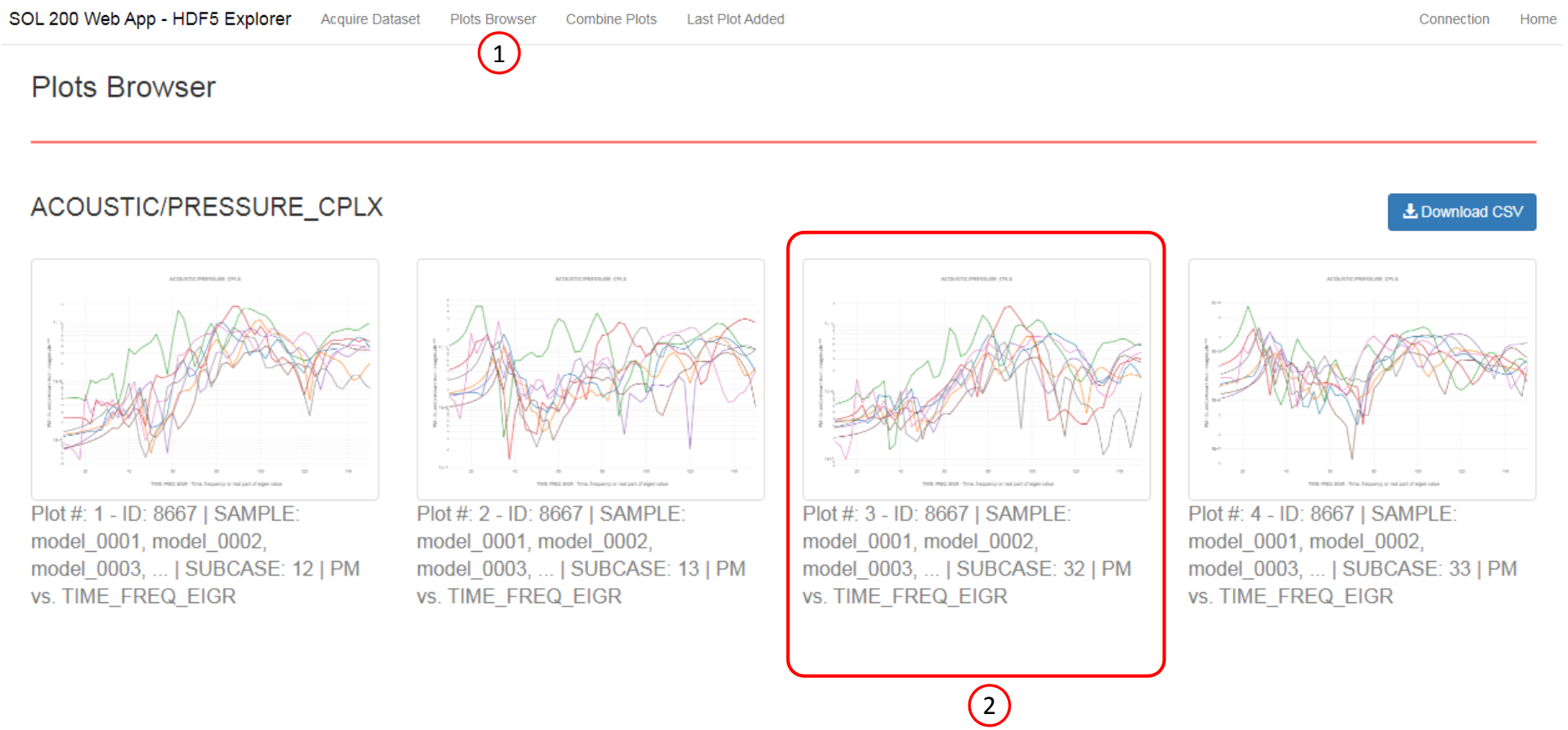
Review Results

1. A window appears asking to start the HDF5 Explorer
2. Select all 8 H5 files
3. Click Continue



HDF5 Explorer

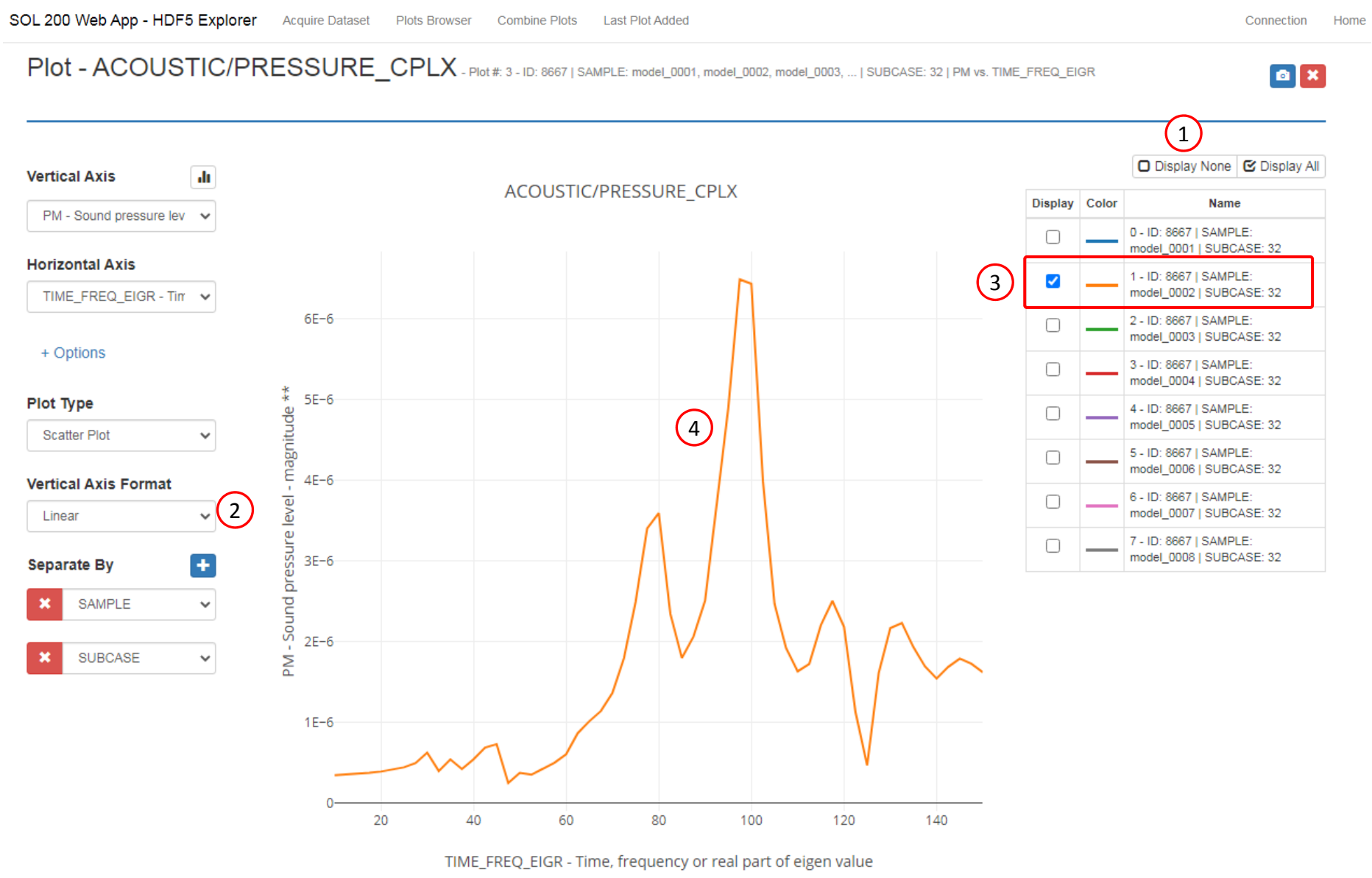
1. Navigate to the Plots Browser section
2. Click the indicated icon



HDF5 Explorer

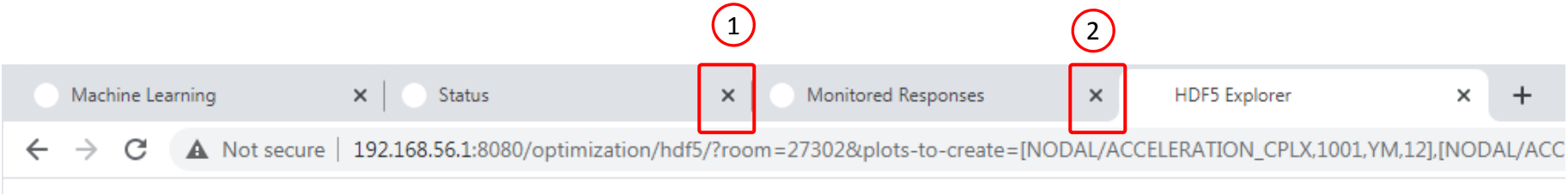
1. Click Display None to hide all the plotted traces
2. Set the Vertical Axis Format to Linear
3. Select only the 2nd trace which corresponds to the pressure at grid 8867, subcase 32, sample 2
4. The corresponding trace is now plotted

This trace will be used to compare the MSC Nastran response and predicted responses



Close Pages

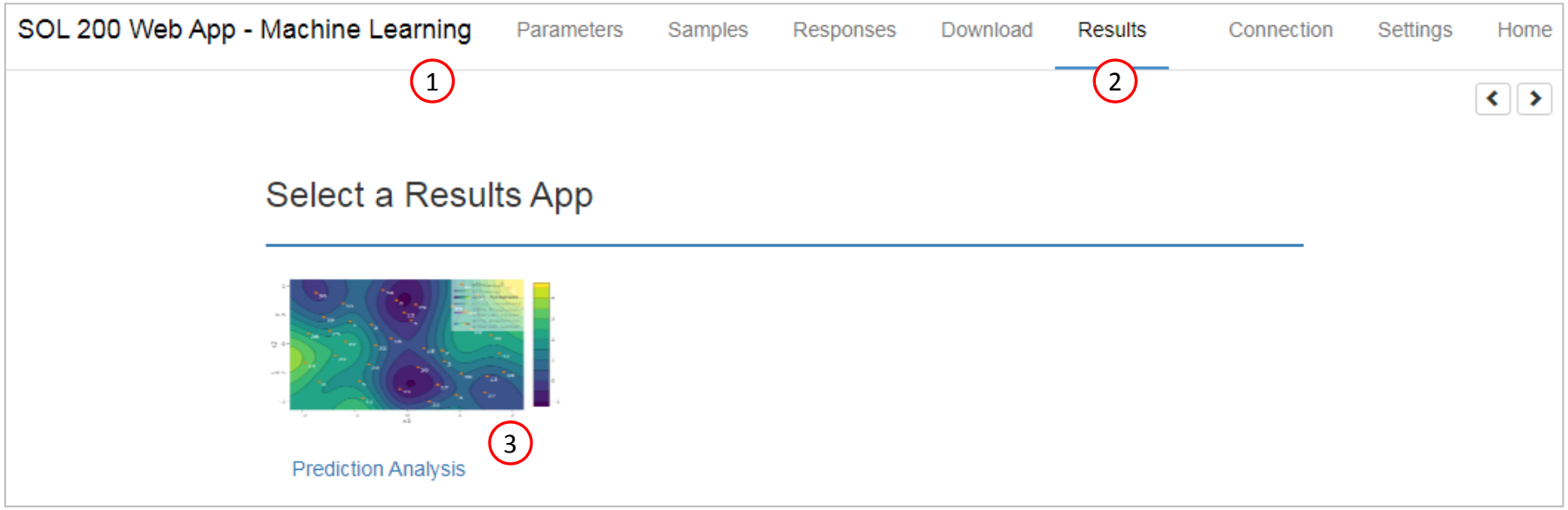
1. The Status page can be closed
2. The Monitored Responses page can be closed

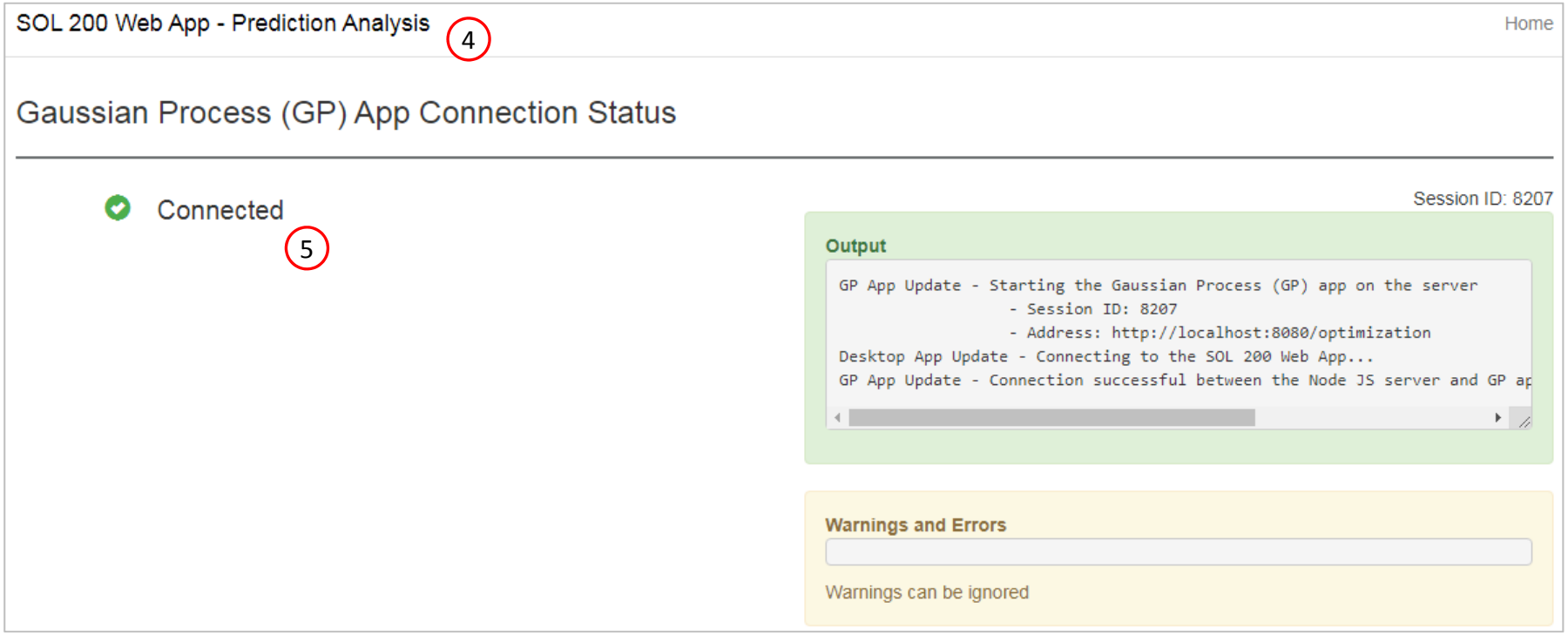


Determining Parameter Relevance (Parameter/Variable Screening)

Prediction Analysis Web App

1. Return to the Machine Learning web app
2. Click Results
3. Click Prediction Analysis
4. The Prediction Analysis web app is now open
5. Ensure it says Connected

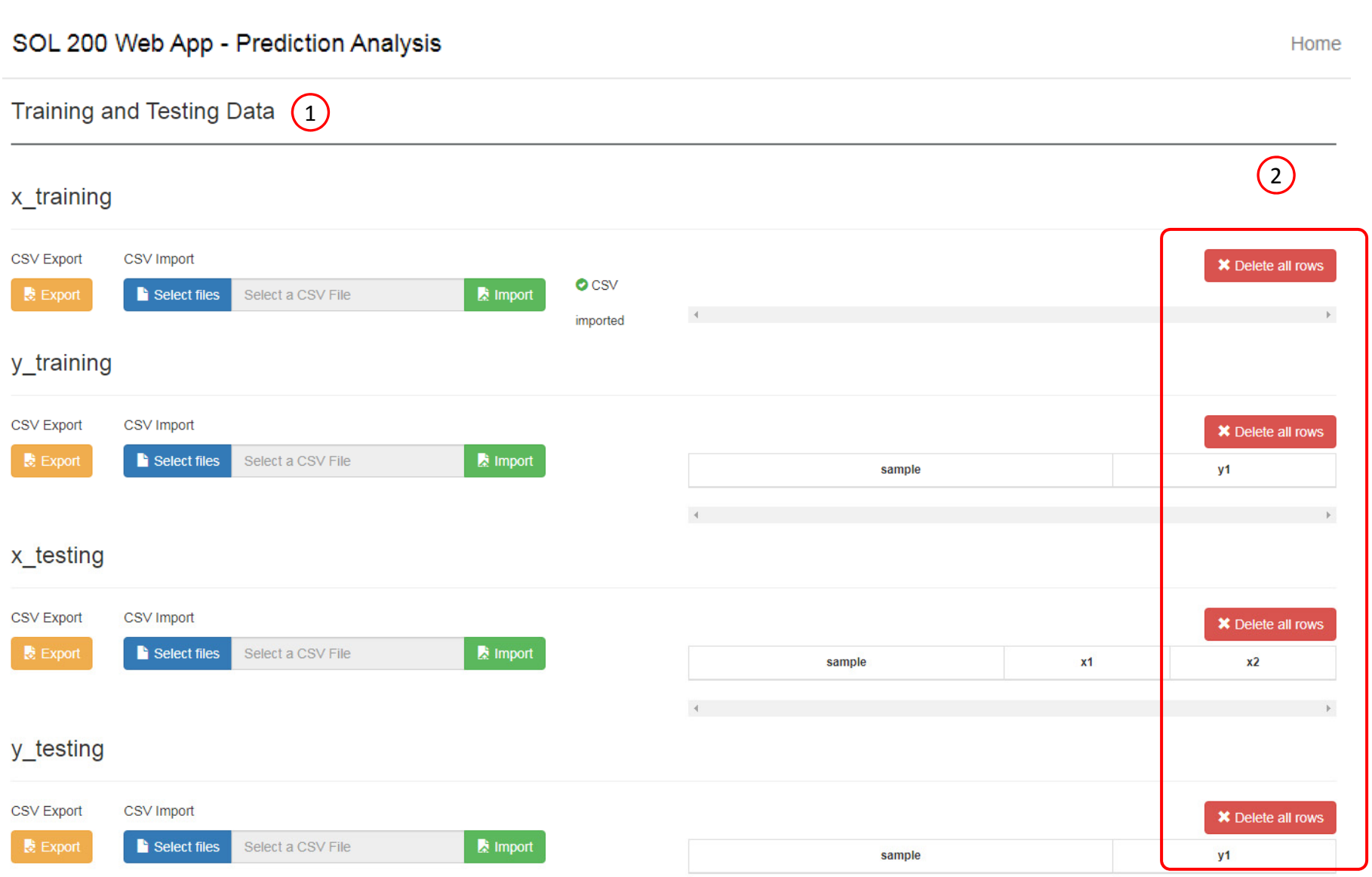




Training Data

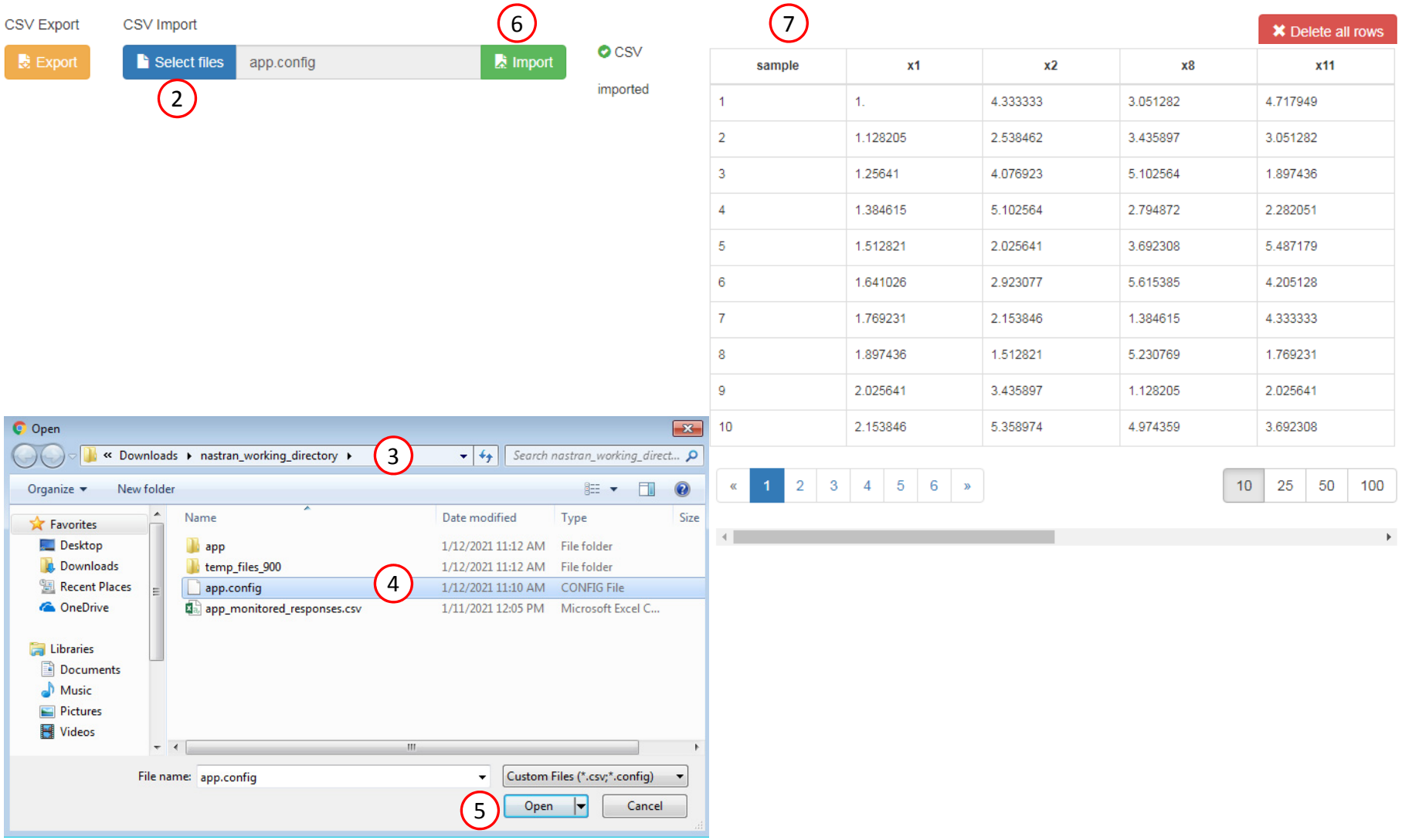
1. Navigate to the Training and Testing Data section
2. Delete any previous table data by clicking the four (4) buttons named Delete all rows

- **x_training, y_training** - This specifies the x inputs and y outputs used to train the surrogate model.
- **x_testing, y_testing** - This specifies the x inputs and y outputs used to calculate the Normalized Root Mean Square Error (NRMSE) between the predicted values and actual MSC Nastran responses. This testing data is optional.
- **x_prediction** – The x inputs at which to make predictions.



