Workshop – Prediction Analysis, Dynamic Impact of a Rigid Sphere on a Woven Fabric

AN MSC NASTRAN MACHINE LEARNING WEB APP TUTORIAL

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

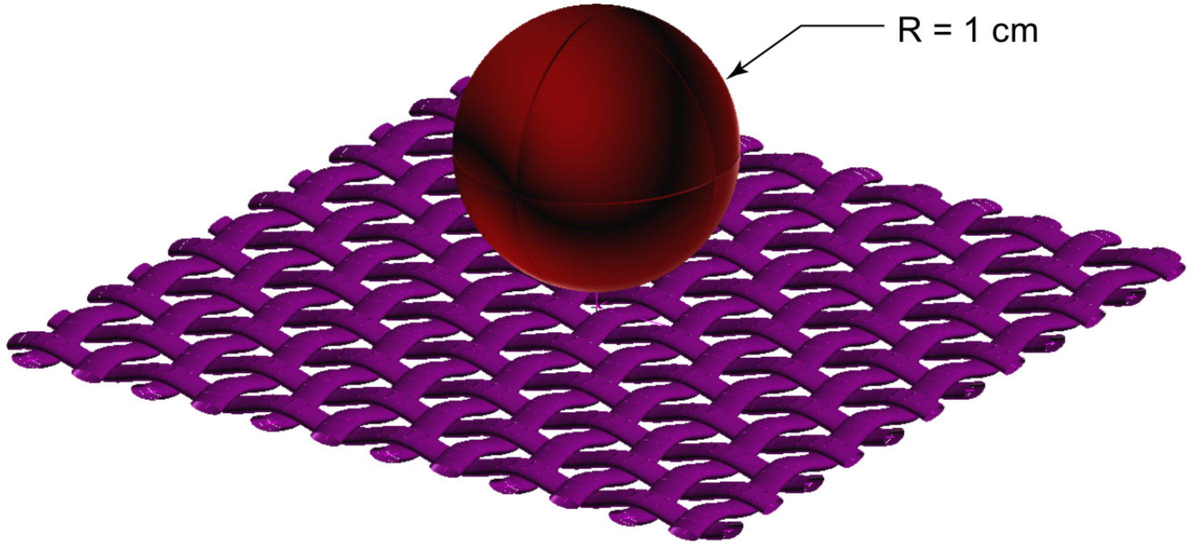
Goal: Prediction Analysis

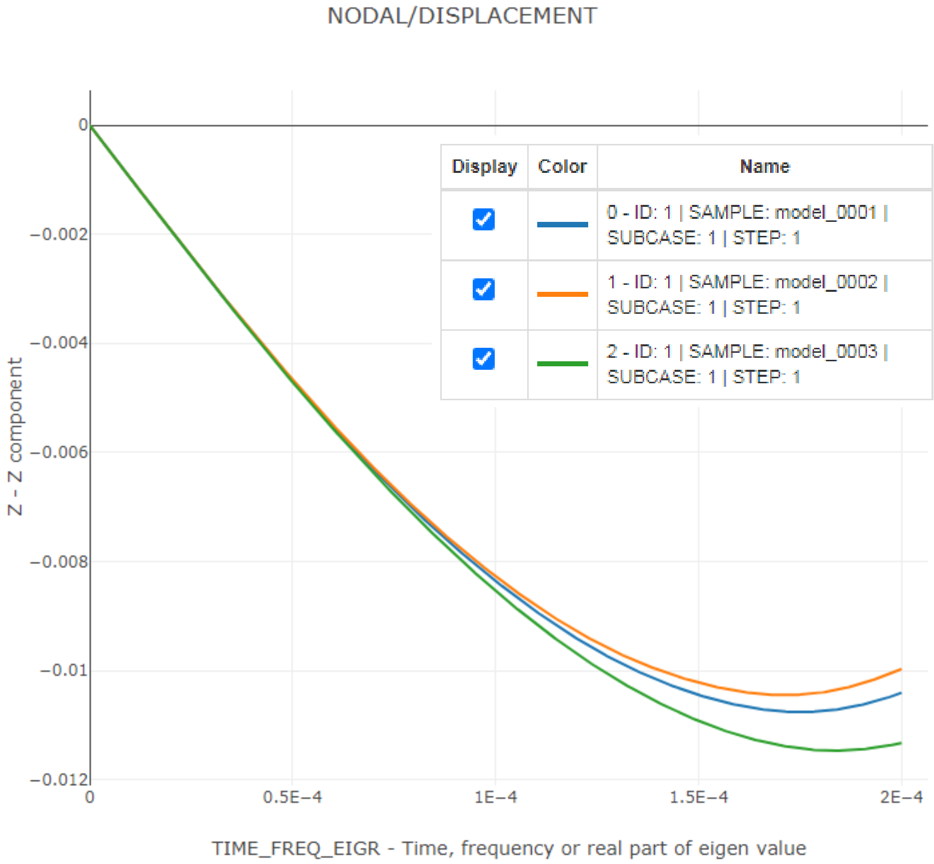
This tutorial consists of multiple parts

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. Creating Plots with the HDF5 Explorer
   - The HDF5 Explorer web app is used to create displacement vs. time plots.
4. Performing Predictions
   - Gaussian process (GP) regression is used to train a surrogate model and perform predictions.
   - The prediction performance of the surrogate model is evaluated.

Details of the Structural Model

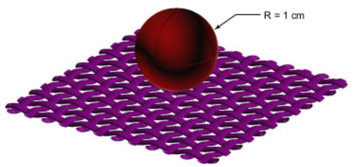
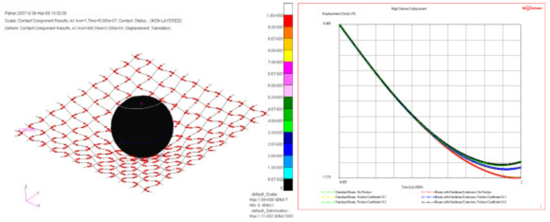
1. Perform nonlinear transient analysis, with contact, for different levels of friction
2. Create a history plot of z-displacements of the rigid sphere



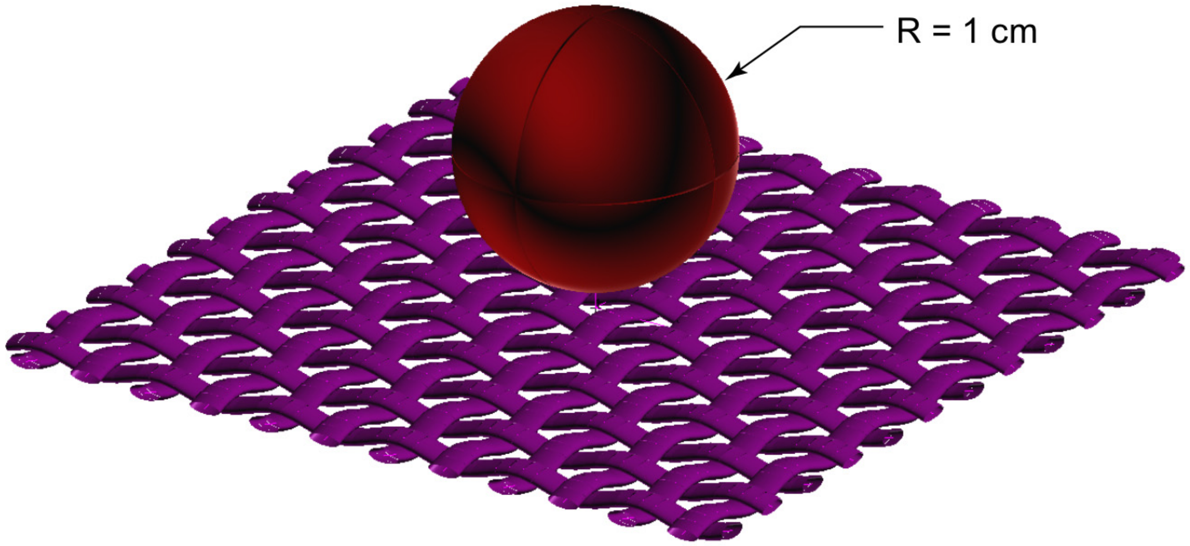


Details of the Structural Model

Summary

Title	Chapter 47: Dynamic Impact of a Rigid Sphere on a Woven Fabric
Features	Beam-to-beam contact, beam-to-rigid contact, dynamic contact, bilinear Coulomb friction model, isotropic elastic material, nonlinear property extensions to beam elements
Geometry	
Material properties	$E = 10GPa$, $\rho = 1500kg/m^3$
Analysis characteristics	Nonlinear transient analysis with adaptive time stepping and geometric nonlinearity due to large displacements and large rotations
Boundary conditions	Fabric is clamped on all four sides; sliding, frictional contact between the beam elements of the fabric and between the fabric and the sphere.
Applied loads	The rigid sphere hits the fabric at the center with an initial velocity of $100m/s$.
Element type	2-node thin elastic beam element with transverse shear effects
FE results	1. Deformed shape and contact status 2. History plot of z-displacements of the rigid sphere 3. Frictional contact forces 

MSC Nastran Demonstration Problems Manual - Implicit Nonlinear, Chapter 28 - Dynamic Impact of a Rigid Sphere on a Woven Fabric



Problem Statement

Design Variables

x1: Friction of yarns parallel to x direction, initial body approach

x2: Friction of yarns parallel to y direction, initial body approach

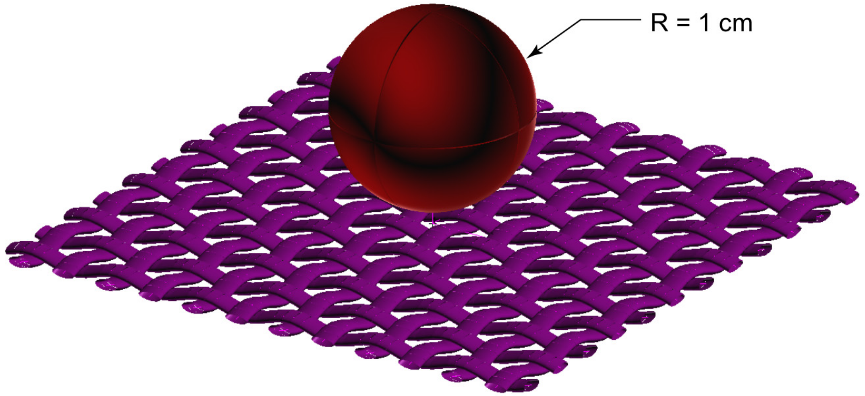
x3: Friction of yarns parallel to x direction

x4: Friction of yarns parallel to y direction

$0.0 < x1 < 1.0$

Samples

Batch set 1 – 20 run LHS Design
Batch set 2 – 8 run LHS Design
Batch set 3 – 3 run User-defined Design



Monitored Responses

r1: Displacement, z component, of rigid sphere, max response across all time steps

r2: Magnitude of displacement ($\sqrt{x^2 + y^2 + z^2}$) of rigid sphere, max response across all time steps

r3: Displacement, z component, of rigid sphere at time step 0.0001

r4: Magnitude of displacement ($\sqrt{x^2 + y^2 + z^2}$) of rigid sphere at time step 0.0001

All displacements are monitored at node 1, which is the center of the woven fabric