Training Data

1. Navigate to the section titled x_training
2. Click Select files
3. Navigate to the folder named nastran_working_directory which contains data for 55 runs
4. Select the file app.config
5. Click Open
6. Click Import
7. The table is now loaded with the x inputs for all 55 runs



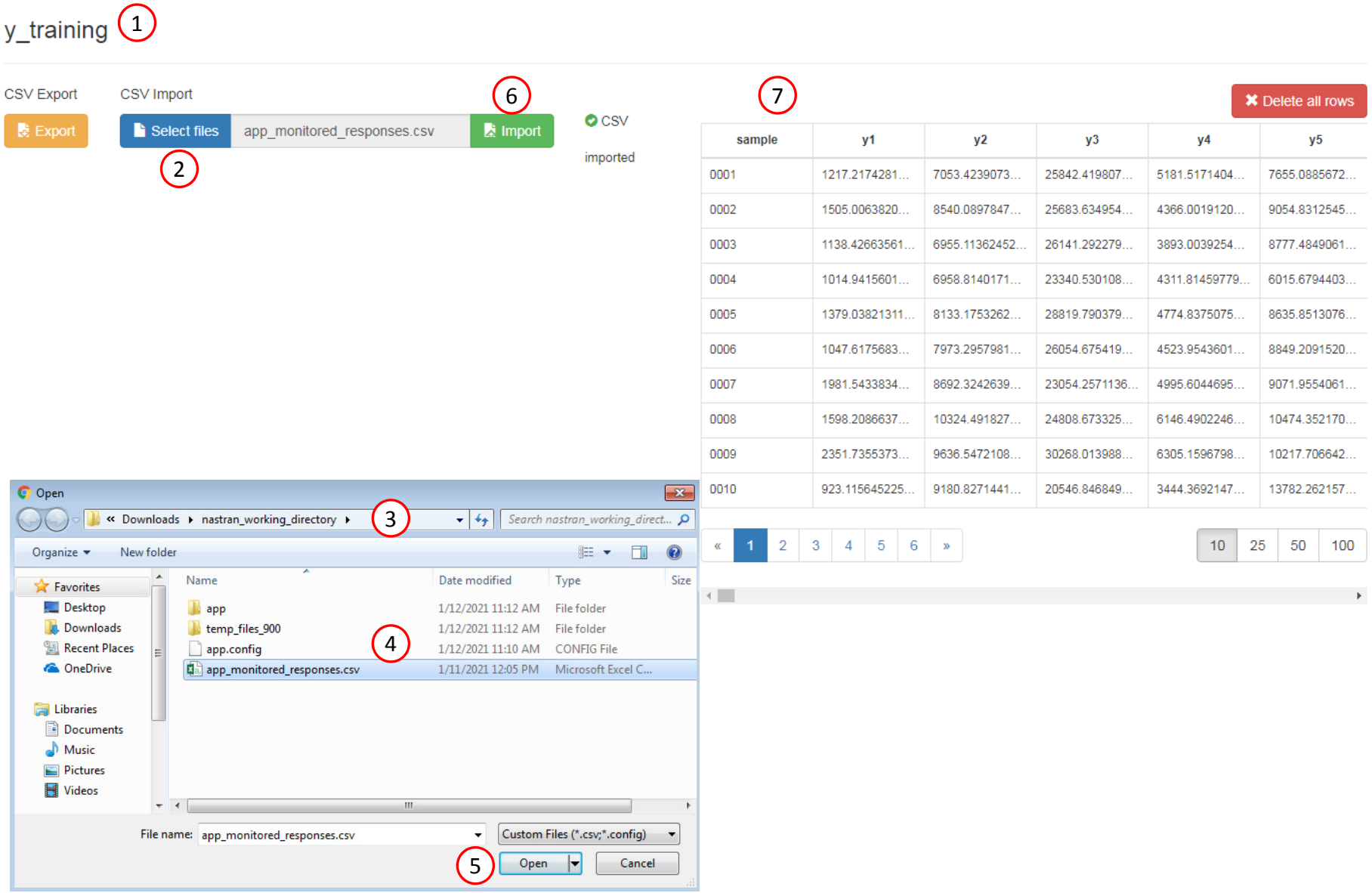
sample	x1	x2	x8	x11
1	1.	4.333333	3.051282	4.717949
2	1.128205	2.538462	3.435897	3.051282
3	1.25641	4.076923	5.102564	1.897436
4	1.384615	5.102564	2.794872	2.282051
5	1.512821	2.025641	3.692308	5.487179
6	1.641026	2.923077	5.615385	4.205128
7	1.769231	2.153846	1.384615	4.333333
8	1.897436	1.512821	5.230769	1.769231
9	2.025641	3.435897	1.128205	2.025641
10	2.153846	5.358974	4.974359	3.692308

« 1 2 3 4 5 6 »

10 25 50 100

Training Data

1. Navigate to the section titled y_training
2. Click Select files
3. Navigate to the folder named nastran_working_directory which contains data for 55 runs
4. Select the file app_monitored_responses.csv
5. Click Open
6. Click Import
7. The table is now loaded with the y outputs (monitored responses) for all 55 runs



sample	y1	y2	y3	y4	y5
0001	1217.2174281...	7053.4239073...	25842.419807...	5181.5171404...	7655.0885672...
0002	1505.0063820...	8540.0897847...	25683.634954...	4366.0019120...	9054.8312545...
0003	1138.42663561...	6955.11362452...	26141.292279...	3893.0039254...	8777.4849061...
0004	1014.9415601...	6958.8140171...	23340.530108...	4311.81459779...	6015.6794403...
0005	1379.03821311...	8133.1753262...	28819.790379...	4774.8375075...	8635.8513076...
0006	1047.6175683...	7973.2957981...	26054.675419...	4523.9543601...	8849.2091520...
0007	1981.5433834...	8692.3242639...	23054.2571136...	4995.6044695...	9071.9554061...
0008	1598.2086637...	10324.491827...	24808.673325...	6146.4902246...	10474.352170...
0009	2351.7355373...	9636.5472108...	30268.013988...	6305.1596798...	10217.706642...
0010	923.115645225...	9180.8271441...	20546.846849...	3444.3692147...	13782.262157...

« 1 2 3 4 5 6 »

10 25 50 100

Perform Regression

1. Click Perform Regression and the surrogate model will be fitted
2. The regression is complete when the following status message is visible:
   - Process complete
3. The output will be used on the next page

SOL 200 Web App - Prediction Analysis

Home

Regression

Data	Link to Table	Status	Status Description
x_training	Link		Ready
y_training	Link		Ready
x_testing (Optional)	Link		Ready
y_testing (Optional)	Link		Ready

Perform Regression (1)

Process complete (2)

Click here to view the Regression Results section

(3)

Output

```
GP App Update - Saving initial data
GP App Update - Summary of Automatic Relevance Determination (ARD)
                ARD measures predictive relevance of parameters and is used for paramet
                - High Value: The parameter xi is relevant
                - Low Value:  The parameter xi is irrelevant and could potentially be s
Kernel: Matern52
| Response   |          x1 |        x2 |           x3 |           x4 |           x5 |
|:-----------|-----------:|---------:|-----------:|-----------:|-----------:|-------
| y1         | 4.41523     | 11.181   | 0.659106     | 2.17256e-09 | 3.3067e-09   | 1.8521
| y2         | 2.6569      |  3.0316  | 3.96957      | 1.37152e-07 | 1.21214      | 0.0482
| y3         | 1.43826     |  5.22752 | 9.84035e-07  | 1.20974e-06 | 0.433083     | 1.4890
| y4         | 0.0857389   | 22.2011  | 2.80218      | 0.0084688   | 1.54202e-09  | 0.0129
| y5         | 0.00394936  | 73.9887  | 0.0320619    | 0.119963    | 0.248584     | 4.7087
| y6         | 0.532546    |  8.6371  | 0.777735     | 5.41834e-05 | 2.99273      | 0.0472
| y7         | 0.383766    | 31.5844  | 3.9199e-09   | 0.616215    | 5.33463e-09  | 0.0254
| y8         | 0.0615319   | 49.5679  | 2.03028e-08  | 1.21104     | 2.07824e-08  | 2.2841
| y9         | 0.31014     |  7.12581 | 1.19458      | 4.37308e-08 | 0.289277     | 0.0793
    Parameters listed in decreasing order of relevance: x2, x8, x1, x11, x3, x5, x9, x4
Kernel: Exponential
| Response   |           x1 |        x2 |           x3 |           x4 |           x5 |
|:-----------|------------:|---------:|------------:|------------:|------------:|------
| y1         | 0.633904     | 3.97626  | 8.68101e-10 | 5.9275e-10  | 9.24688e-10 | 6.455
| y2         | 0.119435     | 0.338008 | 0.102887    | 4.80711e-10 | 4.06709e-10 | 0.049
| y3         | 0.0342023    | 0.391405 | 2.72361e-09 | 6.14333e-09 | 0.0271812   | 8.122
| y4         | 0.00116244   | 0.155004 | 0.0221579   | 5.60043e-11 | 4.89368e-11 | 1.120
| y5         | 3.82391e-11  | 0.41135  | 2.14606e-11 | 2.50395e-11 | 1.47319e-11 | 3.482
| y6         | 9.32315e-06  | 1.35509  | 0.0606396   | 1.84373e-06 | 0.230813    | 3.064
| y7         | 0.0097128    | 1.41159  | 4.10616e-10 | 3.07655e-10 | 1.83933e-10 | 3.214
| y8         | 0.0515579    | 7.13954  | 5.35455e-08 | 3.83144e-07 | 6.88943e-08 | 4.176
| y9         | 0.00201582   | 0.273497 | 2.67888e-10 | 2.10806e-10 | 0.0241915   | 2.522
    Parameters listed in decreasing order of relevance: x2, x1, x8, x11, x10, x3, x6, x
Kernel: RBF
```

Automatic Relevance Determination (ARD)

1. Click and hold the bottom right corner of the output window (gray color) and vertically drag to adjust the height of the window. This will make more text visible.
2. For the Output window, move the scroll bar to the very bottom
3. Ensure the following section is visible: Summary of Automatic Relevance Determination (ARD)
4. ARD values for each response with respect to each parameter have been computed

Output

```
GP App Update - Saving initial data
GP App Update - Summary of Automatic Relevance Determination (ARD)
                ARD measures predictive relevance of parameters and is used for paramete
                - High Value: The parameter xi is relevant
                - Low Value:  The parameter xi is irrelevant and could potentially be s
Kernel: Matern52
| Response   |         x1 |       x2 |          x3 |          x4 |          x5 |
|:-----------|----------:|---------:|----------:|----------:|----------:|
| y1         | 4.41523    | 11.181   | 0.659106    | 2.17256e-09 | 3.3067e-09  | 1.8521
| y2         | 2.6569     |  3.0316  | 3.96957     | 1.37152e-07 | 1.21214     | 0.0482
| y3         | 1.43826    |  5.22752 | 9.84035e-07 | 1.20974e-06 | 0.433083    | 1.4890
| y4         | 0.0857389  | 22.2011  | 2.80218     | 0.0084688   | 1.54202e-09 | 0.0129
| y5         | 0.00394936 | 73.9887  | 0.0320619   | 0.119963    | 0.248584    | 4.7087
| y6         | 0.532546   |  8.6371  | 0.777735    | 5.41834e-05 | 2.99273     | 0.0472
| y7         | 0.383766   | 31.5844  | 3.9199e-09  | 0.616215    | 5.33463e-09 | 0.0254
| y8         | 0.0615319  | 49.5679  | 2.03028e-08 | 1.21104     | 2.07824e-08 | 2.2841
| y9         | 0.31014    |  7.12581 | 1.19458     | 4.37308e-08 | 0.289277    | 0.0793
    Parameters listed in decreasing order of relevance: x2, x8, x1, x11, x3, x5, x9, x4,
Kernel: Exponential
| Response   |          x1 |       x2 |          x3 |          x4 |          x5 |
|:-----------|----------:|---------:|----------:|----------:|----------:|
| y1         | 0.633904    | 3.97626  | 8.68101e-10 | 5.9275e-10  | 9.24688e-10 | 6.455
| y2         | 0.119435    | 0.338008 | 0.102887    | 4.80711e-10 | 4.06709e-10 | 0.049
| y3         | 0.0342023   | 0.391405 | 2.72361e-09 | 6.14333e-09 | 0.0271812   | 8.122
| y4         | 0.00116244  | 0.155004 | 0.0221579   | 5.60043e-11 | 4.89368e-11 | 1.120
| y5         | 3.82391e-11 | 0.41135  | 2.14606e-11 | 2.50395e-11 | 1.47319e-11 | 3.482
| y6         | 9.32315e-06 | 1.35509  | 0.0606396   | 1.84373e-06 | 0.230813    | 3.064
| y7         | 0.0097128   | 1.41159  | 4.10616e-10 | 3.07655e-10 | 1.83933e-10 | 3.214
| y8         | 0.0515579   | 7.13954  | 5.35455e-08 | 3.83144e-07 | 6.88943e-08 | 4.176
| y9         | 0.00201582  | 0.273497 | 2.67888e-10 | 2.10806e-10 | 0.0241915   | 2.52
    Parameters listed in decreasing order of relevance: x2, x1, x8, x11, x10, x3, x6, x
Kernel: RBF
```

Automatic Relevance Determination (ARD)

1. A single line lists the most relevant parameters, in decreasing order, across all responses. Parameters x1, x2, x8 and x11 are the most relevant, and the other parameters can be optionally removed.

2. During the regression, 3 different kernel functions are used. As a result, there will be 3 sets of ARD values. As shown, the Exponential kernel function has produced a similar list of relevant parameters x1, x2, x8 and x11.

3. If desired, more relevant parameters can be determined, but it is expected some disagreement may occur as indicated. The parameter selection process is left to your judgement. For example, when you repeat this example, you may find these parameters as the most relevant: x1, x2 x3 and x8.

- For large dimension problems, i.e. problems with 10 or more parameters, the training data to fit the surrogate model may require 10-20 runs per parameter, possibly more. There is a need to reduce the dimensionality of the problem.
- As an example, suppose computation constraints limit us to 40 runs and the goal is to use 10 runs per parameter, the problem needs to be reduced to 4 parameters. This page demonstrates the parameter selection process.

Output

```
GP App Update - Saving initial data
GP App Update - Summary of Automatic Relevance Determination (ARD)
                ARD measures predictive relevance of parameters and is used for paramete
                - High Value: The parameter xi is relevant
                - Low Value:  The parameter xi is irrelevant and could potentially be s
Kernel: Matern52
| Response   |         x1 |       x2 |          x3 |          x4 |          x5 |
|:-----------|----------:|---------:|----------:|----------:|----------:|
| y1         | 4.41523    | 11.181   | 0.659106    | 2.17256e-09 | 3.3067e-09  | 1.8521
| y2         | 2.6569     |  3.0316  | 3.96957     | 1.37152e-07 | 1.21214     | 0.0482
| y3         | 1.43826    |  5.22752 | 9.84035e-07 | 1.20974e-06 | 0.433083    | 1.4890
| y4         | 0.0857389  | 22.2011  | 2.80218     | 0.0084688   | 1.54202e-09 | 0.0129
| y5         | 0.00394936 | 73.9887  | 0.0320619   | 0.119963    | 0.248584    | 4.7087
| y6         | 0.532546   |  8.6371  | 0.777735    | 5.41834e-05 | 2.99273     | 0.0472
| y7         | 0.383766   | 31.5844  | 3.9199e-09  | 0.616215    | 5.33463e-09 | 0.0254
| y8         | 0.0615319  | 49.5679  | 2.03028e-08 | 1.21104     | 2.07824e-08 | 2.2841
| y9         | 0.31014    |  7.12581 | 1.19458     | 4.37308e-08 | 0.289277    | 0.0793
    Parameters listed in decreasing order of relevance: x2, x8, x1, x11, x3, x5, x9, x4
Kernel: Exponential
| Response   |          x1 |       x2 |          x3 |          x5 |
|:-----------|----------:|---------:|----------:|----------:|
| y1         | 0.633904    | 3.97626  | 8.68101e-10 | 5.9275e-10  | 9.24688e-10 | 6.455
| y2         | 0.119435    | 0.338008 | 0.102887    | 4.80711e-10 | 4.06709e-10 | 0.049
| y3         | 0.0342023   | 0.391405 | 2.72361e-09 | 6.14333e-09 | 0.0271812   | 8.122
| y4         | 0.00116244  | 0.155004 | 0.0221579   | 5.60043e-11 | 4.89368e-11 | 1.120
| y5         | 3.82391e-11 | 0.41135  | 2.14606e-11 | 2.50395e-11 | 1.47319e-11 | 3.48
| y6         | 9.32315e-06 | 1.35509  | 0.0606396   | 1.84373e-06 | 0.230813    | 3.064
| y7         | 0.0097128   | 1.41159  | 4.10616e-10 | 3.07655e-10 | 1.83933e-10 | 3.214
| y8         | 0.0515579   | 7.13954  | 5.35455e-08 | 3.83144e-07 | 6.88943e-08 | 4.176
| y9         | 0.00201582  | 0.273497 | 2.67888e-10 | 2.10806e-10 | 0.0241915   | 2.522
    Parameters listed in decreasing order of relevance: x2, x1, x8, x11, x10, x3, x6, x
Kernel: RBF
```

1

2

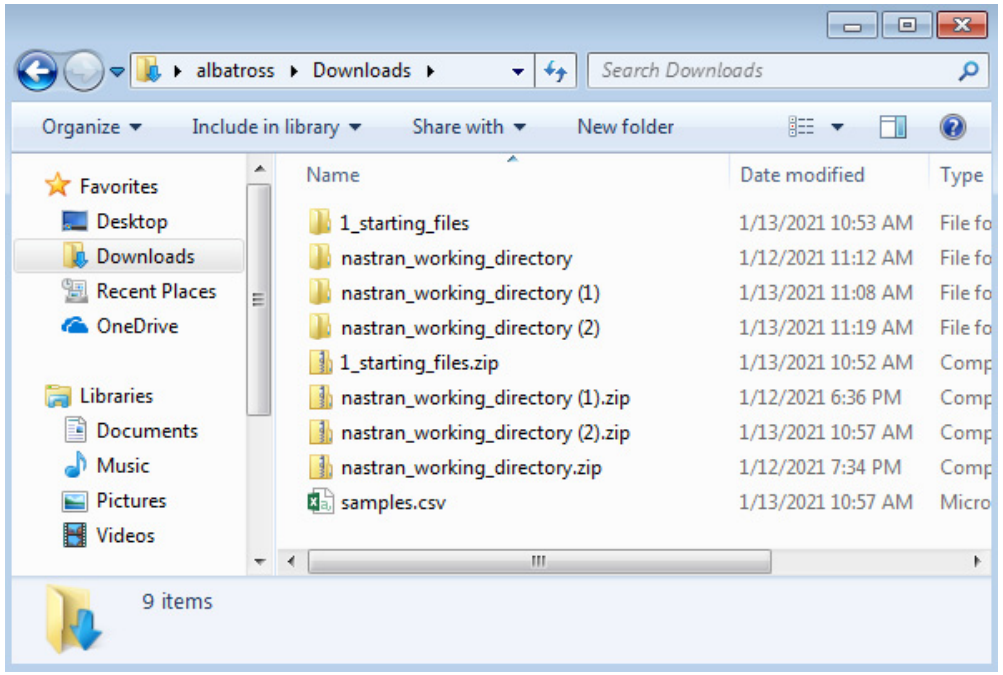
3

Samples

It has been determined that 4 parameters x1, x2, x8 and x11 should be kept, and the other 7 parameters should be removed.

The next batch, Batch 2, has been configured previously for 4 parameters and 40 runs.

The following pages go over the regression process, making predictions and comparing the predictions to MSC Nastran outputs.