Problem Statement, Continued

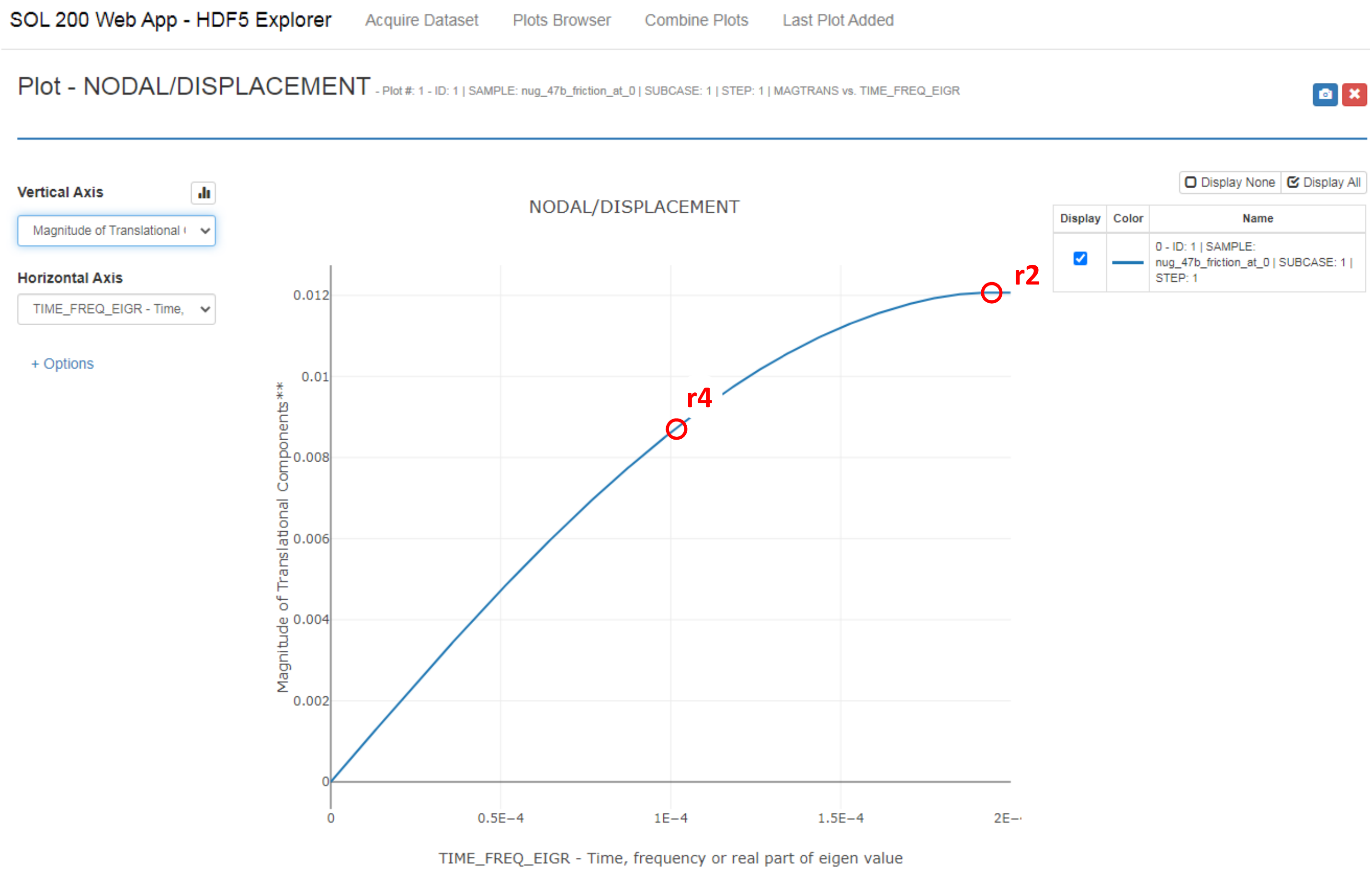
The responses defined in this tutorial correspond to points on the displacement vs. time plot

- Response r1 is the max displacement, z component, across all time steps, in this case the max displacement is negative
- Response r3 is the displacement, z component, at time step .0001

Problem Statement, Continued

The responses defined in this tutorial correspond to points on the displacement vs. time plot

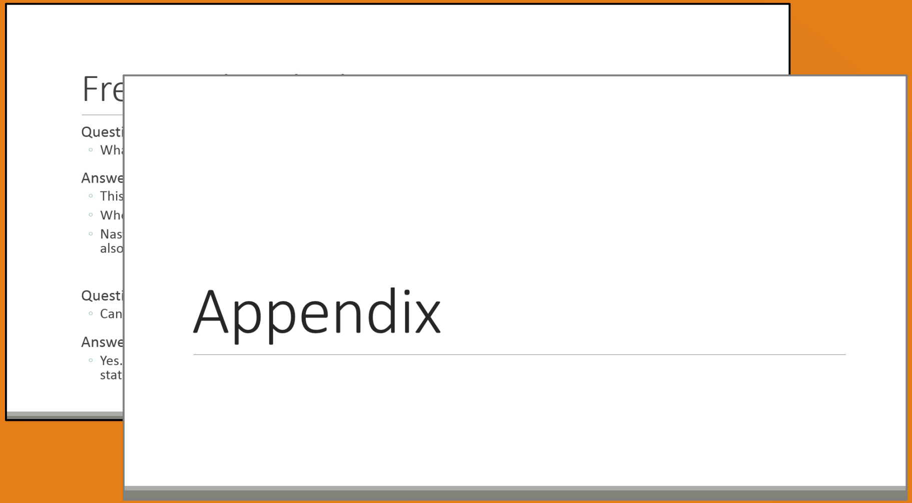
- Response r2 is the max displacement, magnitude, across all time steps
- Response r4 is the displacement, magnitude, at time step .0001



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



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 HDF5 Explorer to:
    1. Create plots
4. Use the Prediction Analysis web app to:
    1. Determine parameter relevance (parameter/variable screening)
    2. Perform predictions

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.

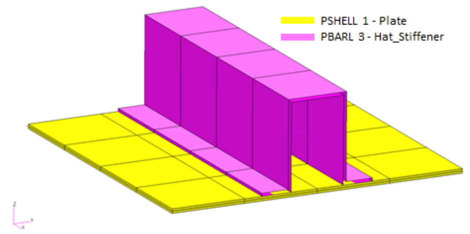
Compatibility

- 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.

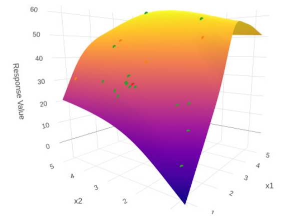
Benefits

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

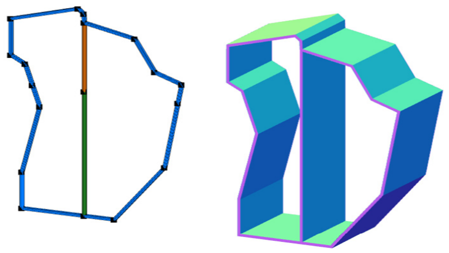
Web Apps



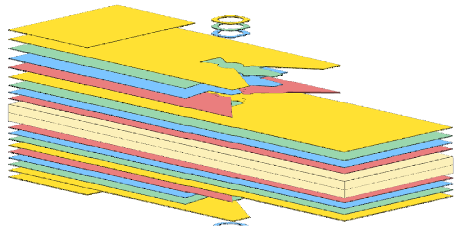
Web Apps for MSC Nastran SOL 200
Pre/post for MSC Nastran SOL 200. Support for size, topology, topometry, topography, multi-model optimization.



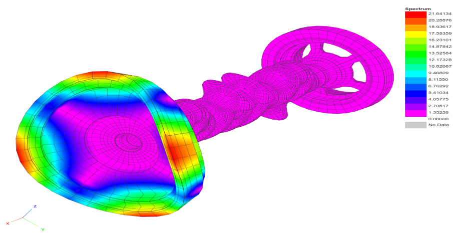
Machine Learning Web App
Bayesian Optimization for nonlinear response optimization (SOL 400)



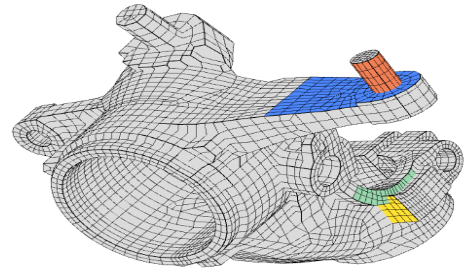
PBMSECT Web App
Generate PBMSECT and PBRSECT entries graphically



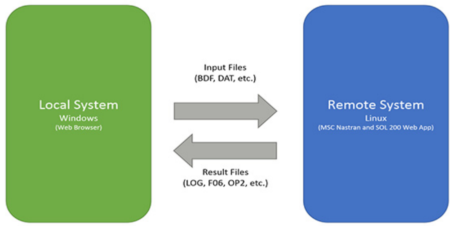
Ply Shape Optimization Web App
Optimize composite ply drop-off locations, and generate new PCOMPG entries



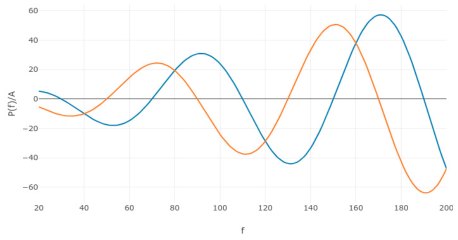
Post-processor Web App
View MSC Nastran results in a web browser on Windows and Linux



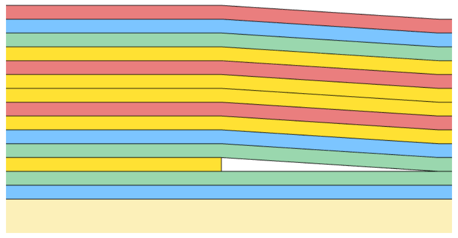
Shape Optimization Web App
Use a web application to configure and perform shape optimization.



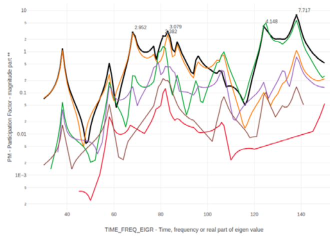
Remote Execution Web App
Run MSC Nastran jobs on remote Linux or Windows systems available on the local network



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



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



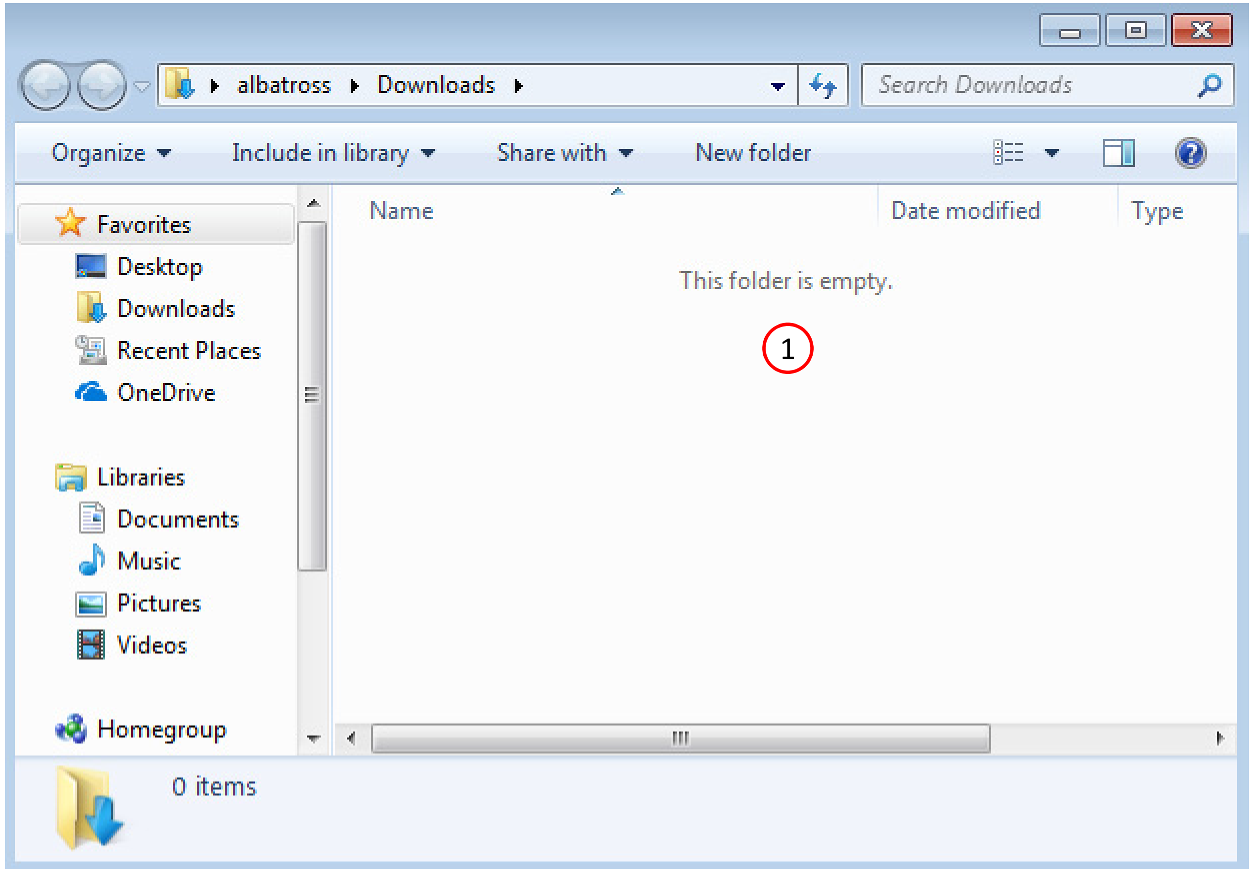
HDF5 Explorer Web App
Create graphs (XY plots) using data from the H5 file