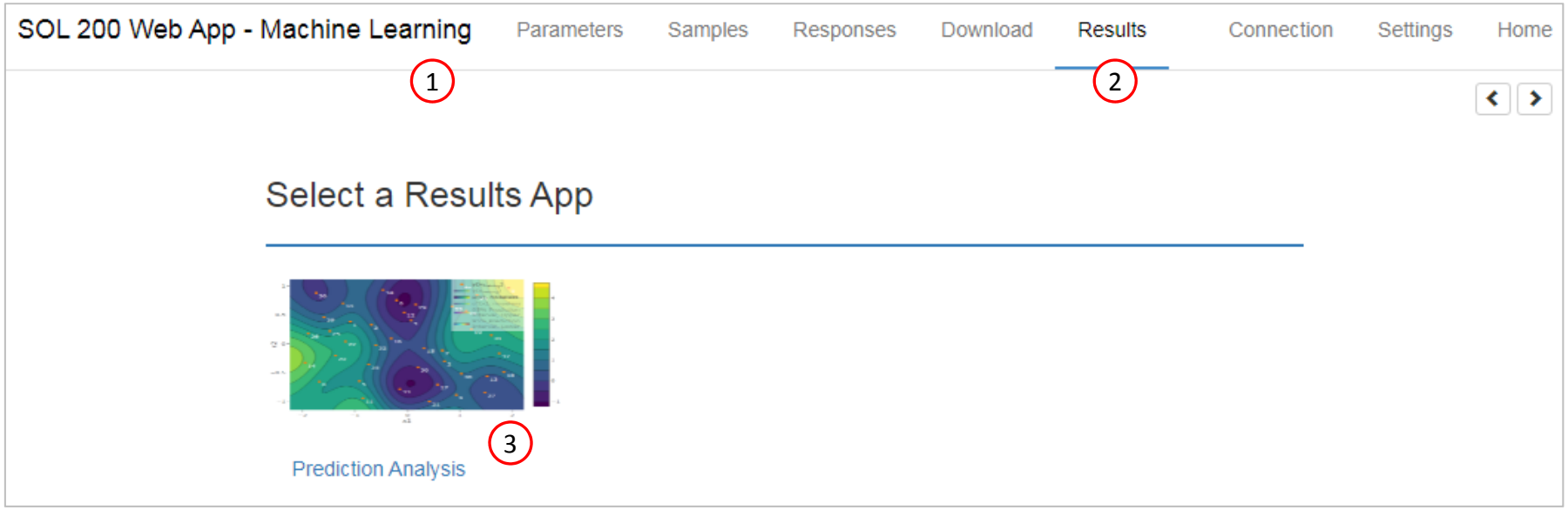


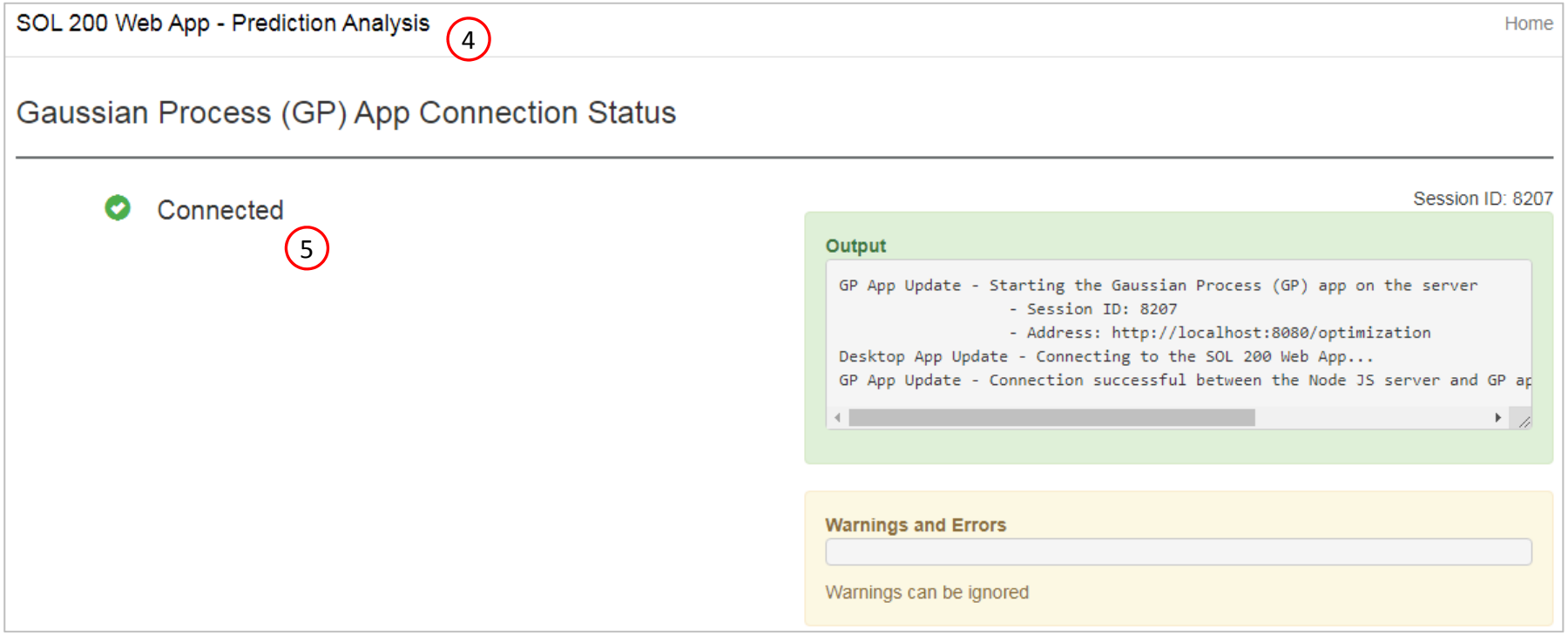
Batch	File Name	Number of Runs	Number of Parameters	Purpose
1	nastran_working_directory.zip	55	11	This configuration includes 11 parameters. The goal is to use the data from the 55 run set to screen parameters and reduce the problem to 4 parameters. Automatic relevance determination (ARD) is used to identify the 4 most relevant parameters.
2	nastran_working_directory (1).zip	40	4	This configuration includes 4 parameters. The goal of this 40 run set is to produce training data to fit the surrogate model and make predictions.
3	nastran_working_directory (2).zip	8	4	This is an 8 run configuration. This set is used to compare the predicted responses with MSC Nastran responses.

Performing Predictions

Prediction Analysis Web App

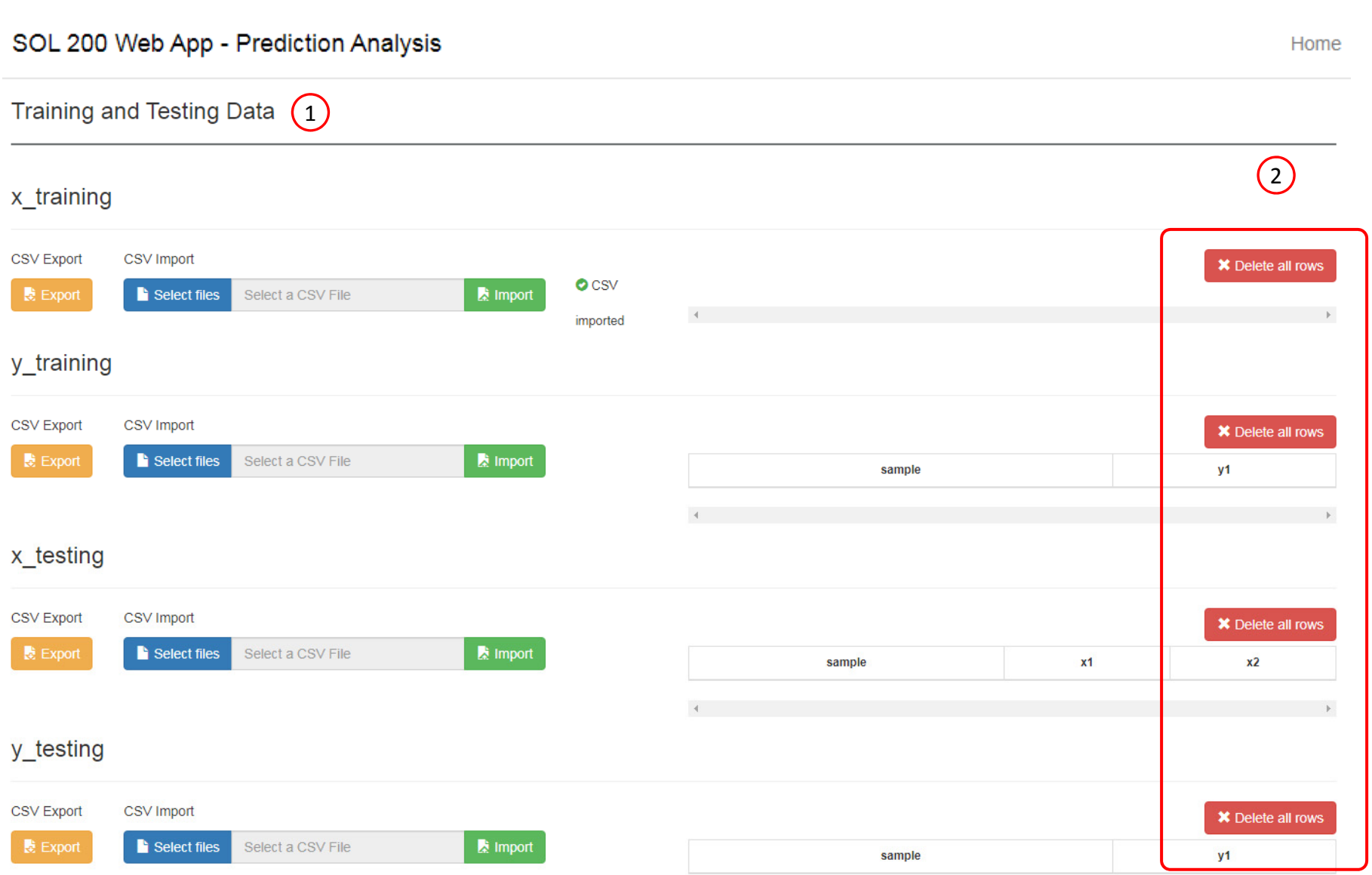
1. Return to the Machine Learning web app
2. Click Results
3. Click Prediction Analysis
4. The Prediction Analysis web app is now open
5. Ensure it says Connected





Training Data

1. Navigate to the Training and Testing Data section
2. Delete any previous table data by clicking the four (4) buttons named Delete all rows



Training Data

1. Navigate to the section titled x_training
2. Click Select files
3. Navigate to the folder named nastran_working_directory (1) which contains data for 40 runs
4. Select the file app.config
5. Click Open
6. Click Import
7. The table is now loaded with the x inputs for all 40 runs

Training and Testing Data

x_training (1)

CSV Export

Export

CSV Import

Select files (2) app.config Import (6)

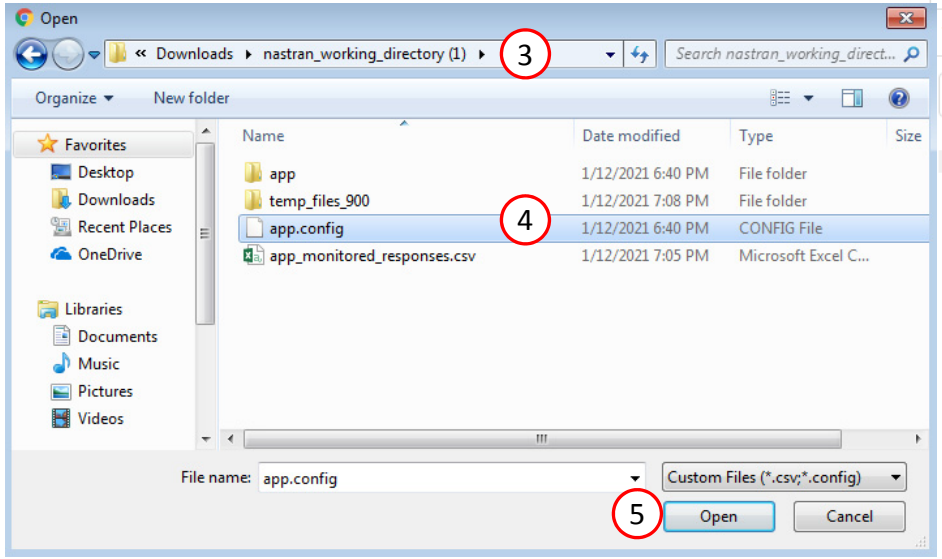
CSV imported

Delete all rows

(7)

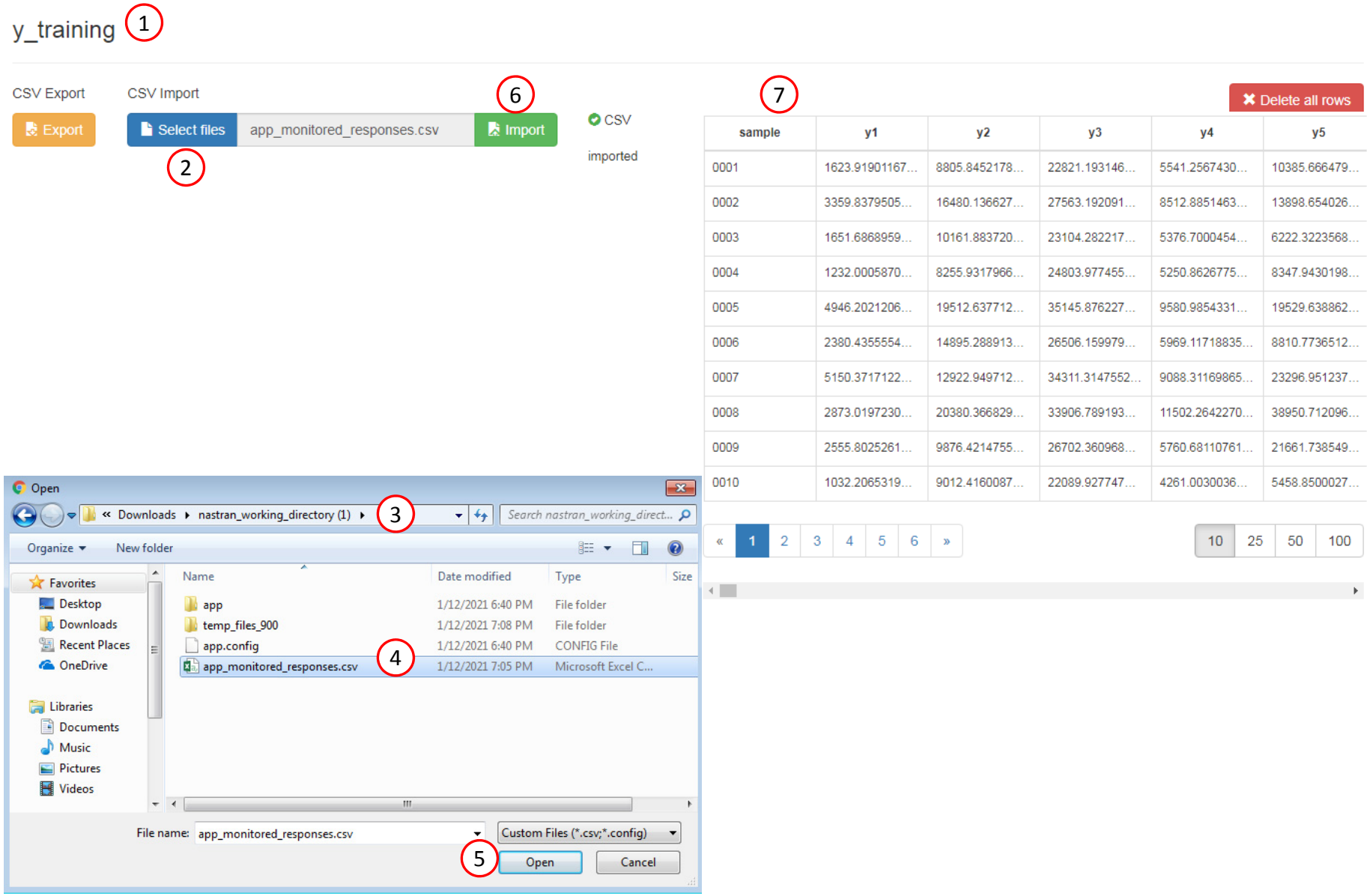
sample	x1	x2	x8	x11
1	1.	4.333333	3.051282	4.717949
2	1.128205	2.538462	3.435897	3.051282
3	1.25641	4.076923	5.102564	1.897436
4	1.384615	5.102564	2.794872	2.282051
5	1.512821	2.025641	3.692308	5.487179
6	1.641026	2.923077	5.615385	4.205128
7	1.769231	2.153846	1.384615	4.333333
8	1.897436	1.512821	5.230769	1.769231
9	2.025641	3.435897	1.128205	2.025641
10	2.153846	5.358974	4.974359	3.692308

« 1 2 3 4 5 6 » 10 25 50 100



Training Data

1. Navigate to the section titled y_training
2. Click Select files
3. Navigate to the folder named nastran_working_directory (1) which contains data for 40 runs
4. Select the file app_monitored_responses.csv
5. Click Open
6. Click Import
7. The table is now loaded with the y outputs (monitored responses) for all 40 runs



Perform Regression

1. Click Perform Regression and the surrogate model will be fitted
2. The regression is complete when the following status message is visible:
   - Process complete

SOL 200 Web App - Prediction Analysis

Home

Regression

Data	Link to Table	Status	Status Description
x_training	Link		Ready
y_training	Link		Ready
x_testing (Optional)	Link		Ready
y_testing (Optional)	Link		Ready

Perform Regression (1)

Process complete (2)

Click here to view the Regression Results section

Output

```
| y3          |  6.34332     |  22.8637   |  0.285728 | 12.5891     |
| y4          |  0.329643    |   7.79946  |  7.49135  |  3.58932    |
| y5          |  0.00412772  | 298.861    |  0.9722   |  0.00234721 |
| y6          |  0.65093     |  20.7999   | 22.9172   |  3.70404    |
| y7          |  0.274844    |  35.1077   |  1.39711  |  3.72269    |
| y8          |  0.00739204  | 105.864    |  6.33735  |  2.76692    |
| y9          |  0.22452     |  47.8042   |  0.824128 |  4.19834    |
    Parameters listed in decreasing order of relevance: x2, x8, x11, x1
GP App Update - Sending initial data to the web browser
GP App Update - Sending complete
```

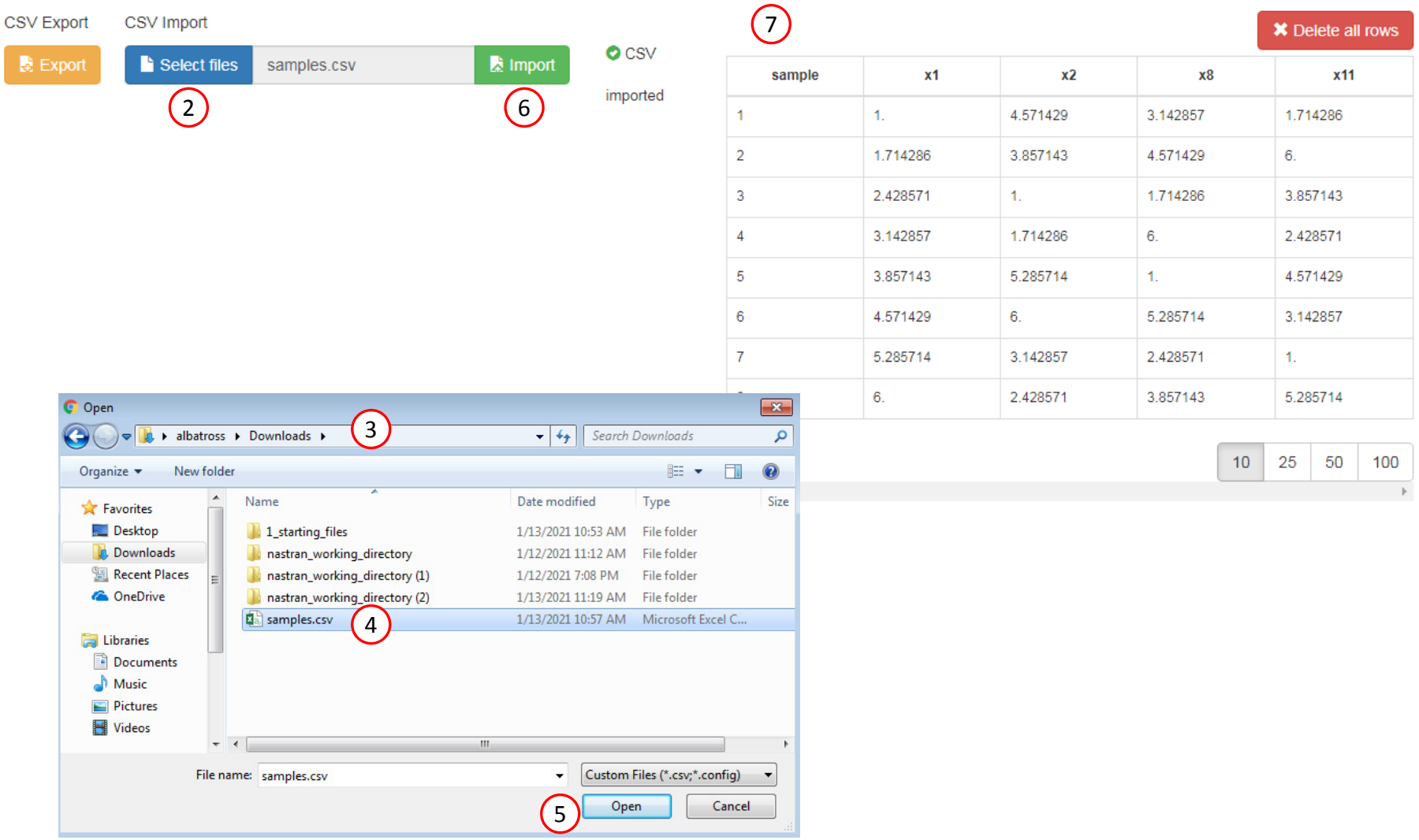
Warnings and Errors

```
/home/apricot/PycharmProjects/python-app/venv/lib/python3.6/site-packages/GPy/kern/src/st
/home/apricot/PycharmProjects/python-app/venv/lib/python3.6/site-packages/GPy/kern/src/st
/home/apricot/PycharmProjects/python-app/venv/lib/python3.6/site-packages/GPy/kern/src/st
/home/apricot/PycharmProjects/python-app/venv/lib/python3.6/site-packages/GPy/kern/src/st
/home/apricot/PycharmProjects/python-app/venv/lib/python3.6/site-packages/GPy/kern/src/st
/home/apricot/PycharmProjects/python-app/venv/lib/python3.6/site-packages/paramz/transfor
/home/apricot/PycharmProjects/python-app/venv/lib/python3.6/site-packages/GPy/kern/src/rb
/home/apricot/PycharmProjects/python-app/venv/lib/python3.6/site-packages/GPy/kern/src/st
/home/apricot/PycharmProjects/python-app/venv/lib/python3.6/site-packages/GPy/kern/src/st
```