Configuring The Problem Statement

Before Starting

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

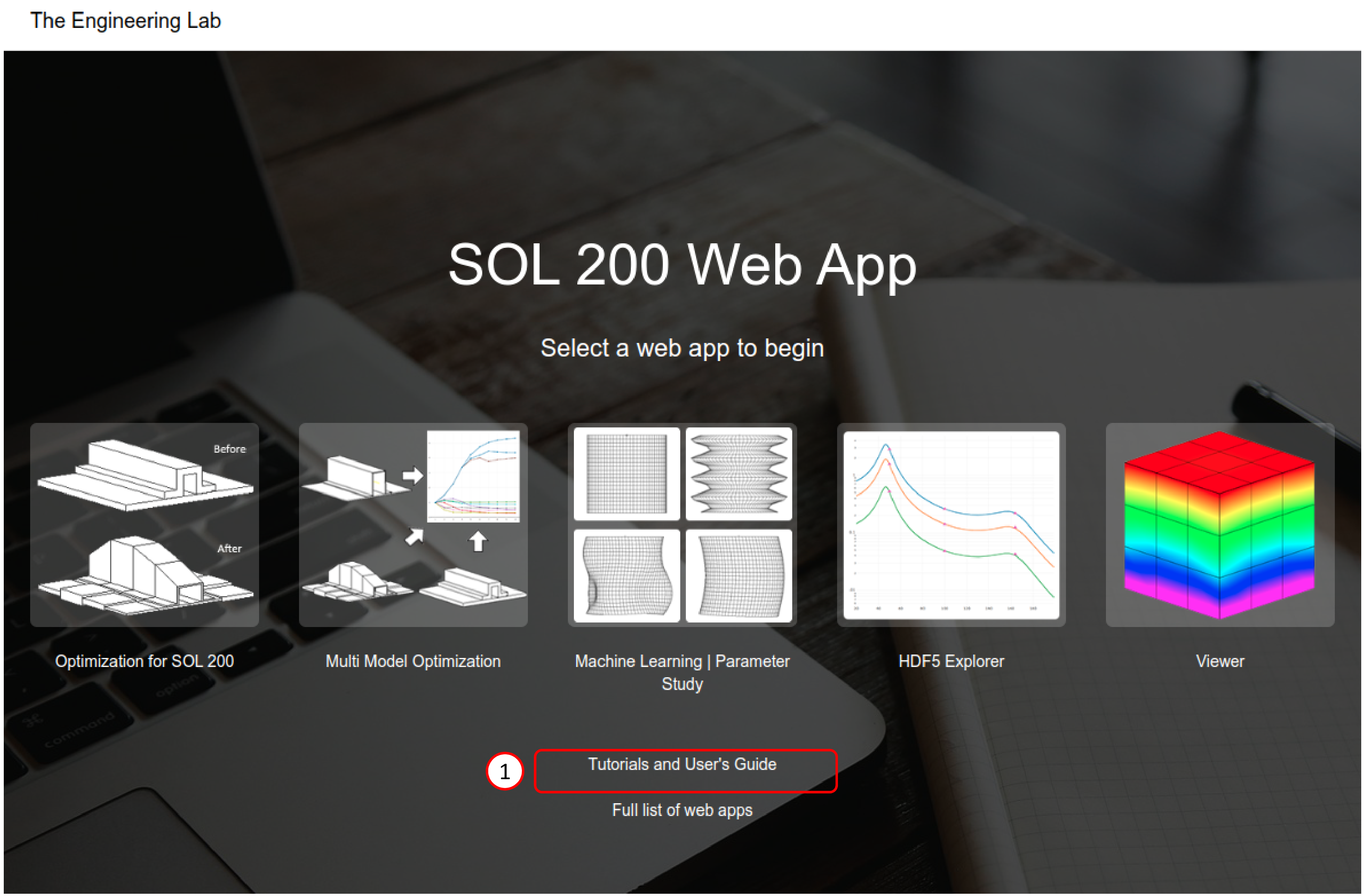
- Throughout this workshop, you will be working with multiple file types and directories such as:
    - .bdf/.dat
    - nastran_working_directory
    - .f06, .log, .pch, .h5, etc.
- To minimize confusion with files and folders, it is encouraged to start with a clean directory.



Go to the User's Guide

1. Click on the indicated link

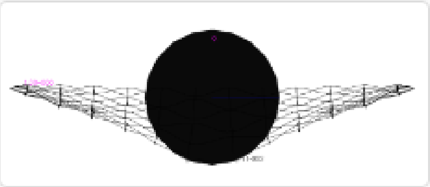
- The necessary BDF files for this tutorial are available in the Tutorials section of the User's Guide.



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.

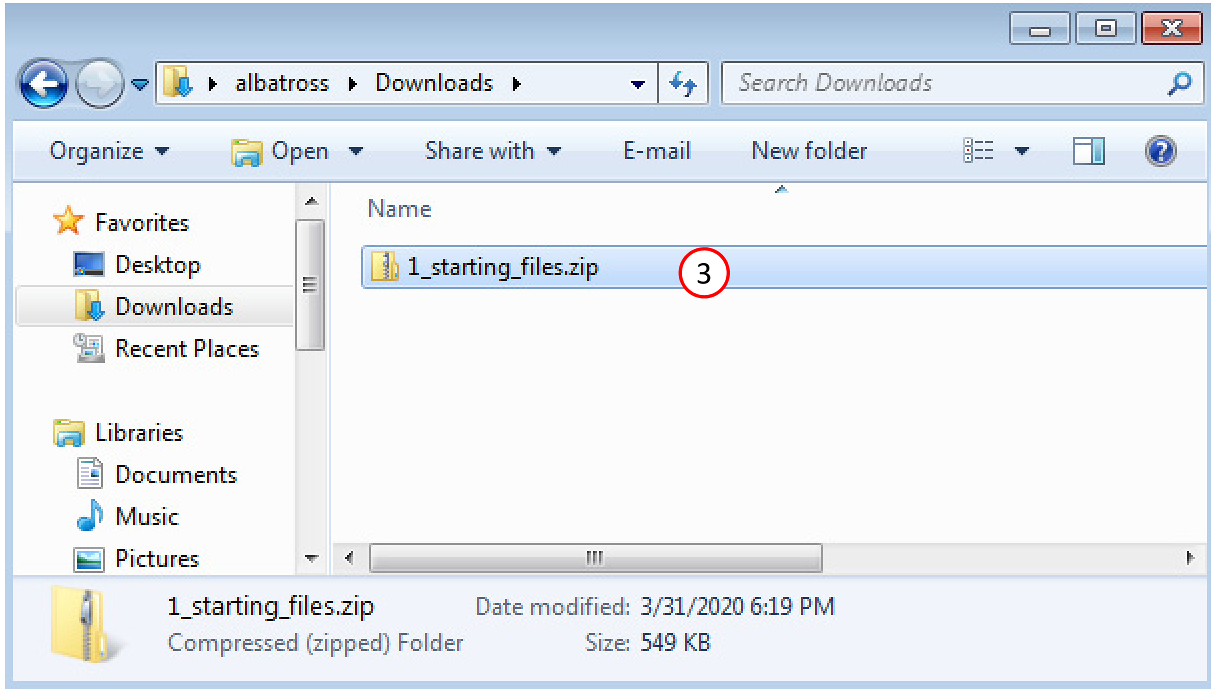


Parameter Study, Dynamic Impact of a Rigid Sphere on a Woven Fabric (1)

Consider a transient analysis of a rigid sphere impacting a woven fabric. The parameters allowed to vary include the friction coefficients. The response of interest are the displacements.

This tutorial describes how to configure multiple MSC Nastran runs to generate training data. Gaussian process regression is used to train a surrogate model and make predictions. The prediction performance of the surrogate model is also evaluated. Also discussed are instructions to create displacement vs. time plots .

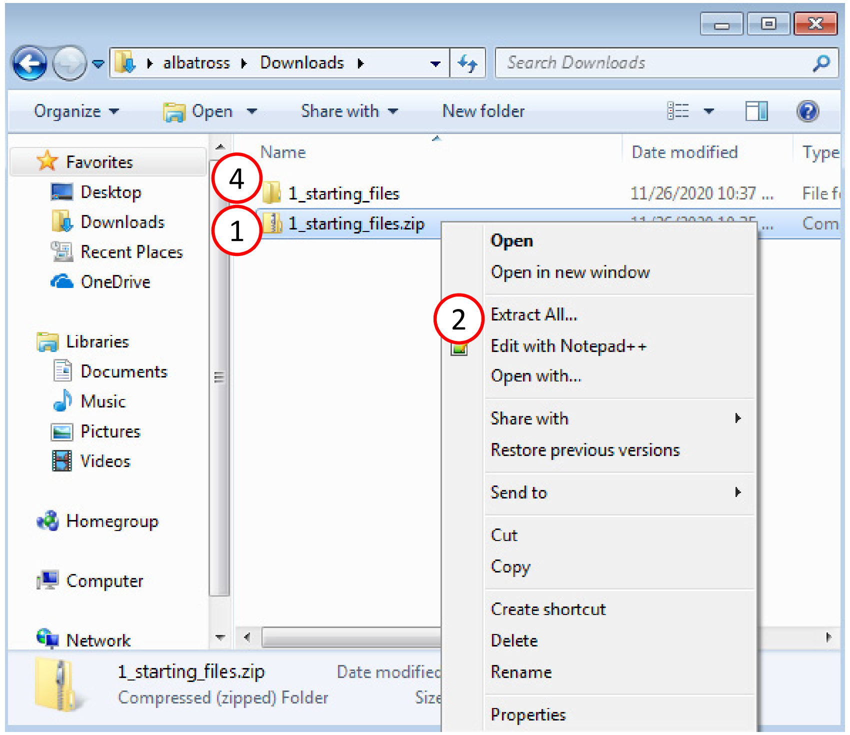
Starting Files: Link (2)
Solution BDF Files: Link