Warnings can be ignored

Perform Prediction

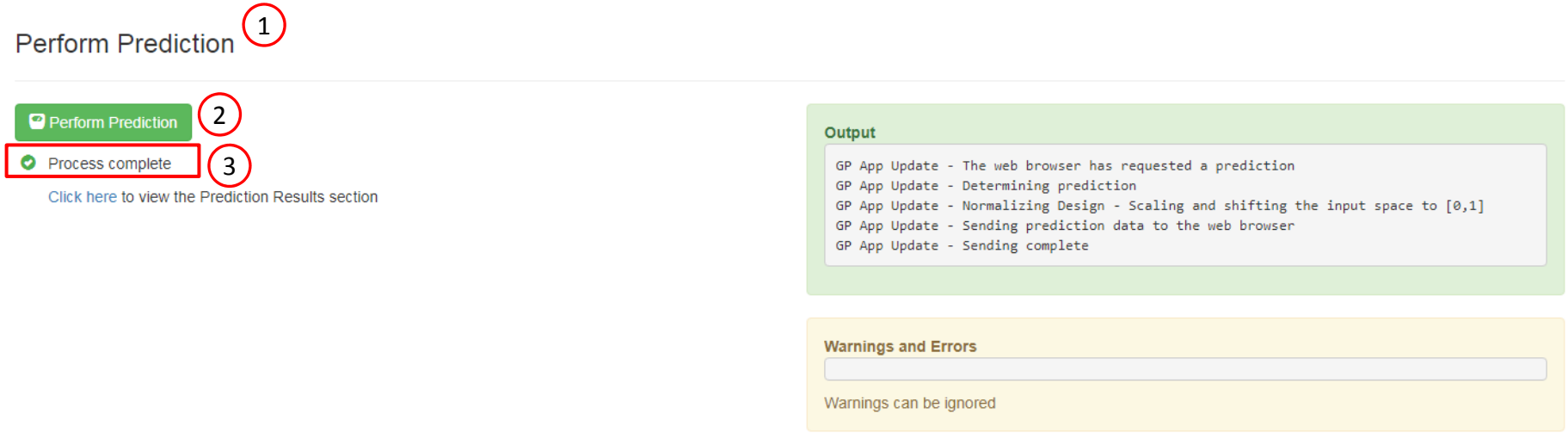
1. Navigate to the section titled x_prediction
2. Click Select files
3. Navigate to the location of the file named samples.csv
4. Select the file samples.csv
5. Click Open
6. Click Import
7. The table is now loaded with the x inputs for 8 runs



Perform Prediction

1. Navigate to the section titled Perform Prediction
2. Click Perform Prediction
3. The prediction is complete when the following status message is visible:
   - Process complete

- Note that the predictions are performed seemingly instantly



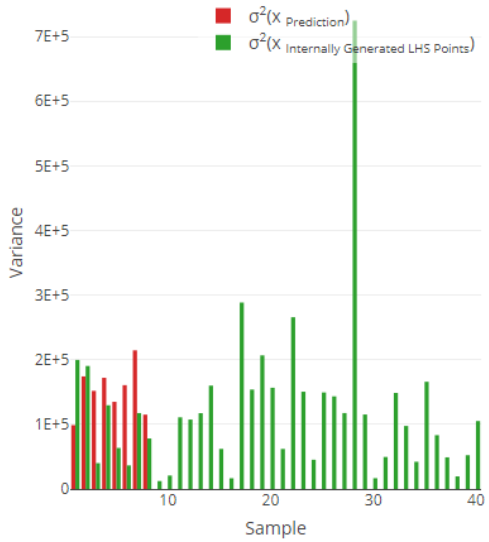
Variance

1. Navigate to the section titled Variance

Variance 1

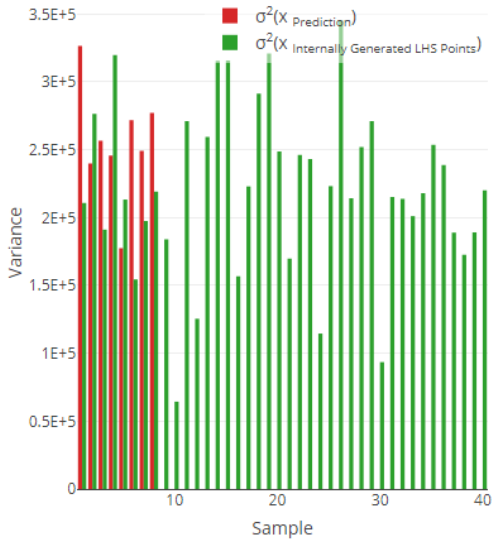
Matern52

NRMSE:



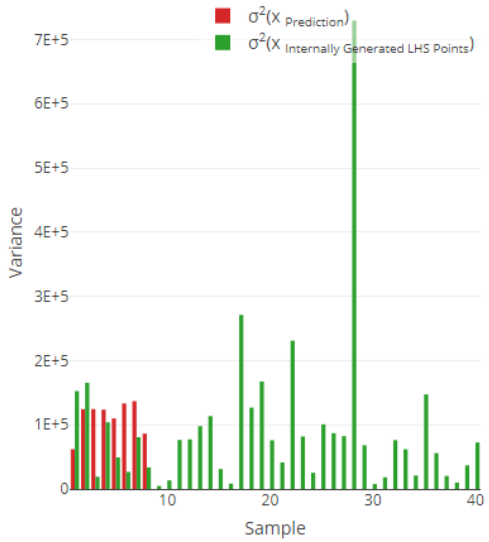
Exponential

NRMSE:



RBF

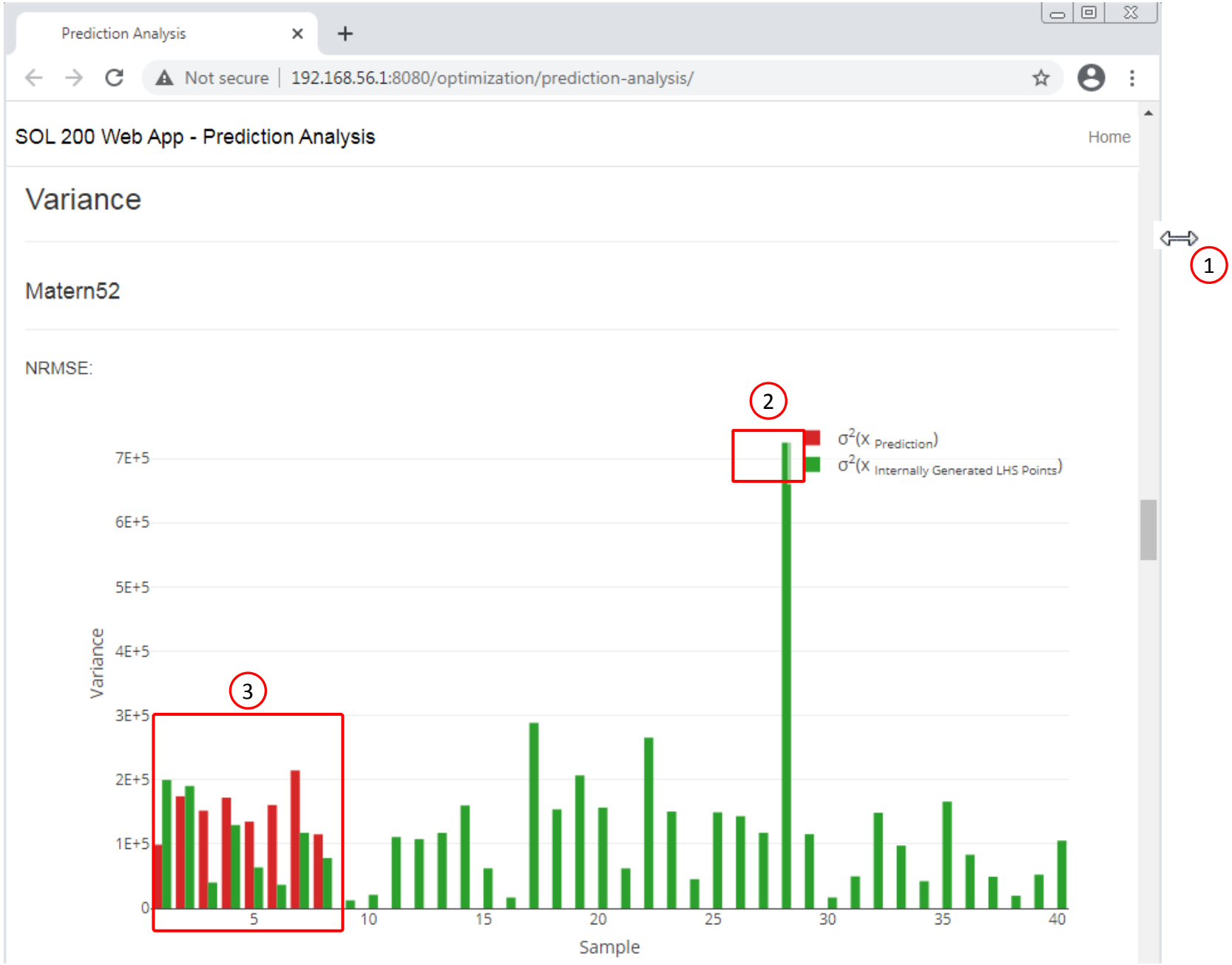
NRMSE:



Variance

1. Resize the window to fit half the screen, this causes the plot to be increased in size
2. A high bar indicates a high prediction uncertainty, or a high variance, and is indication that we do not have enough information to conclude the prediction is credible at that prediction point.
3. Predictions have been made at 8 samples and are indicated by 8 red bars
   - When making predictions, the prediction uncertainty should ideally be low, like in this example

- In this tutorial, variance (σ^2) is used to gauge the prediction uncertainty. Sometimes, you will see this prediction uncertainty expressed as the standard deviation (σ).



Pressure vs. Frequency

For frequency responses and after a prediction is performed, Response vs. Frequency plots are automatically generated.

1. Navigate to the section titled XYPLOT
2. Set Select a response to r8
3. Set Select a sample to 2
4. Set Include 95% Prediction Intervals to Yes
5. Set the Vertical Axis Format to Linear
6. The predicted plots are now displayed. Since 3 kernel functions were used during regression, there are 3 predicted plots.

Comparison of Prediction with MSC Nastran

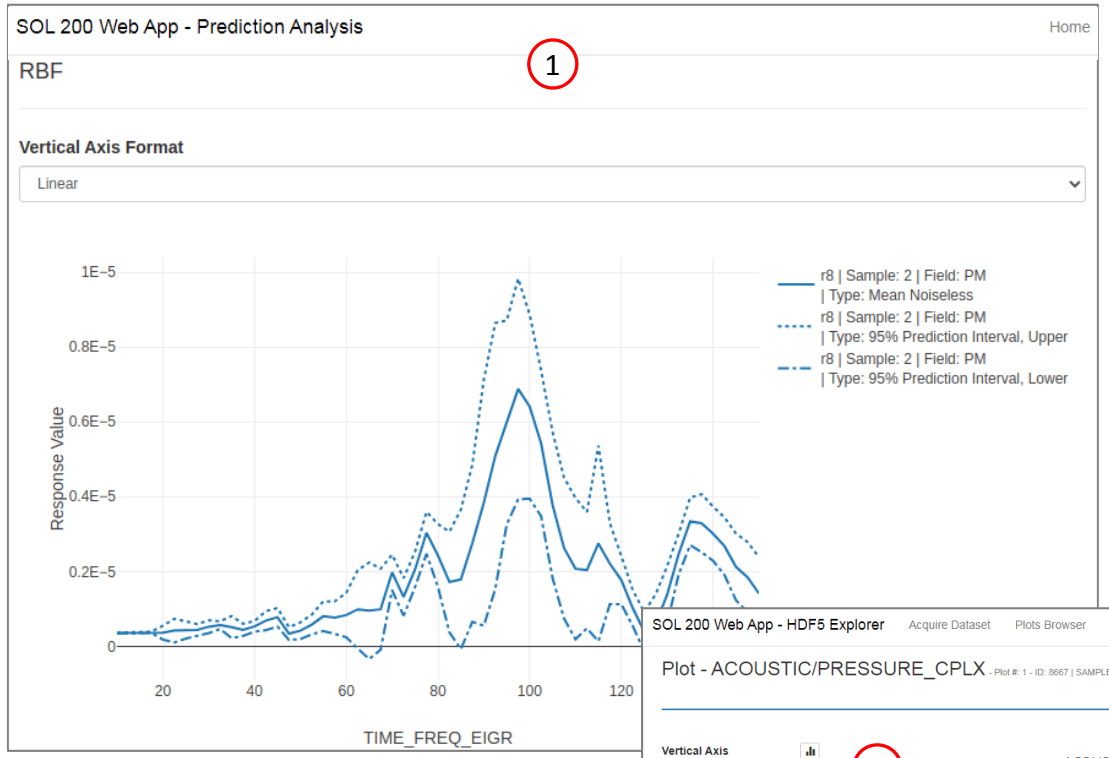
Recall that batch 2 was used to produce the training data and fit the surrogate model. Batch 3 contained 8 sample points.

1. The surrogate model was used to predict the output responses at the 8 sample points. The predicted response vs. frequency plot is displayed.

2. MSC Nastran was used to evaluate all 8 sample points and the HDF5 Explorer was used to display the true response vs. frequency plots.

A comparison can be made between the prediction and MSC Nastran output.

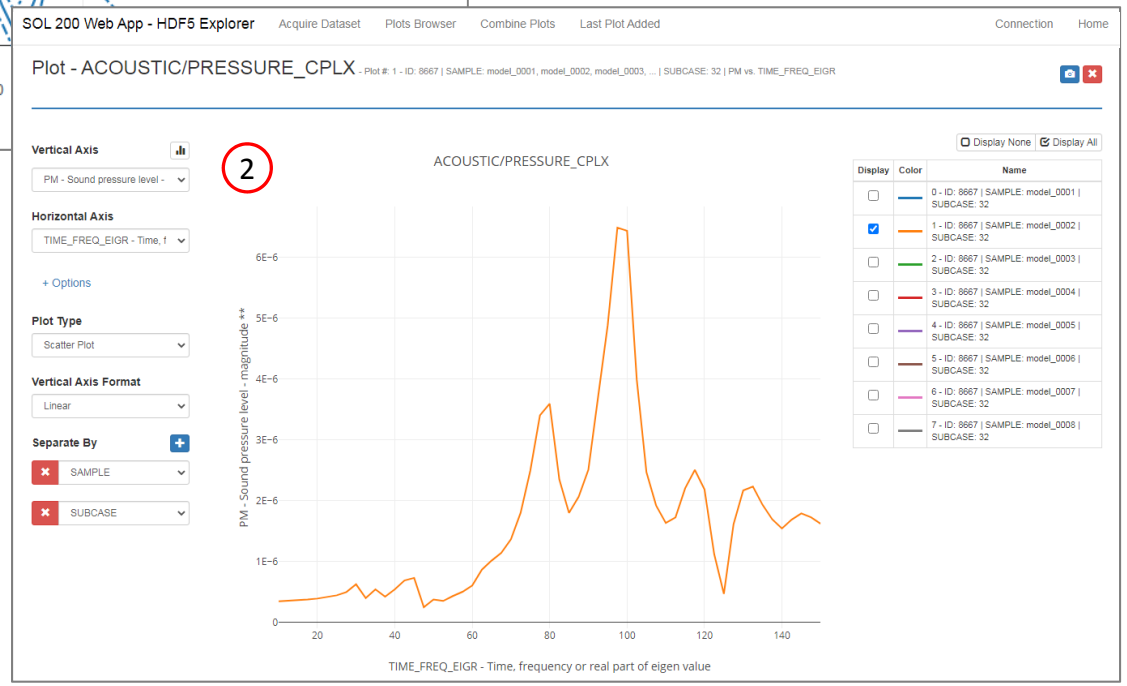
- In this tutorial, variance (σ^2) is used to gauge the prediction uncertainty. Sometimes, you will see this prediction uncertainty expressed as the standard deviation (σ).



Predicted response

95% prediction interval

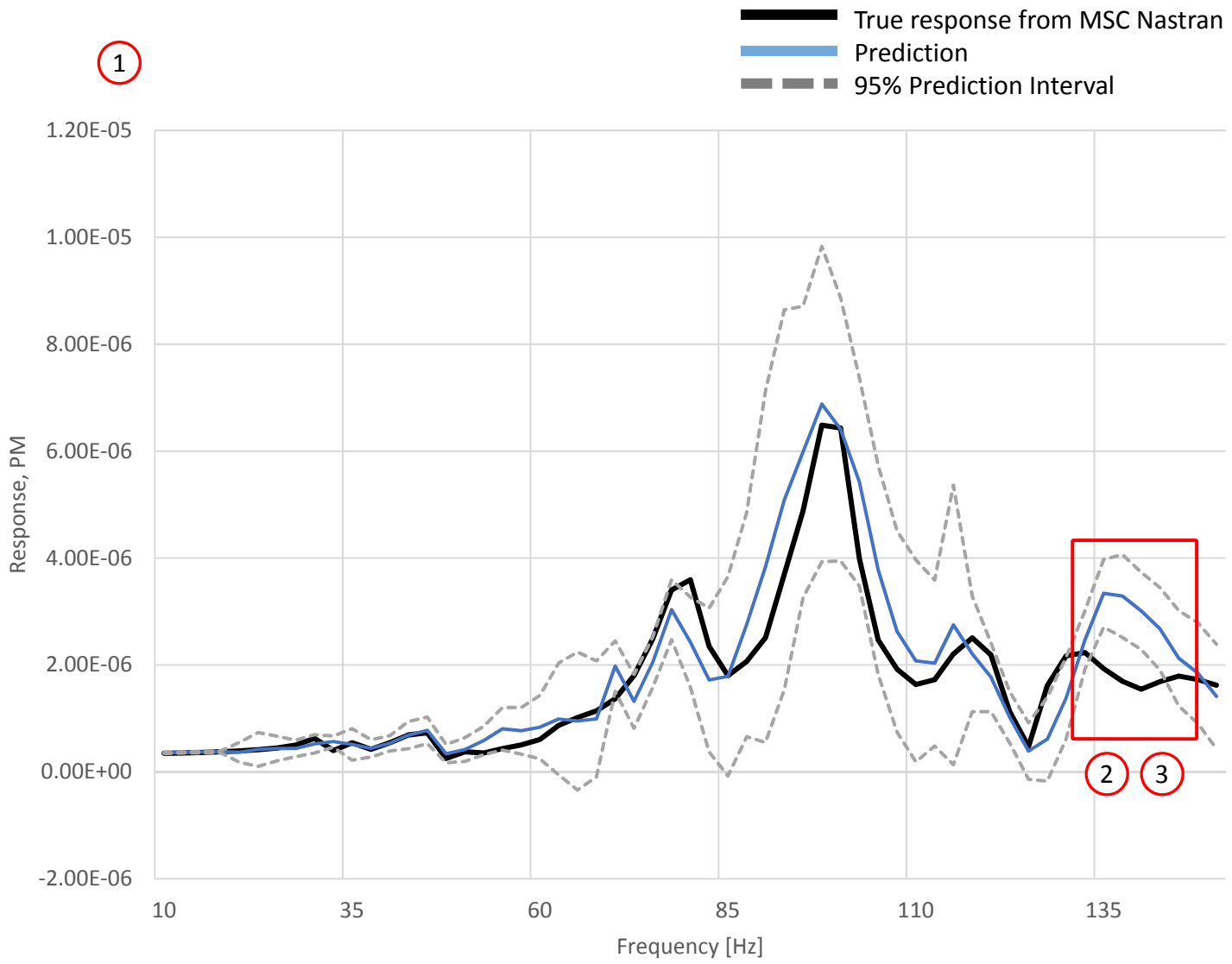
True response from MSC Nastran



Comparison of Prediction with MSC Nastran

1. Optional - Excel was used to overlap the MSC Nastran output over the predicted response
2. Note that the 95% prediction interval does not guarantee the true value is within this interval.
3. With a limited number of samples, the surrogate model poorly predicts the true response between 80-100Hz

- In some cases, using more samples improves the surrogate model. You are encouraged to repeat this exercise but with additional samples. For example, this prediction used 40 samples. Perhaps repeat this prediction with 50, 60 or 70 samples.