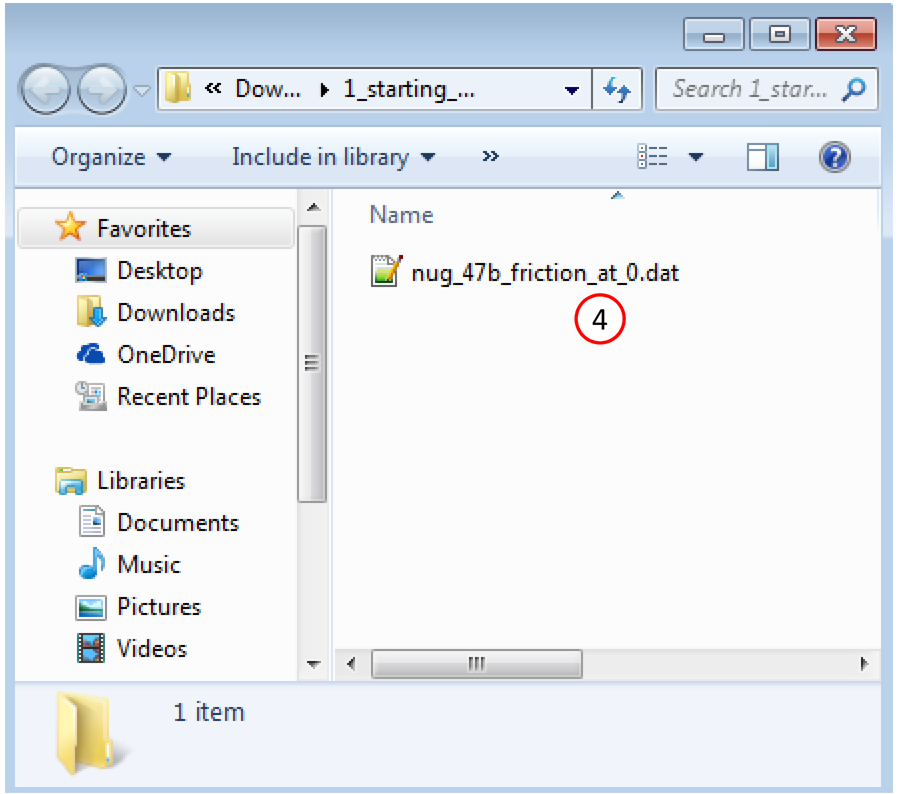


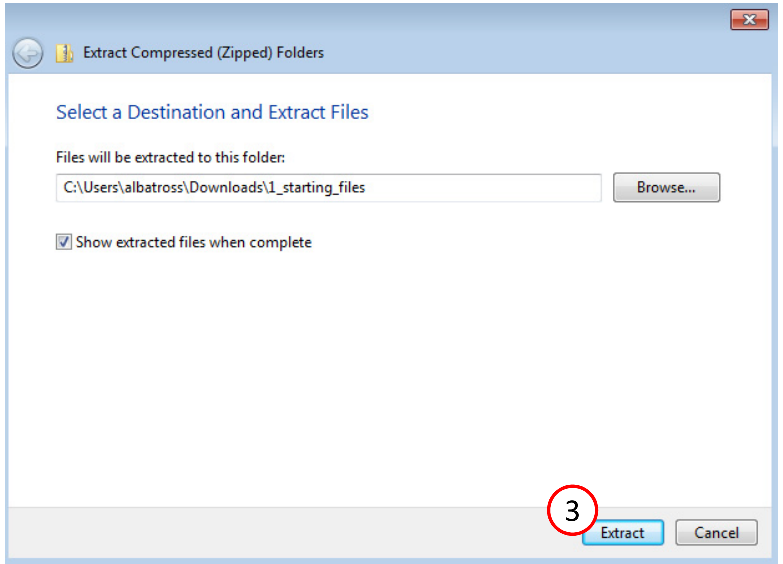
Obtain Starting Files

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.