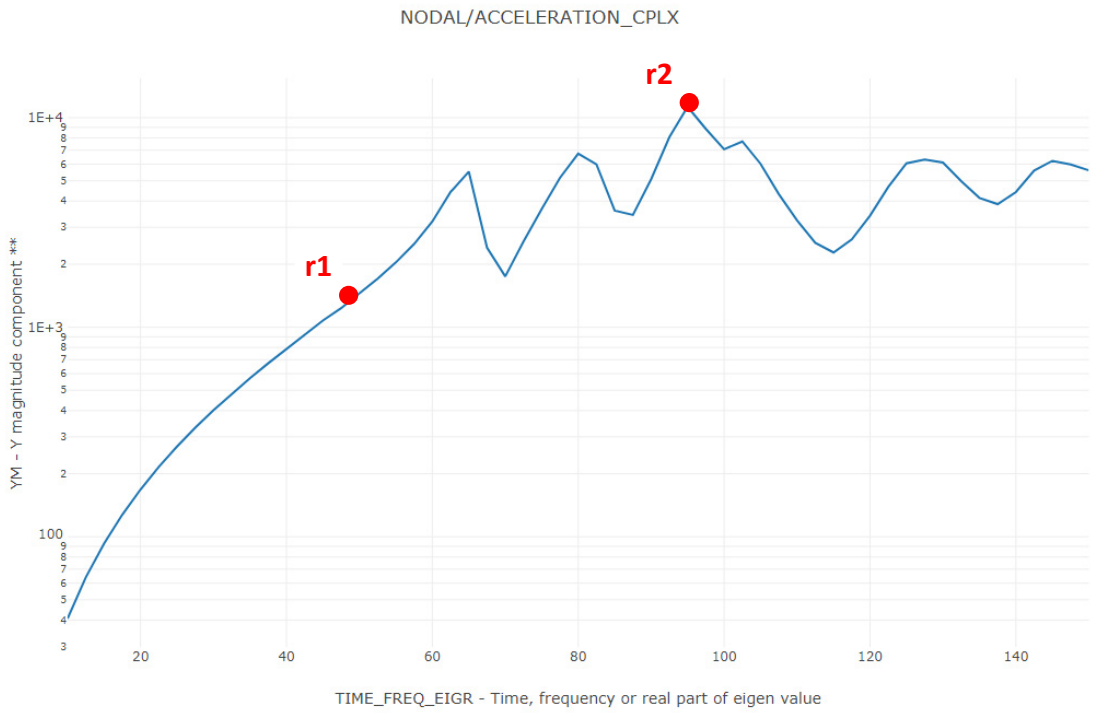


Creating Response vs. Frequency Plots with the HDF5 Explorer

Responses

Recall the following

- r1 is the response at 50Hz
- r2 is the maximum responses across all frequencies



ID: 1001 | SUBCASE: 12 | YM vs. TIME_FREQ_EIGR

Start Desktop App

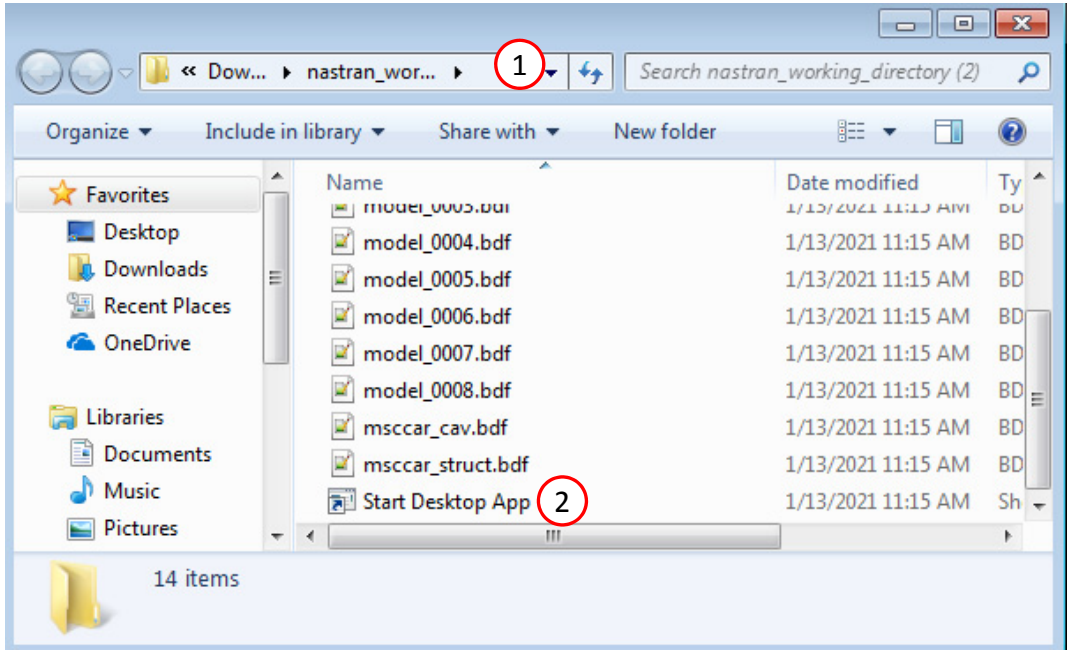
1. Open this folder: nastran_working_directory (2)
2. Inside of the new folder, double click on Start Desktop App
3. Click Open, Run or Allow Access on any subsequent windows

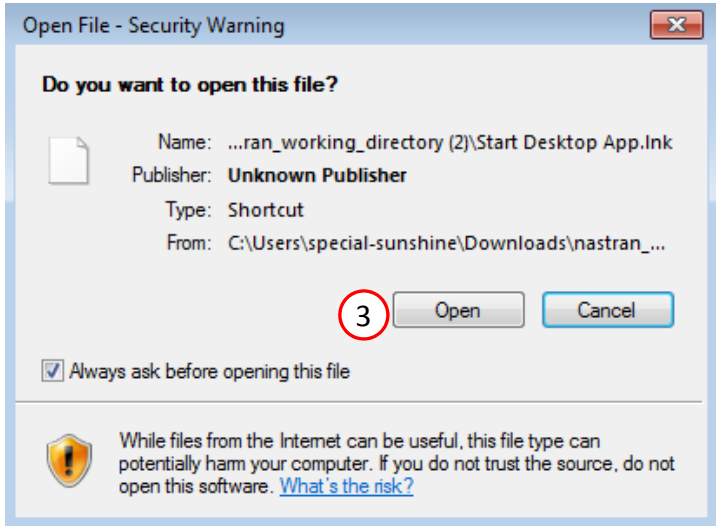
Using Linux?

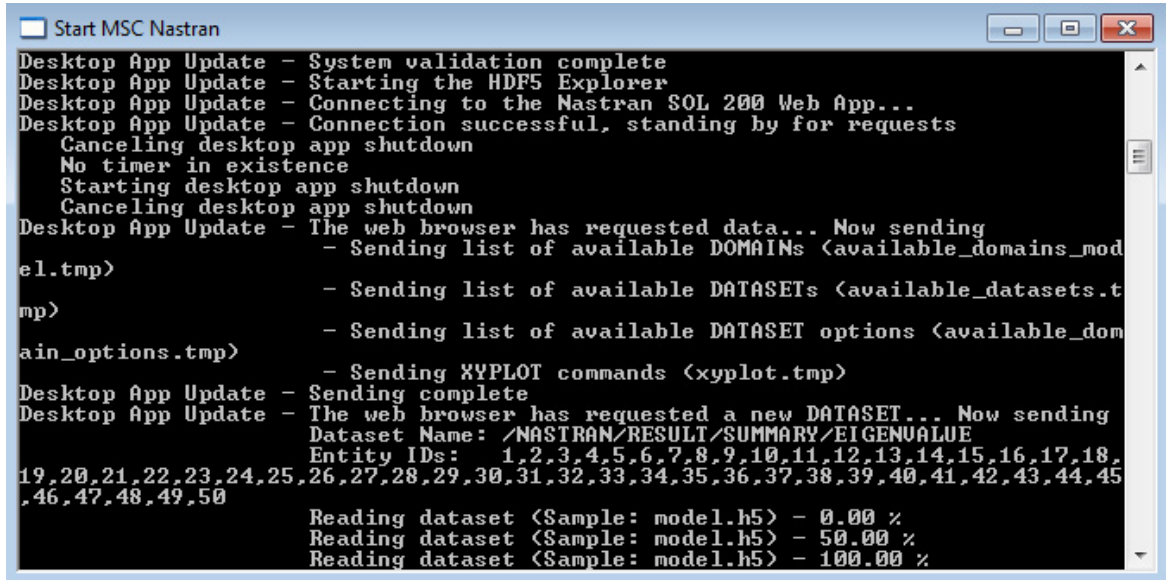
Follow these instructions:
1) Open Terminal
2) Navigate to the nastran_working_directory
   cd ./nastran_working_directory
3) Use this command to start the process
   ./Start_MSC_Nastran.sh

In some instances, execute permission must be granted to the directory. Use this command. This command assumes you are one folder level up.

sudo chmod -R u+x ./nastran_working_directory



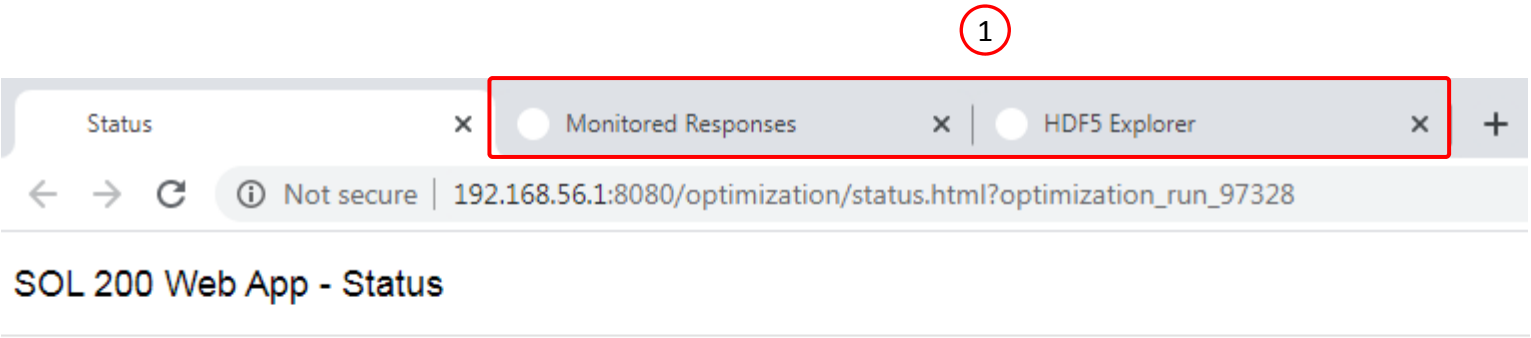




Results

Multiple web apps are automatically opened to display the results.

1. Use the tabs to switch between each web app
2. A description of each web app is given in the table.



2

Name of Web App	Purpose	Description
Monitored Responses	• The response value from each sample can be compared.	• After each MSC Nastran analysis, the response values are extracted from the H5 file and contained in a file named app_monitored_responses.csv. The Monitored Responses web app is used to create a bar chart of the values contained in this CSV file.
HDF5 Explorer	• This web app is used to probe each H5 file and generate XY plots.	

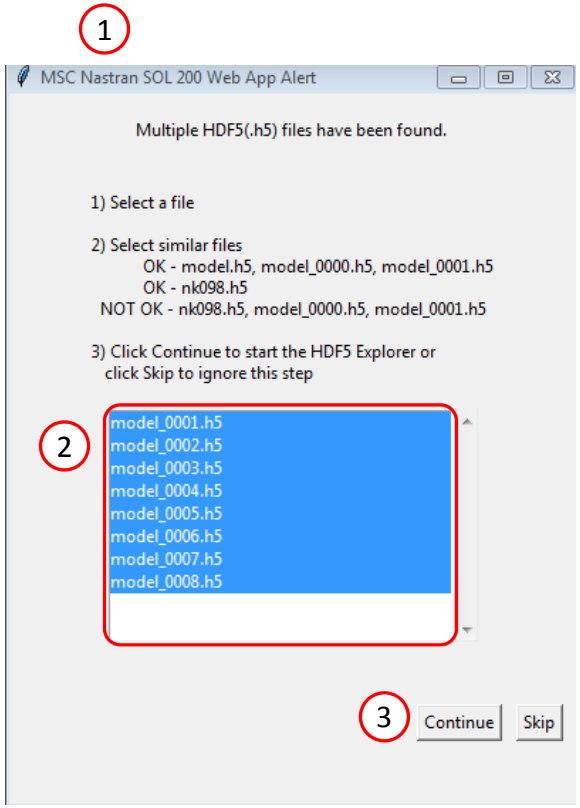
Review Results

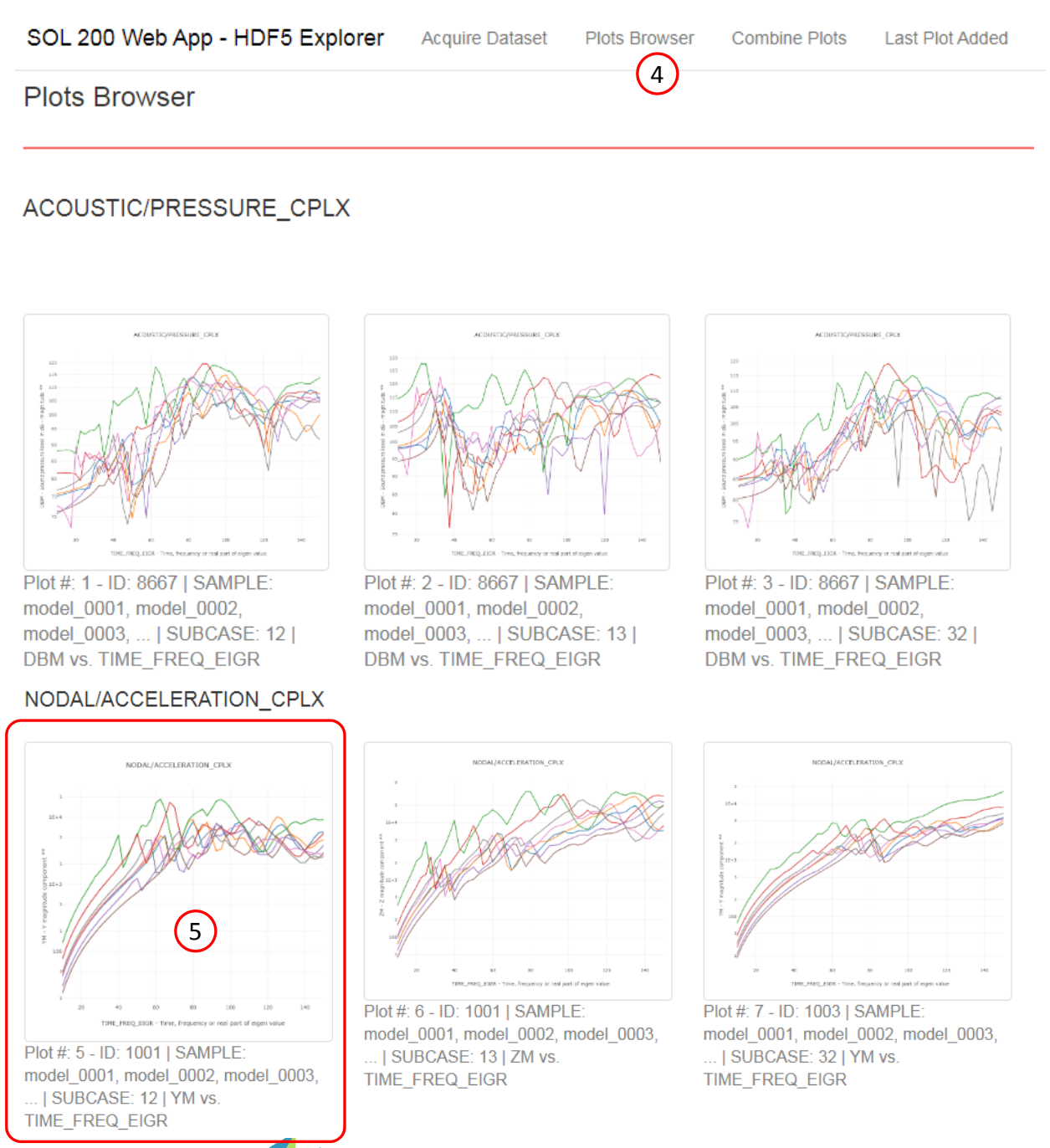
The following steps describe how to start the HDF5 Explorer and display the plots for responses r1 and r2.

1. A new window is opened
2. Select all H5 files in the list
3. Click Continue
4. Click Plots Browser
5. Click the indicated plot:
   - Plot #: 5 - ID: 1001 | SAMPLE: model_0001, model_0002, model_0003, ... | SUBCASE: 12 | YM vs. TIME_FREQ_EIGR

The HDF5 Explorer is broken into sections.

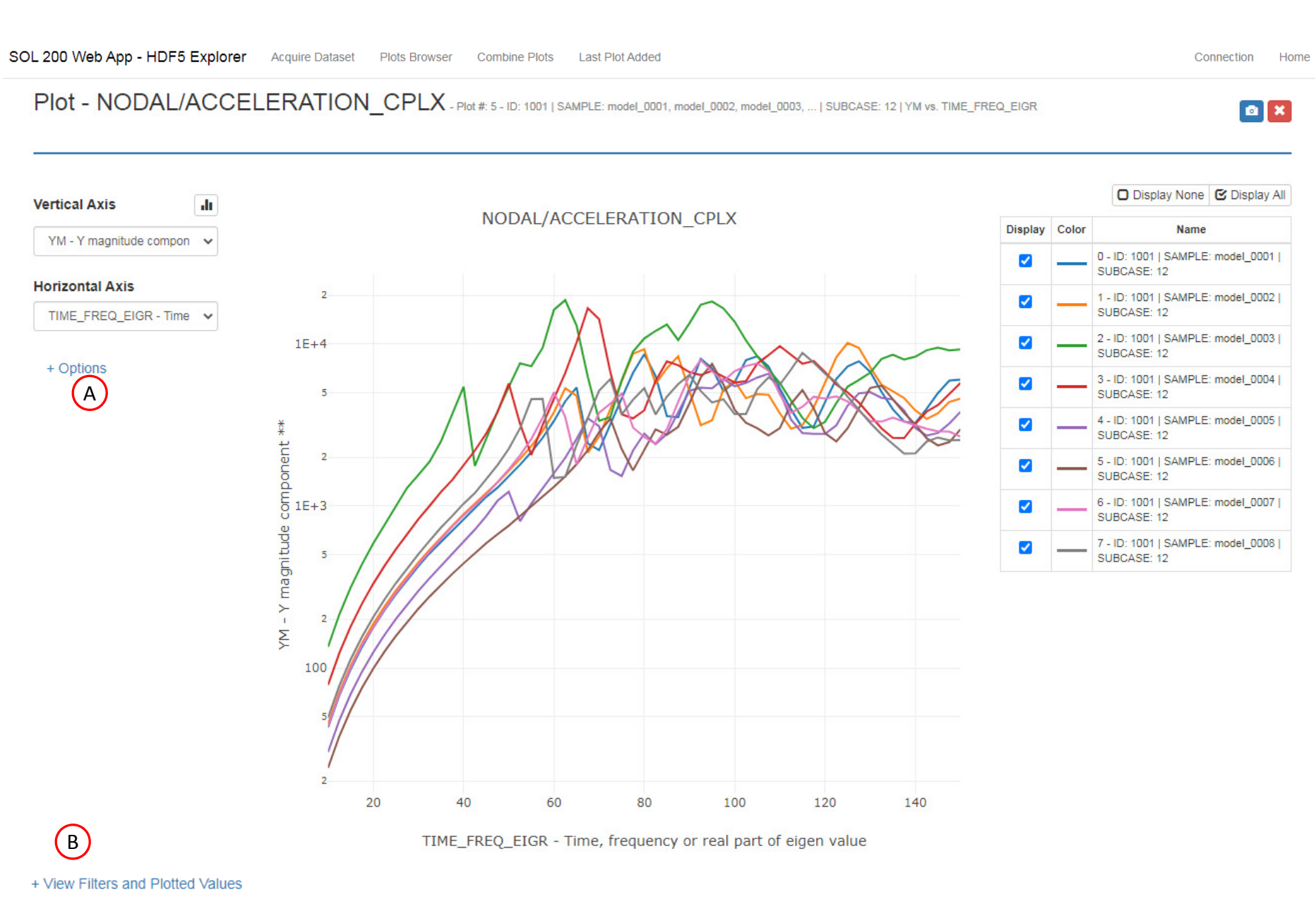
- Acquire Dataset – Specific datasets from the H5 file can be extracted in this section.
- Plots Browser – Use this section to navigate every plot created.
- Combine Plots – This section allows you to combine multiple plots. For example, you can create Load vs. Displacement plots in this section.
- Last Plot Added – This display the last plot that was created.





Review Results

This plot will be referenced later



The plots in the HDF5 explorer have additional functionalities that are hidden by default. Click on any of the following to show the extra functions.

A. + Options
B. + View Filters and Plotted Values

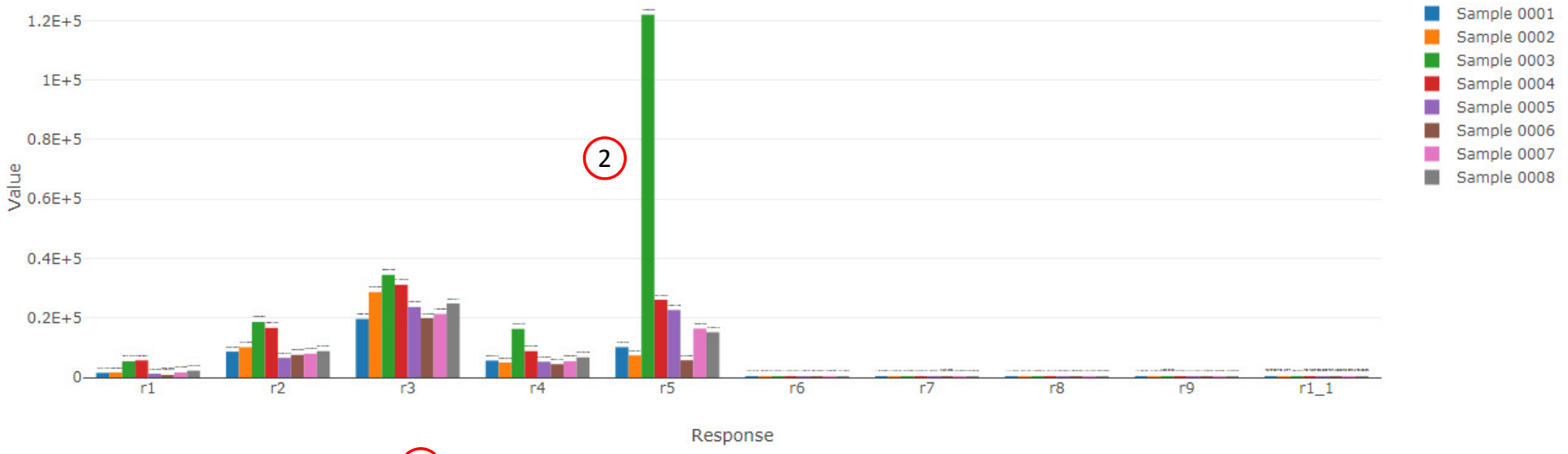
Users are encouraged to experiment with the additional functions.

Review Results

1. The Monitored Responses web app is opened
2. The value of each response and for each sample is displayed in a bar chart
3. A table lists the values for each response and sample.

A. The table titled Monitored Response can be interacted with. Each column in the table contains filters. Once a filter is modified, the Bar Chart will instantly update.
B. Additional functions include the ability to highlight the MAX and MIN bars, download a CSV file and reset the filters.

SOL 200 Web App - Monitored Responses (1) Home



(B)

Monitored Responses Display MAX and MIN | Download CSV | Reset Filters

Label	Dataset Name	Field	Field Description
r1 r1_1 r1_2 r1_3	ACOUSTIC/PRESSURE_CPLX NODAL/ACCELERATION_CPLX (A)	DBM YM ZM	Sound pressure level in dB - magr Y magnitude component ** Z magnitude component **
r1	NODAL/ACCELERATION_CPLX	YM	Y magnitude component **
r2	NODAL/ACCELERATION_CPLX	YM	Y magnitude component **
r3	NODAL/ACCELERATION_CPLX	ZM	Z magnitude component **
r4	NODAL/ACCELERATION_CPLX	YM	Y magnitude component **

Monitored Responses from Each Sample (3)

0001	0002	0003	0004	
1526.125681263411	1646.542449357661	5431.856987635404	5706.046062108631	1
8657.530528587466	10151.6078119792	18656.548989469935	16649.137630152713	6
19648.168717343582	28702.664023028425	34493.15381275541	31158.639324650096	2
5643.971287579098	4963.355450686416	16309.51034127708	8814.994819594214	5

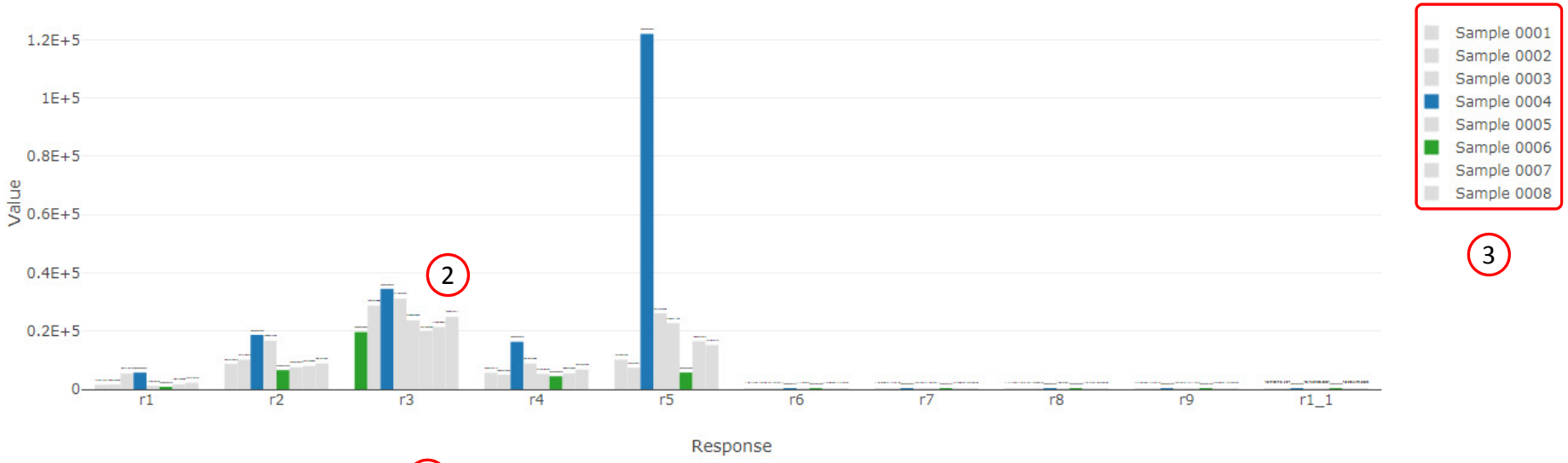
Review Results

1. Click Display MAX and MIN
2. The bars are now colored blue, green and gray
3. The legend is displayed on the top right corner

- When Display MAX and MIN is clicked, for each response the maximum bar is colored blue and the minimum is colored green.
- The coloring in the legend on the top right corner is only accurate for the first response displayed. In the figure shown, for response r1, sample 4 produces the maximum response and sample 6 produces the minimum response.

SOL 200 Web App - Monitored Responses

Home



Monitored Responses Display MAX and MIN | Download CSV | Reset Filters

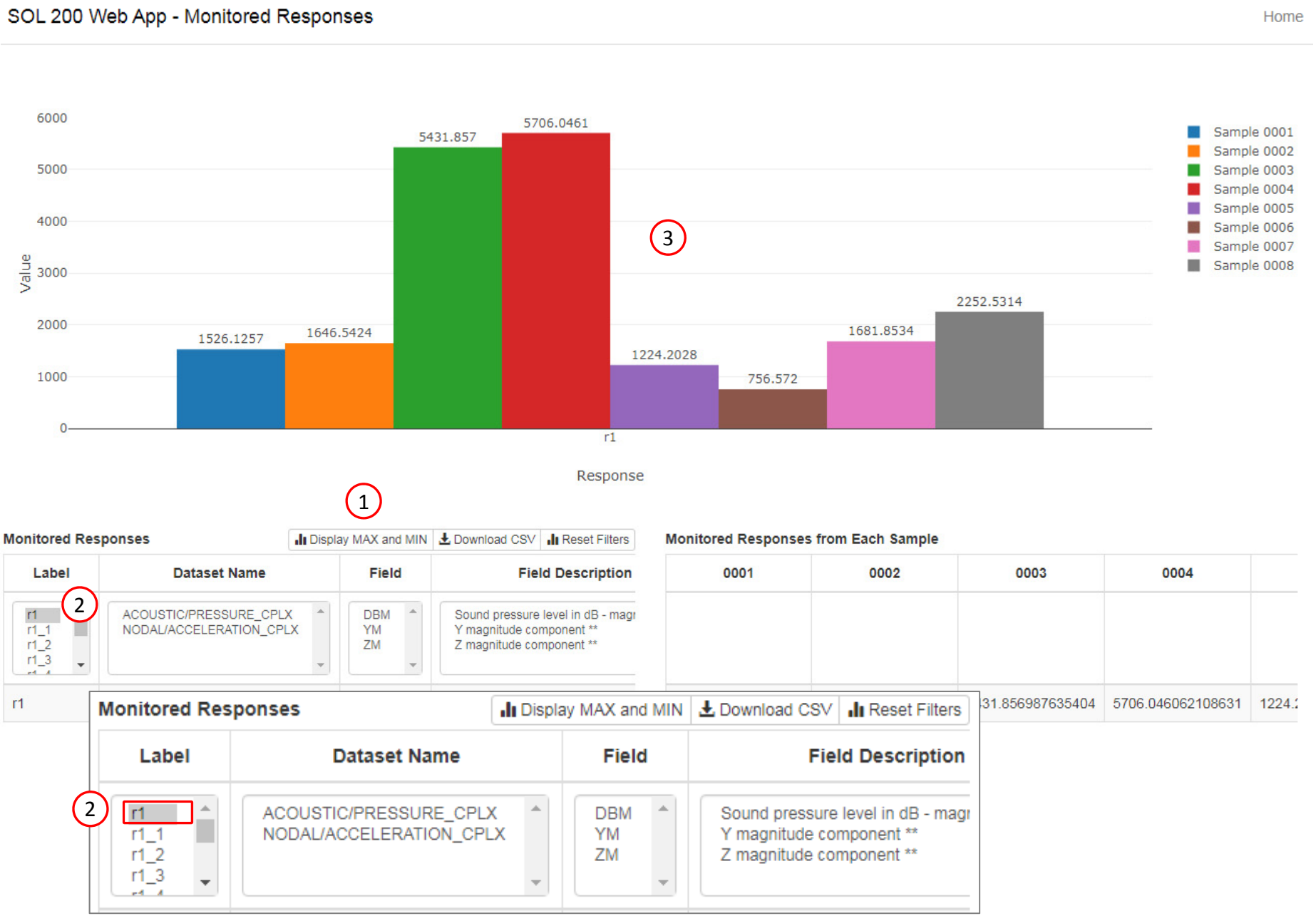
Label	Dataset Name	Field	Field Description
r1 r1_1 r1_2 r1_3	ACOUSTIC/PRESSURE_CPLX NODAL/ACCELERATION_CPLX	DBM YM ZM	Sound pressure level in dB - magr Y magnitude component ** Z magnitude component **
r1	NODAL/ACCELERATION_CPLX	YM	Y magnitude component **
r2	NODAL/ACCELERATION_CPLX	YM	Y magnitude component **
r3	NODAL/ACCELERATION_CPLX	ZM	Z magnitude component **
r4	NODAL/ACCELERATION_CPLX	YM	Y magnitude component **
r5	NODAL/ACCELERATION_CPLX	ZM	Z magnitude component **
r6	ACOUSTIC/PRESSURE_CPLX	DBM	Sound pressure level in dB - ma

Monitored Responses from Each Sample

0001	0002	0003	0004	
1526.125681263411	1646.542449357661	5431.856987635404	5706.046062108631	1
8657.530528587466	10151.6078119792	18656.548989469935	16649.137630152713	6
19648.168717343582	28702.664023028425	34493.15381275541	31158.639324650096	2
5643.971287579098	4963.355450686416	16309.51034127708	8814.994819594214	5
10180.927393382006	7386.50209251185	122054.75754985167	26125.939837904127	2
114.1514155253656	114.94181882212138	118.76114036753917	119.51549857017466	1

Review Results

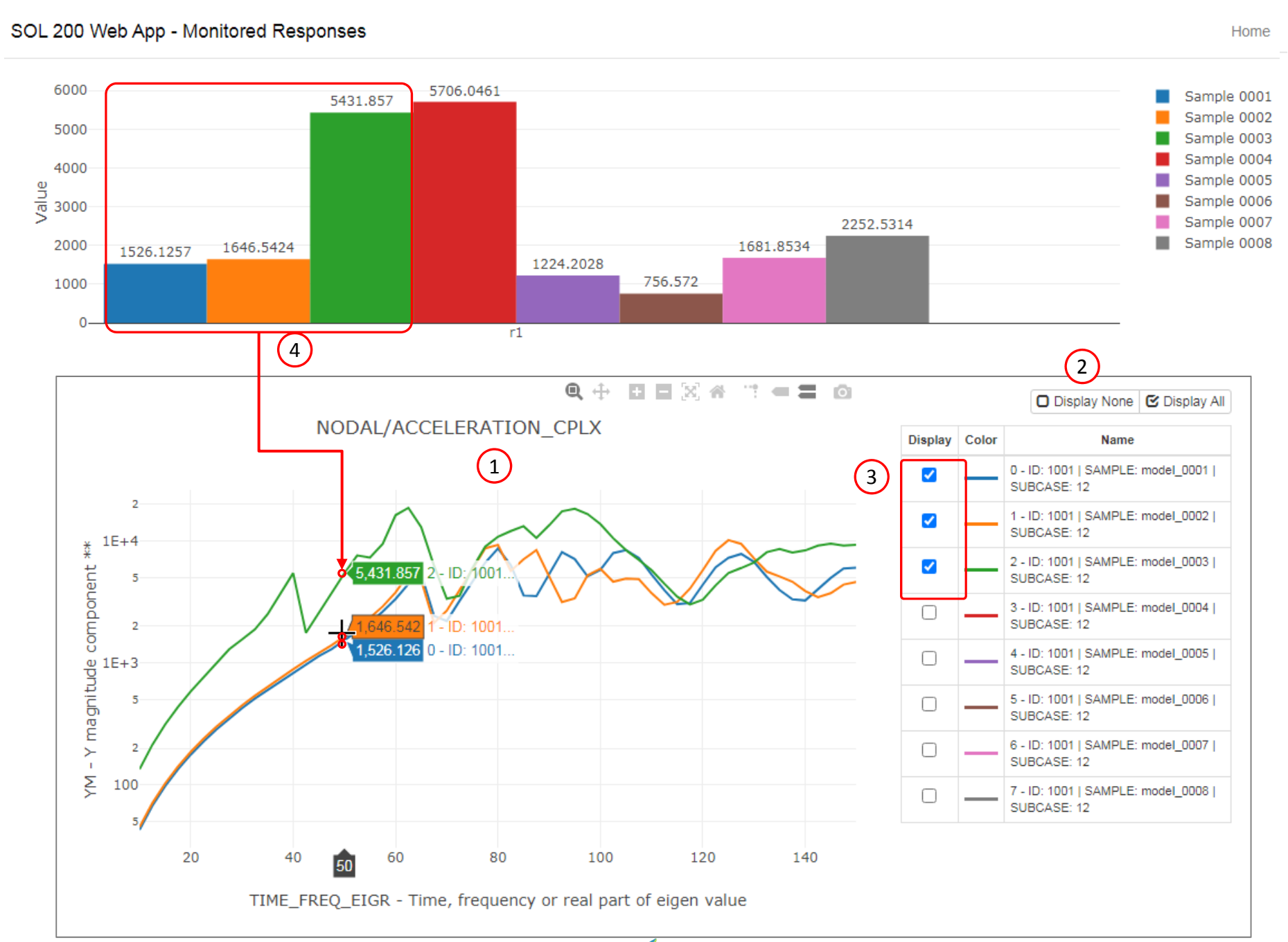
1. Click Display MAX and MIN
2. In the filters, select the following:
   - Label: r1
3. Only the responses for response r7 are now shown



Review Results

1. Refer to the plot that was previously shown
2. Click Display None
3. Mark the checkboxes for the first 3 rows (Samples 0, 1 and 2)
4. The response values that were extracted and displayed in the bar chart match the values at 50Hz in the Acceleration vs. Frequency plot

- Refer to the Appendix for an explanation on the use of the following:
  - Monitor the maximum or minimum response, whichever has the greatest absolute value: Yes, No or blank

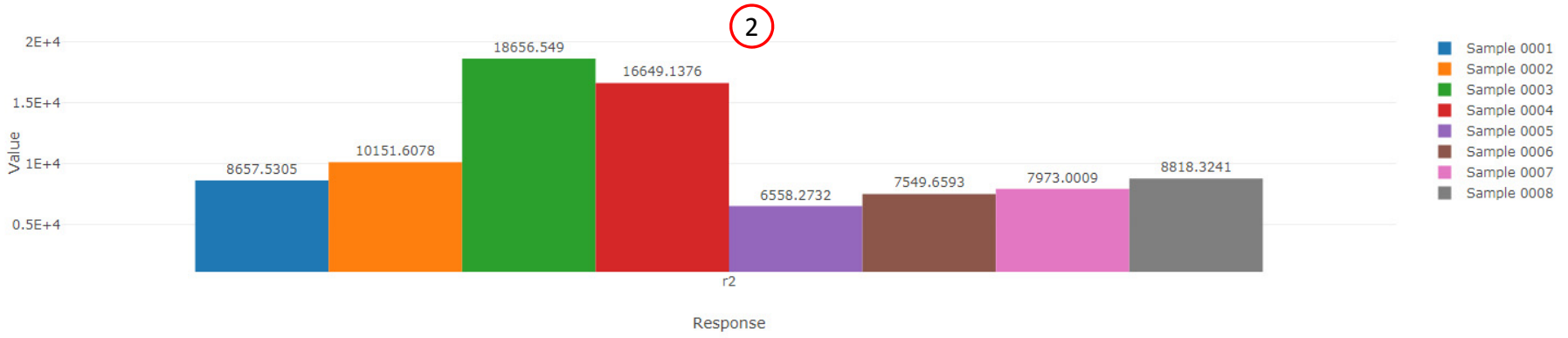


Review Results

1. In the filters, select only response r2
2. Only the responses for response r2 are now shown

SOL 200 Web App - Monitored Responses

Home



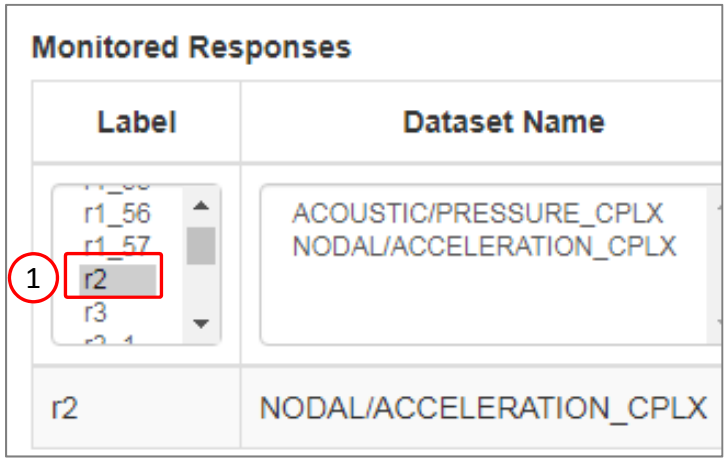
Monitored Responses

Display MAX and MIN | Download CSV | Reset Filters

Label	Dataset Name	Field	Field Description
r1_56 r1_57 r2 r3 (1)	ACOUSTIC/PRESSURE_CPLX NODAL/ACCELERATION_CPLX	DBM YM ZM	Sound pressure level in dB - magnitude ** Y magnitude component ** Z magnitude component **
r2	NODAL/ACCELERATION_CPLX	YM	Y magnitude component **

Monitored Responses from Each Sample

0001	0002	0003	0004	0005
8657.530528587466	10151.6078119792	18656.548989469935	16649.137630152713	6558.273211742



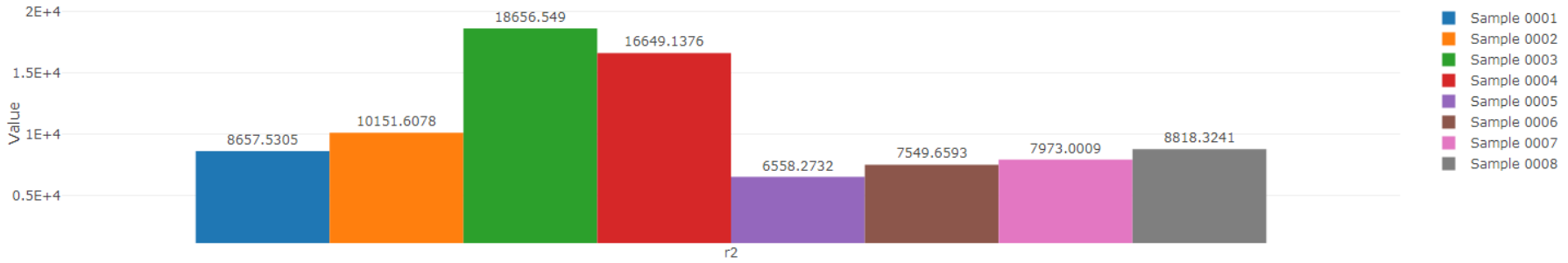
Review Results

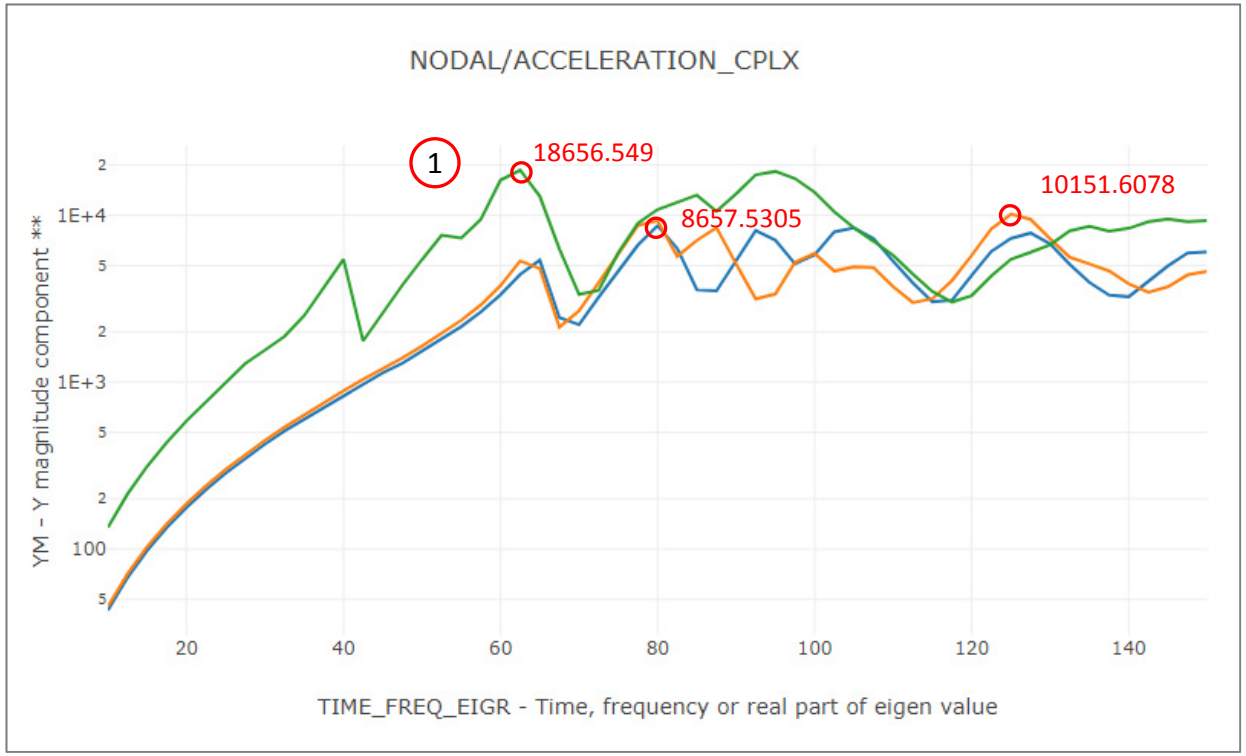
1. The response values that were extracted and displayed in the bar chart match the peak values in the Acceleration vs. Frequency plot

- Refer to the Appendix for an explanation on the use of the following:
  - Monitor the maximum or minimum response, whichever has the greatest absolute value: Yes, No or blank

SOL 200 Web App - Monitored Responses

Home





End of Tutorial

Appendix

Appendix Contents

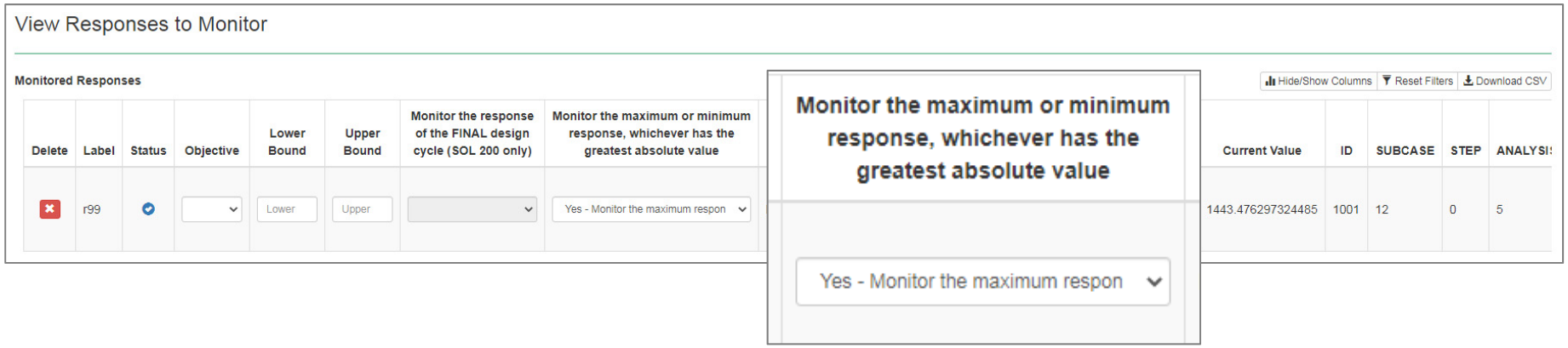
- Response Configuration
  - Monitor the maximum or minimum response, whichever has the greatest absolute value: Yes, No or blank
- How to import and edit previous files
- What is Gaussian Process Regression?

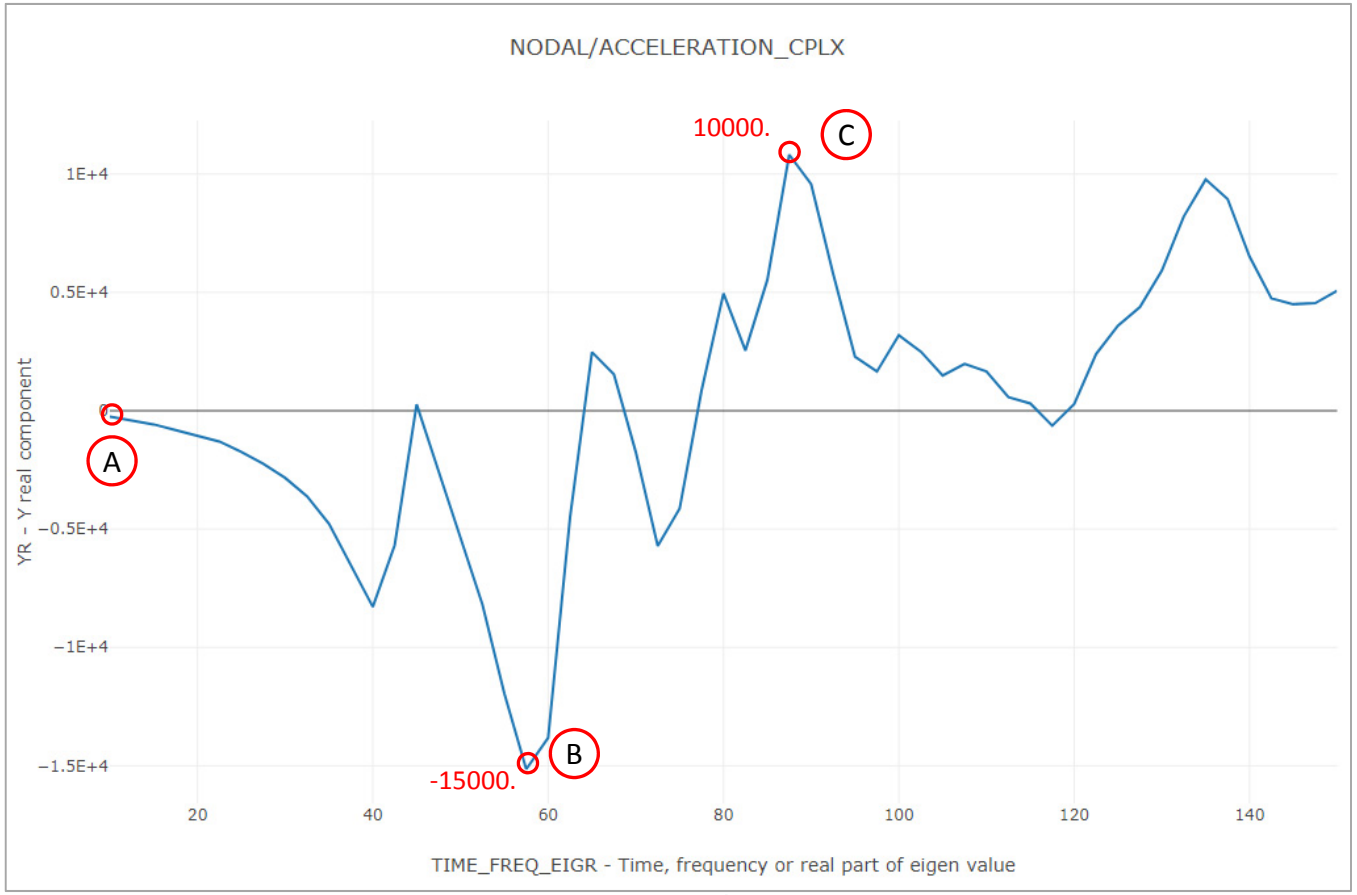
Response Configuration

During this tutorial, this option was used:

- Monitor the maximum or minimum response, whichever has the greatest absolute value : Yes

Suppose response r99 is configured for 10 seconds and corresponds to point A on the plot. When Yes is used for the option, the response furthest from the horizontal axis is monitored. In this example, points B and c are furthest from the horizontal axis. Since point B is furthest from the horizontal axis, a value of -15000.0 is monitored.





How to import and edit previous files

How to import and edit previous files

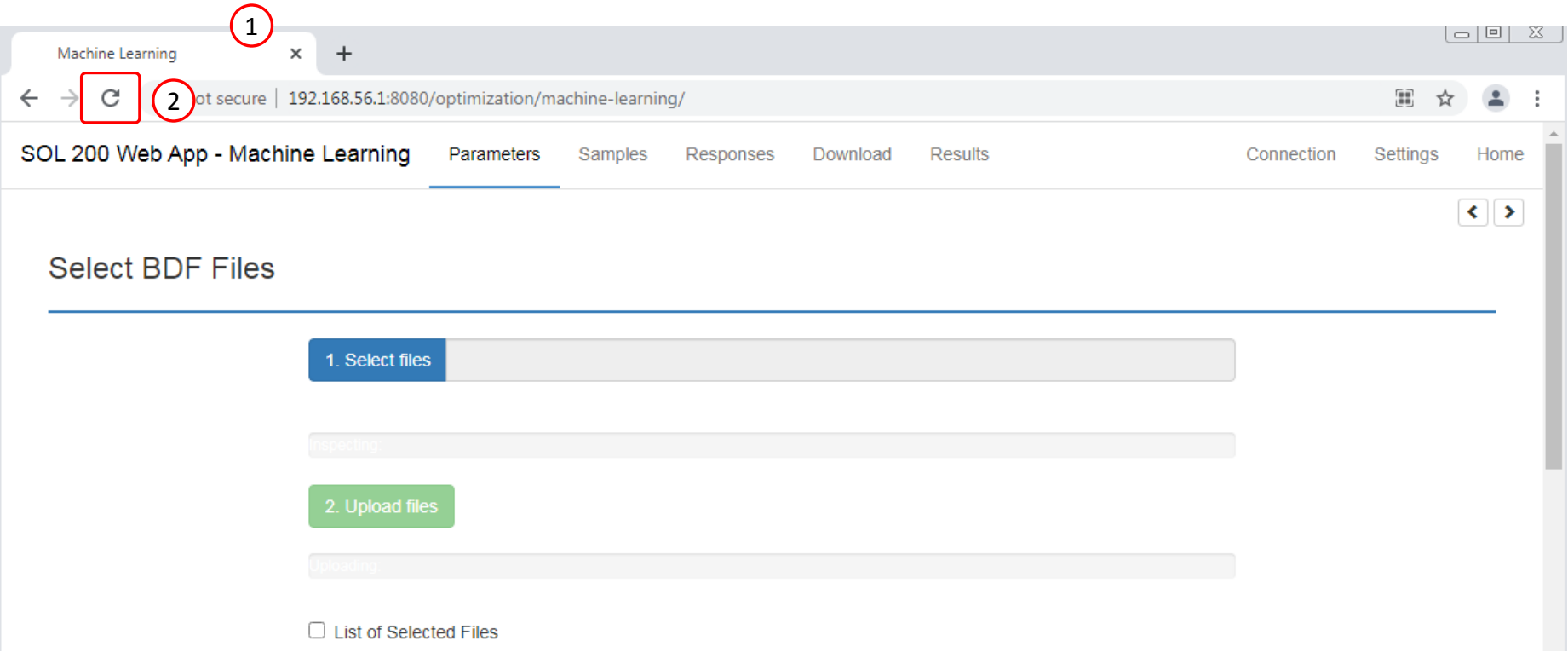
The parameters, samples and responses are contained in the following files

- app.config
- BDF files

These files may be imported back to the Machine Learning web app, and any parameters, samples and responses can be reconfigured

Import

1. Return to the window or tab that has the Machine Learning web app opened
2. Refresh the web page to start a new session

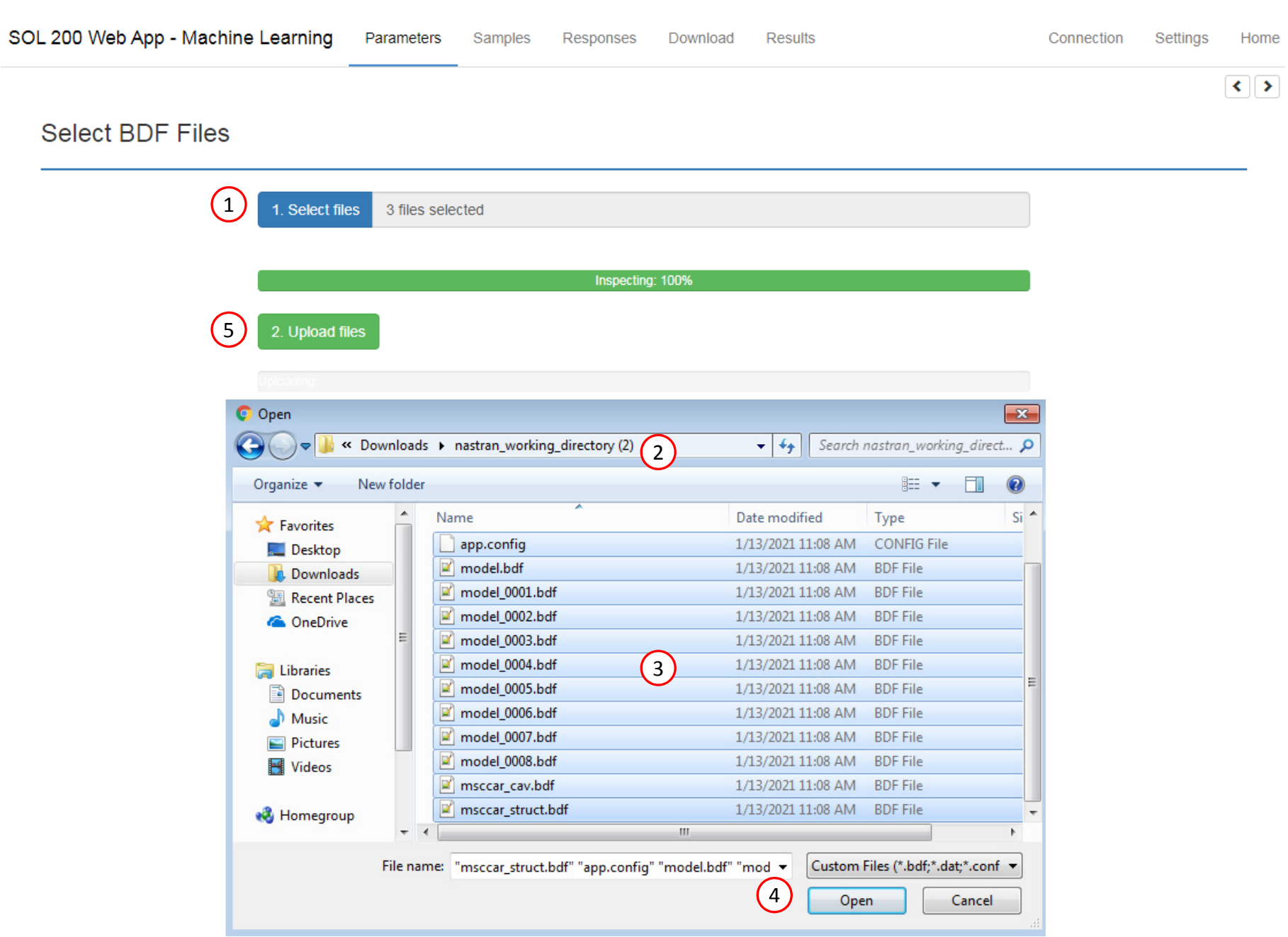


- Refreshing the page is only required when the *Select files* button is disabled.

Import

1. Click Select Files
2. Navigate to the folder named nastran_working_directory (2)
3. Select all the BDF files AND the app.config file.
4. Click Open
5. Click Upload files

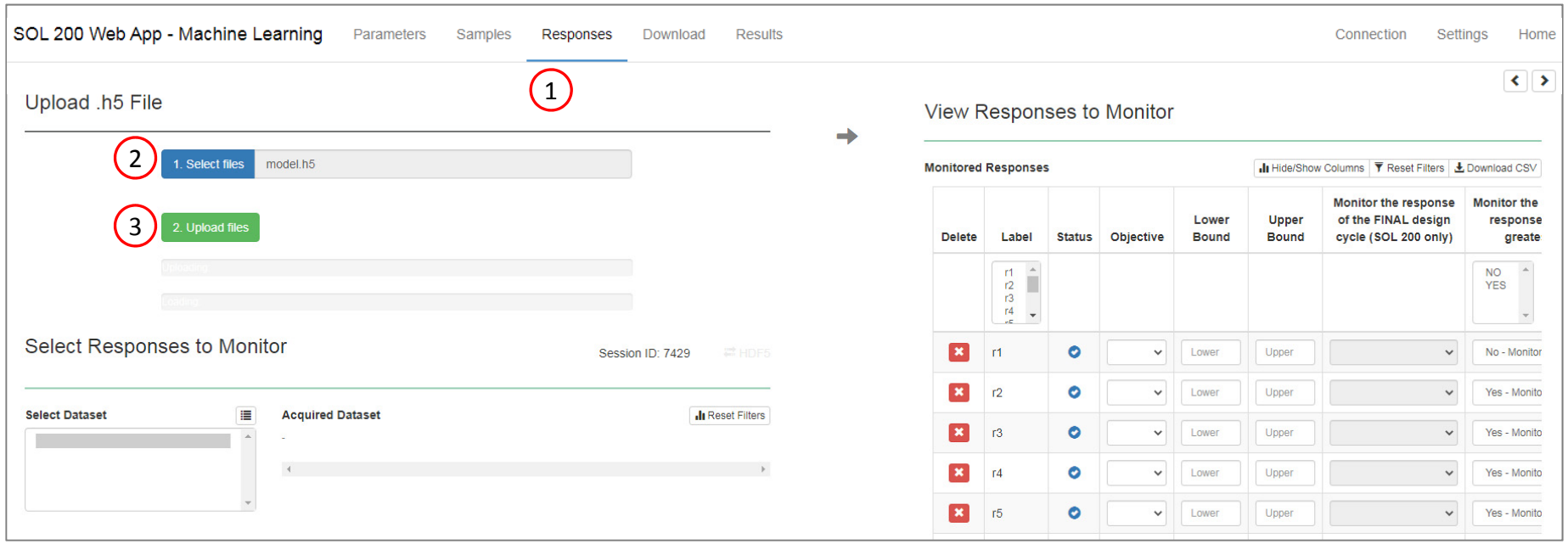
- All imports require the app.config file to be selected.

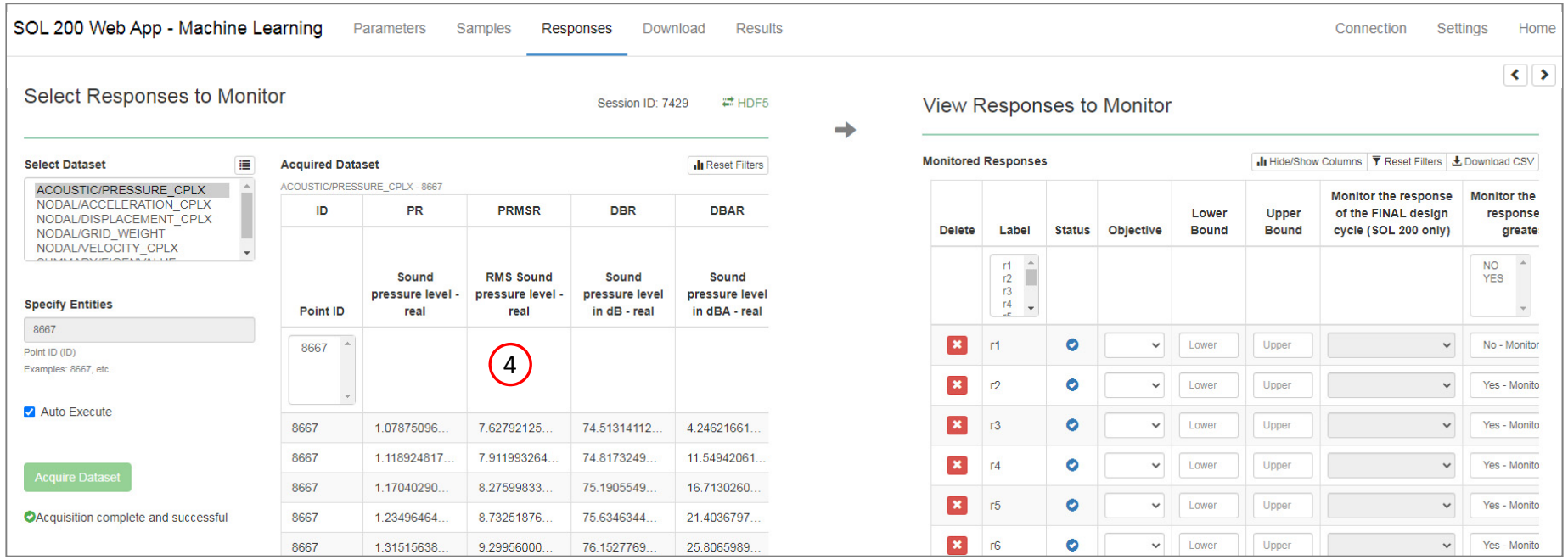


Import

For the Response section, the H5 file will need to be re-uploaded.

1. Click Responses
2. Select the H5 file
3. Click Upload
4. Data from the H5 is loaded and ready to use





Import

After import, any Parameter, Samples or Responses can be modified.

SOL 200 Web App - Machine Learning | Parameters | Samples | Responses | Download | Results | Connection | Settings | Home

Select BDF Files

1. Select files — 4 files selected

Inspecting: 100%

2. Upload files

Uploading: 100 %

List of Selected Files

Select Parameters

```
$__1___||__2___||__3___||__4___||__5___||__6___||__7___||__8___||__9___||__10__|


EIGRL   1               225.
EIGRL   2               300.
FORCE   212     1001            500.    0.0     1.0     0.0
FORCE   213     1001            1000.   0.0     0.0     1.0
FORCE   232     1003            500.    0.0     1.0     0.0
FORCE   233     1003            1000.   0.0     0.0     1.0
FREQ1   5       10.     2.5     56
MAT1    7       210000.0        0.3     7.90E-06
MAT1    8       62000.0         0.24    2.30E-06
MAT10   6               1.23E-12340000.0
PARAM   G       0.06
PARAM   GFL     0.12
PARAM   LFREQ   0.1
PARAM   PREFDB  2.E-11
PARAM   WTMASS  .001
PSHELL  1       7       %x1%    7       1.0             0.833333
```

Configure Parameters

Delete	Parameter	Status	Low	High	Comments
✖	x1	✔	1.	6.	Field 4 of PSHE
✖	x2	✔	1.	6.	Field 4 of PSHE
✖	x8	✔	1.	6.	Field 4 of PSHE
✖	x11	✔	1.	6.	Field 4 of PSHE

What is Gaussian Process Regression?

Gaussian Process Regression Overview

Training Data

D_n: Training data X_n (inputs) and Y_n (outputs)

Kernel (Covariance Function)*

$k(x, x') = \Sigma(x, x')$

MVN Conditioning Equations

$$\mu(\mathcal{X}) = \Sigma(\mathcal{X}, X_n)\Sigma_n^{-1}Y_n \qquad \text{(Prediction Model)}$$

$$\Sigma(\mathcal{X}) = \Sigma(\mathcal{X}, \mathcal{X}) - \Sigma(\mathcal{X}, X_n)\Sigma_n^{-1}\Sigma(\mathcal{X}, X_n)^\top$$

Predicted Values

Mean: $\mu(x)$

Prediction Uncertainty

Variance: $\sigma^2(x)$

Sometimes expressed as $\Sigma(x)$

* Hyperparameter optimization is part of the procedure but not covered in this presentation

** $\mu(x)$: This function corresponds to the mean function or kriging model. This function is the prediction model, also known as the surrogate model, meta model or emulator.

Multivariate Normal (MVN) Conditioning Equations

The following must be calculated: Covariance Matrix, Mean and Variance

Covariance Matrix

$$\Sigma = \begin{pmatrix} \Sigma(\chi,\chi) & \Sigma(\chi, X_n) \\ \Sigma(X_n,\chi) & \Sigma_n = \Sigma(X_n, X_n) \end{pmatrix}$$

X_n: Training locations
χ: Testing (predictive) locations

Apply the covariance function $\Sigma(x, x')$ (kernel $k(x, x')$)

- $\Sigma(\chi,\chi)$: Covariance between testing (predictive) locations and themselves
- $\Sigma(\chi, X_n)$: Covariance between testing (predictive) and training locations
- $\Sigma(\chi, X_n)$: Covariance between training and testing (predictive) locations, which is the transpose of $\Sigma(\chi, X_n)$
- $\Sigma_n = \Sigma(X_n, X_n)$: Covariance between training locations and themselves

MVN Conditioning Equations (Mean and Variance)

Also referred to as "Gaussian process regression," "kriging" or "kriging equations"

$$\text{mean} \quad \mu(\mathcal{X}) = \Sigma(\mathcal{X}, X_n)\Sigma_n^{-1} Y_n$$

Prediction Model (Vary χ to make predictions)

$$\text{and variance} \quad \Sigma(\mathcal{X}) = \Sigma(\mathcal{X},\mathcal{X}) - \Sigma(\mathcal{X}, X_n)\Sigma_n^{-1}\Sigma(\mathcal{X}, X_n)^\top$$

Prediction Uncertainty

Example 1

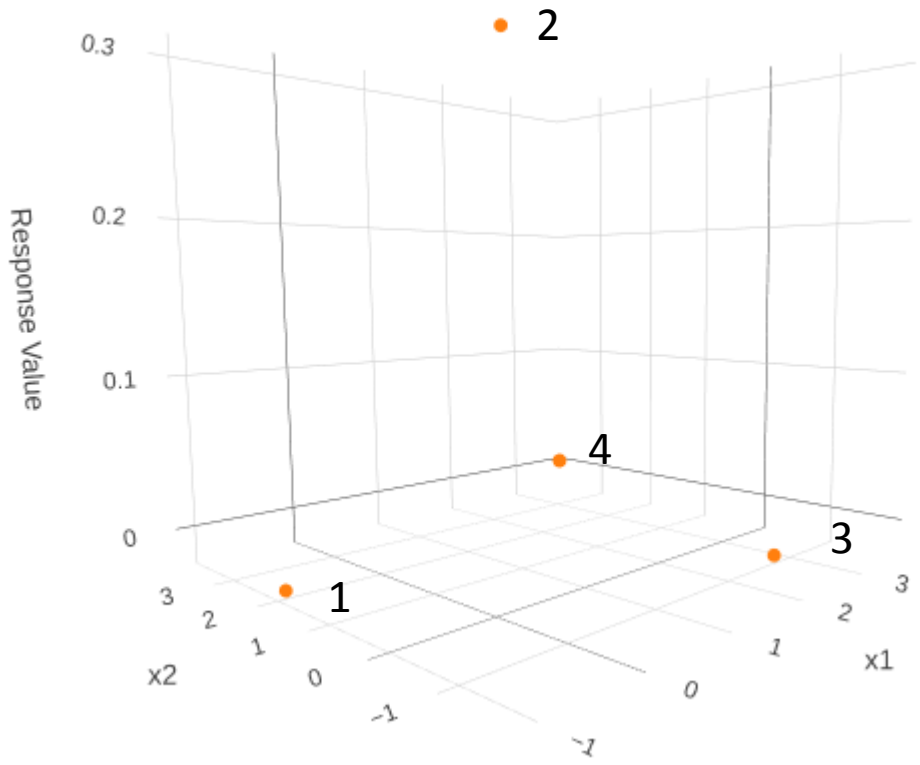
Example 1

Suppose a black box function was executed at 4 different samples (x1, x2 combinations)

With limited data (x and y), what does the response surface look like?

Training Data

Sample	x1	x2	y
1	-1.03	1.76	-1.56E-02
2	.49	.49	3.04E-01
3	1.77	-1.77	3.38E-03
4	3.62	3.76	5.43E-12



Training Data and Testing (Predictive) Locations

Suppose you have the following training data (X_n and Y_n) and testing locations (χ)

- X_n : The training design consists of 4 points
- χ : The test design (locations to make predictions) consists of 2 points

$$X = \begin{bmatrix} \chi \\ X_n \end{bmatrix} = \begin{bmatrix} .35 & .69 \\ .65 & .46 \\ -1.03 & 1.76 \\ .49 & .49 \\ 1.77 & -1.77 \\ 3.62 & 3.76 \end{bmatrix}$$

$$\begin{bmatrix} y* \\ Y_n \end{bmatrix} = \begin{bmatrix} ? \\ ? \\ -1.56e-02 \\ 3.04e-01 \\ 3.38e-03 \\ 5.43e-12 \end{bmatrix}$$

The goal is make predictions ($y*$) for points in χ

Note

- X_n: inputs of the training data
- Y_n: outputs of the training data
- χ or x: inputs of the testing data (predictive locations, i.e. points to make predictions)
- $y*$: predicted outputs
- D_n: Training data X_n and Y_n

X: upper case of Greek letter chi (pronounced kai in English)
χ: lower case of Greek letter chi

Calculation of the Covariance Matrix

1. Select a covariance (kernel) function
   - Many covariance functions (kernels) exist: Radial Basis Function (RBF), Matern 5/2, 3/2, Exponential, …
   - For this example, a form of the RBF covariance function is used. This covariance function is described as the "inverse exponentiated squared Euclidean distance"

$$k(x, x') = \Sigma(x, x') = \exp\{-||x - x'||^2\} = e^{-\|x-x'\|^2}$$

2. Calculate D (Distance Matrix)

$$D = \|X - X\|^2$$

"Norm between X and X, squared"

3. Calculate Σ (Covariance Matrix)

$$\Sigma = e^{-D}$$

Calculation of D

$$D = \begin{bmatrix} \sqrt{(.35 - .35)^2 + (.69 - .69)^2} = 0 & \sqrt{(.35 - .65)^2 + (.69 - .46)^2} = .1429 & \sqrt{(.35 - -1.03)^2 + (.69 - 1.76)^2} = 3.0493 & \sqrt{(.35 - .49)^2 + (.69 - .49)^2} = .0596 & \sqrt{(.35 - 1.77)^2 + (.69 - -1.77)^2} = 8.068 & \sqrt{(.35 - 3.62)^2 + (.69 - 3.76)^2} = 20.1178 \\ .1429 & \sqrt{(.65 - .65)^2 + (.46 - .46)^2} = 0 & \sqrt{(.65 - -1.03)^2 + (.46 - 1.76)^2} = 4.5124 & \sqrt{(.65 - .49)^2 + (.46 - .49)^2} = .0265 & \sqrt{(.65 - 1.77)^2 + (.46 - -1.77)^2} = 6.2273 & \sqrt{(.65 - 3.62)^2 + (.46 - 3.76)^2} = 19.7109 \\ 3.0493 & 4.5124 & \sqrt{(-1.03 - -1.03)^2 + (1.76 - 1.76)^2} = 0 & \sqrt{(-1.0\,3 - .49)^2 + (1.76 - .49)^2} = 3.9233 & \sqrt{(-1.03 - 1.77)^2 + (1.76 - -1.77)^2} = 20.3009 & \sqrt{(-1.03 - 3.62)^2 + (1.76 - 3.76)^2} = 25.6225 \\ .0596 & .0265 & 3.9233 & \sqrt{(.49 - .49)^2 + (.49 - .49)^2} = 0 & \sqrt{(.49 - 1.77)^2 + (.49 - -1.77)^2} = 6.746 & \sqrt{(.49 - 3.62)^2 + (.49 - 3.76)^2} = 20.4898 \\ 8.068 & 6.2273 & 20.3009 & 6.746 & \sqrt{(1.77 - 1.77)^2 + (-1.7\,7 - -1.77)^2} = 0 & \sqrt{(1.77 - 3.62)^2 + (-1.77 - 3.76)^2} = 34.0034 \\ 20.1178 & 19.7109 & 25.6225 & 20.4898 & 34.0034 & \sqrt{(3.62 - 3.62)^2 + (3.76 - 3.76)^2} = 0 \end{bmatrix}$$

Calculation of Σ

$$\Sigma = \begin{bmatrix} e^{0} = 1 & e^{-.1429} = .8668 & e^{-3.0493} = .0474 & e^{-.0596} = .9421 & e^{-8.068} = .0003 & e^{-20.1178} = 1.832\text{e-}9 \\ .8668 & e^{0} = 1 & e^{-4.5124} = .0110 & e^{-.0265} = .9738 & e^{-6.2273} = .0020 & e^{-19.7109} = 2.8\text{e-}9 \\ .0474 & .0110 & e^{0} = 1 & e^{-3.9233} = .0198 & e^{-20.3009} = 1.5\text{e-}9 & e^{-25.6225} = 7.5\text{e} - 12 \\ .9421 & .9738 & .0198 & e^{0} = 1 & e^{-6.746} = .0012 & e^{-20.4898} = 1.263\text{e-}9 \\ .0003 & .0020 & 1.5\text{e-}9 & .0012 & e^{0} = 1 & e^{-34.0034} = 1.7\text{e} - 15 \\ 1.832\text{e-}9 & 2.8\text{e-}9 & 7.5\text{e} - 12 & 1.263\text{e-}9 & 1.7\text{e} - 15 & e^{0} = 1 \end{bmatrix}$$

Calculation of Σ

$$\Sigma = \begin{bmatrix} \Sigma(\chi,\chi) & \Sigma(\chi,X_n) \\ \Sigma(X_n,\chi) & \Sigma_n = \Sigma(X_n,X_n) \end{bmatrix}$$

$\Sigma(\chi,\chi)$:

$e^0 = 1$	$e^{-.1429} = .8668$
.8668	$e^0 = 1$

$\Sigma(\chi,X_n)$:

$e^{-3.0493} = .0474$	$e^{-.0596} = .9421$	$e^{-8.068} = .0003$	$e^{-20.1178} = 1.832\text{e-}9$
$e^{-4.5124} = .0110$	$e^{-.0265} = .9738$	$e^{-6.273} = .0020$	$e^{-19.7109} = 2.8\text{e-}9$

$\Sigma(X_n,\chi)$:

.0474	.0110
.9421	.9738
.0003	.0020
1.832e-9	2.8e-9

$\Sigma_n = \Sigma(X_n,X_n)$:

$e^0 = 1$	$e^{-3.9233} = .0198$	$e^{-20.3009} = 1.5\text{e-}9$	$e^{-25.6225} = 7.5\text{e}-12$
.0198	$e^0 = 1$	$e^{-6.746} = .0012$	$e^{-20.4898} = 1.263\text{e-}9$
1.5e-9	.0012	$e^0 = 1$	$e^{-34.0034} = 1.7\text{e}-15$
7.5e − 12	1.263e-9	1.7e − 15	$e^0 = 1$

Since Σ is symmetric, note that $\Sigma(X_n,\chi) = \Sigma(\chi,X_n)^{\mathrm{T}}$

Calculation of Predictive Quantities

The MVN conditioning equations are used to determine the predictive quantities mean and variance

$$\text{mean} \quad \mu(\mathcal{X}) = \Sigma(\mathcal{X}, X_n)\Sigma_n^{-1}Y_n$$

$$\mu(\chi) = y* = \begin{pmatrix} 0.2849657 \\ 0.2954011 \end{pmatrix}$$ Predicted values for locations in χ

$$\text{and variance} \quad \Sigma(\mathcal{X}) = \Sigma(\mathcal{X}, \mathcal{X}) - \Sigma(\mathcal{X}, X_n)\Sigma_n^{-1}\Sigma(\mathcal{X}, X_n)^\top$$

$$\Sigma(\chi) = \begin{pmatrix} 0.11154162 & -0.05042265 \\ -0.05042265 & 0.05155061 \end{pmatrix}$$ Prediction Uncertainty

The diagonal terms are the variances at prediction points 1 and 2

$$\sigma^2(\chi) = \begin{pmatrix} 0.11154162 \\ 0.05155061 \end{pmatrix}$$

R
Code to replicate this example in R

```r
library(plgp)

eps = sqrt(.Machine$double.eps)

# Training points
X = rbind(c(-1.03,1.76), c(.49,.49), c(1.77,-1.77), c(3.62,3.76))

# The goal is to fit this function: y(x) = x1 * exp(-x1^2 - x2^2)
y = X[,1] * exp(-X[,1]^2 - X[,2]^2)

# Test points
XX = rbind(c(.35, .69),c(.65, .46))
XX

# Sigma 22 (Sigma) and its inverse (Si)
# ##################################################
# Distance among the Training Data
D = distance(X)
Sigma = exp(-D)
Si = solve(Sigma)

# Sigma 11
# ##################################################
# Distance among the Testing Data
DXX = distance(XX)
SXX = exp(-DXX)

# Sigma 12 and Sigma 21 (Transpose of Sigma 12)
# ##################################################
# Distance between training and testing data
DX = distance(XX, X)
SX = exp(-DX)

# Calculate the predictive mean and predictive variance
# ##################################################
# Predictive mean
mup = SX %*% Si %*% y
mup

# Predictive variance
Sigmap = SXX - SX %*% Si %*% t(SX)
Sigmap
```

Output

```
Console   Terminal   Jobs
~/
> # ##################################################
> # Predictive mean
> mup = SX %*% Si %*% y
> mup
          [,1]
[1,] 0.2849657
[2,] 0.2954011
>
> # Predictive variance
> Sigmap = SXX - SX %*% Si %*% t(SX)
> Sigmap
            [,1]        [,2]
[1,] 0.11154162 -0.05042265
[2,] -0.05042265  0.05155061
>
```

Mean

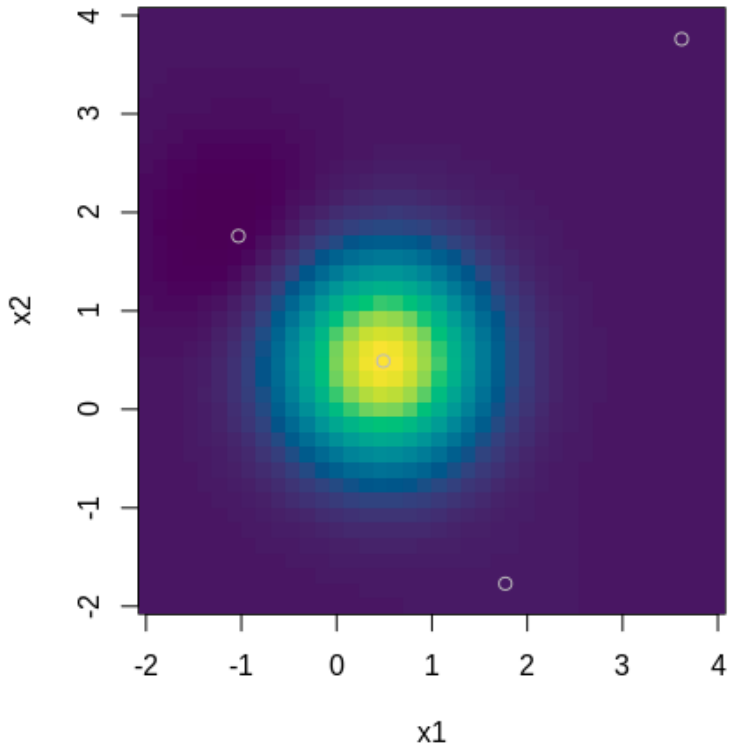
Variance

R
Code to replicate this example in R with Plots

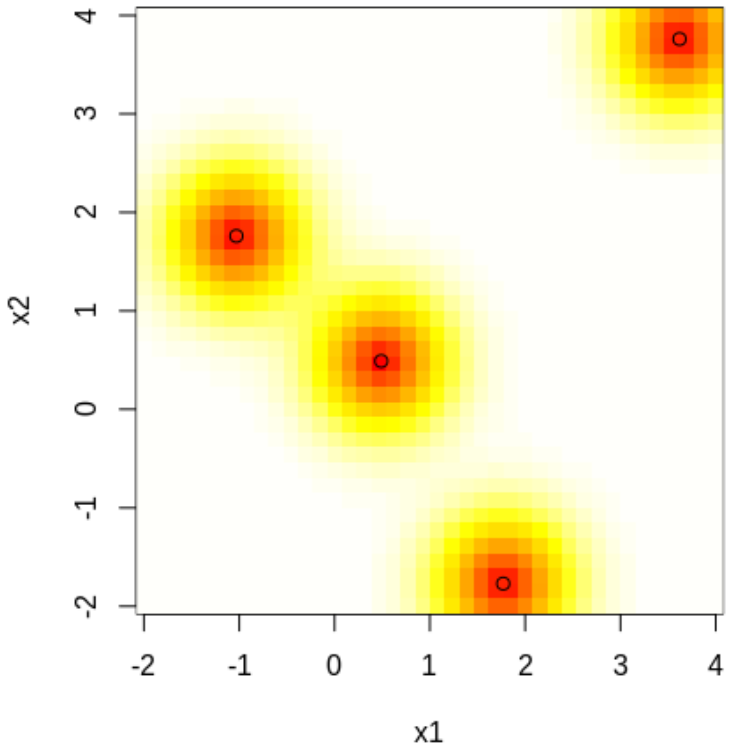
```r
library(plgp)
library(lhs)

eps = sqrt(.Machine$double.eps)

# Training Data
# ################################################
# Training points
number_of_sample_points = 4
X = rbind(c(-1.03,1.76), c(.49,.49), c(1.77,-1.77), c(3.62,3.76))

# Observed values
# The goal is to fit this function: y(x) = x1 * exp(-x1^2 - x2^2)
y = X[,1] * exp(-X[,1]^2 - X[,2]^2)

# Testing Data
# ################################################
# Test points
number_of_test_points_per_axis = 40
xx = seq(-2, 4, length=number_of_test_points_per_axis)
XX = expand.grid(xx, xx)

# Sigma 22 (Sigma) and its inverse (Si)
# ################################################
# Distance among the Training Data
D = distance(X)
Sigma = exp(-D) + diag(eps, nrow(X))
Si = solve(Sigma)

# Sigma 11
# ################################################
# Distance among the Testing Data
DXX = distance(XX)
SXX = exp(-DXX)

# Sigma 12 and Sigma 21 (Transpose of Sigma 12)
# ################################################
# Distance between training and testing data
DX = distance(XX, X)
SX = exp(-DX)

# Calculate the predictive mean and predictive variance
# ################################################
mup = SX %*% Si %*% y
Sigmap = SXX - SX %*% Si %*% t(SX)

# Predictive standard deviation
diag(Sigmap)
sdp = sqrt(diag(Sigmap))

# Figure 5.5
par(mfrow=c(1, 2))
cols_a = hcl.colors(128, palette = "viridis")
cols_b = heat.colors(128)
image(xx, xx, matrix(mup, ncol=length(xx)), xlab='x1', ylab='x2', col=cols_a)
points(X[,1], X[,2])
image(xx, xx, matrix(sdp, ncol=length(xx)), xlab='x1', ylab='x2', col=cols_b)
points(X[,1], X[,2])

# Figure 5.6
persp(xx, xx, matrix(mup, ncol=number_of_test_points_per_axis), theta=-30, phi=30,
xlab='x1', ylab='x2', zlab='y', zlim = c(-.5,.5))
```

Predictive Quantities Mean and Standard Deviation

Mean: $\mu(\chi)$



Standard Deviation: $\sigma(\chi)$
(Square root of variance)



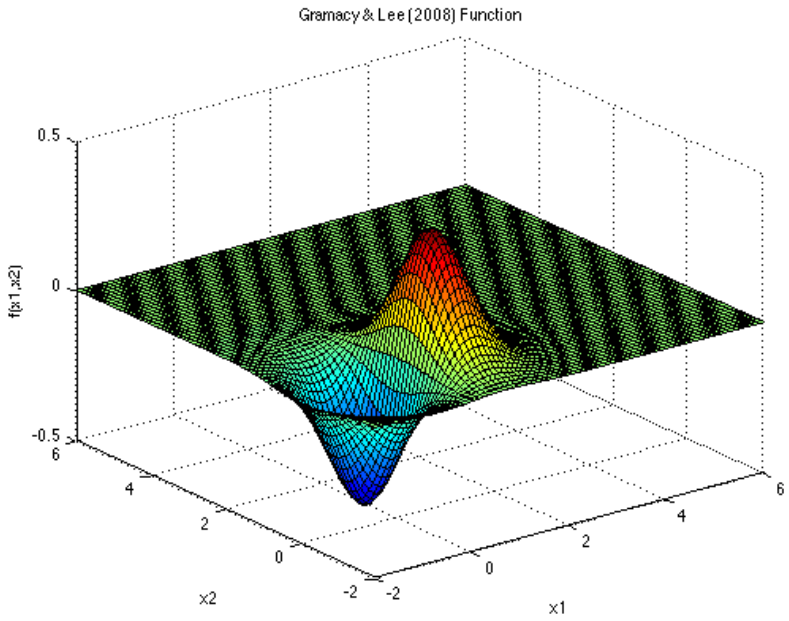
Not Good – High Standard Deviation – High Variance – High Prediction uncertainty (Prediction is not reliable)

Good – Low Standard Deviation – Low Variance – Low Prediction uncertainty (Prediction is reliable)

Prediction uncertainty is lowest near training data locations

Comparison of True Function and Prediction Model

True Function



$$f(\mathbf{x}) = x_1 \exp(-x_1^2 - x_2^2)$$

Source: https://www.sfu.ca/~ssurjano/grlee08.html

Prediction Model ($\mu(\chi)$)