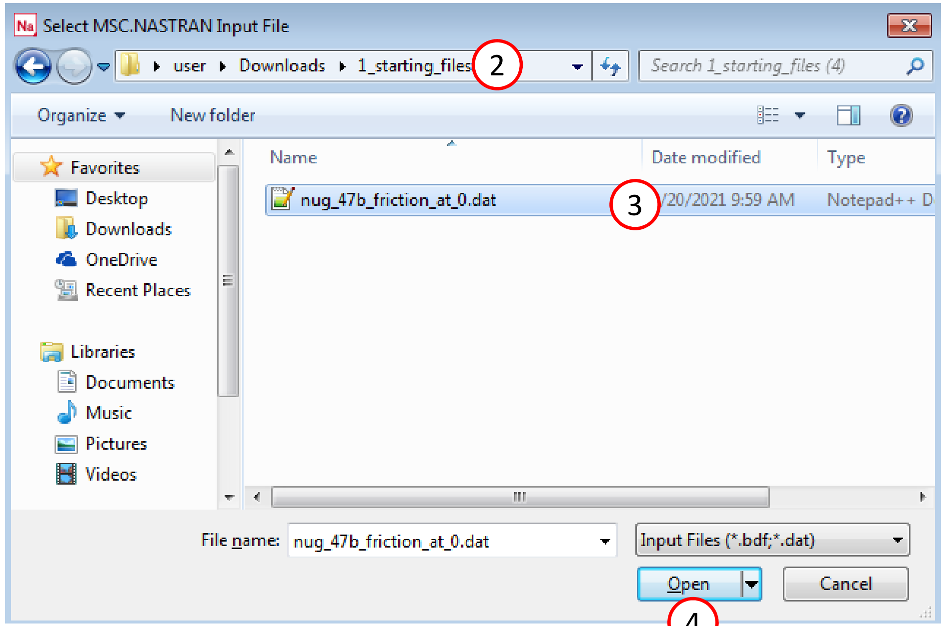


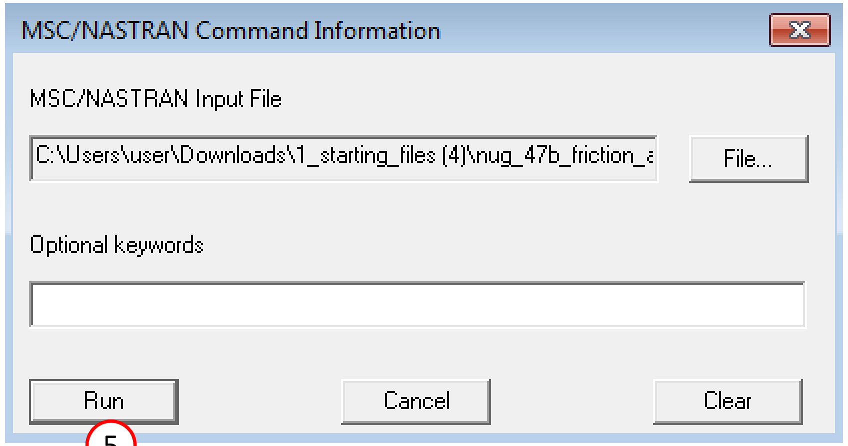
Create the Starting H5 File

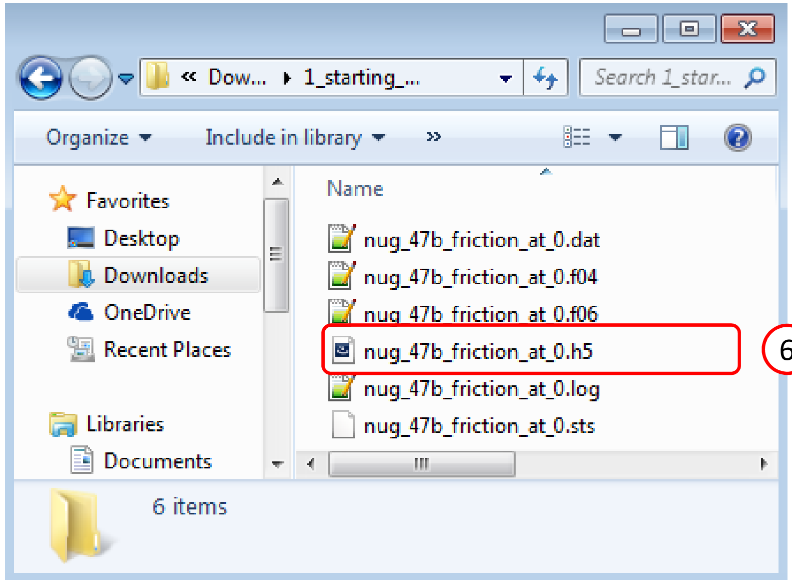
A starting H5 file must be created. This H5 file will be used to configure the responses later on.

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

1





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

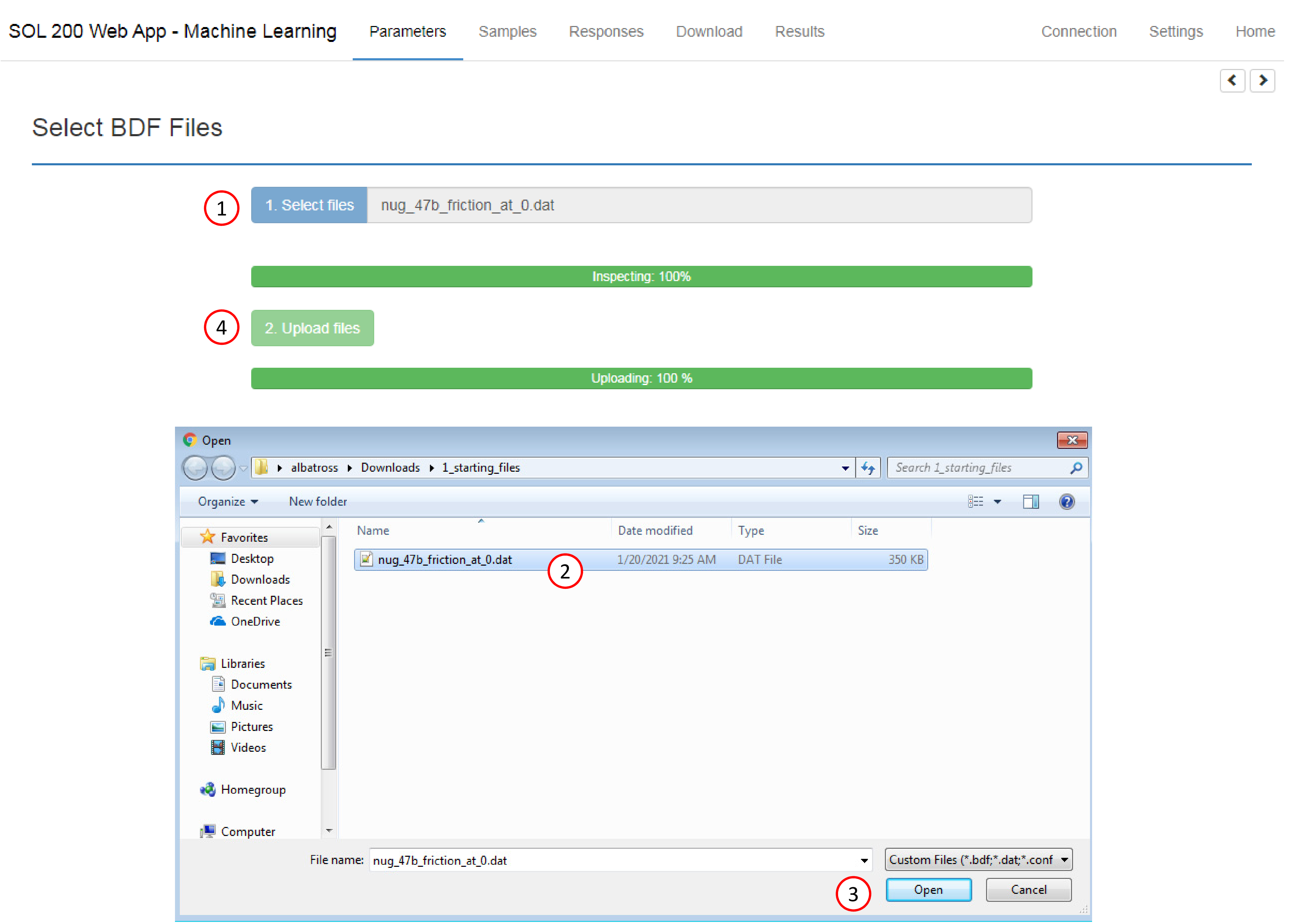
1. Click on the indicated link

- 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.

The Engineering Lab

Select BDF Files

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

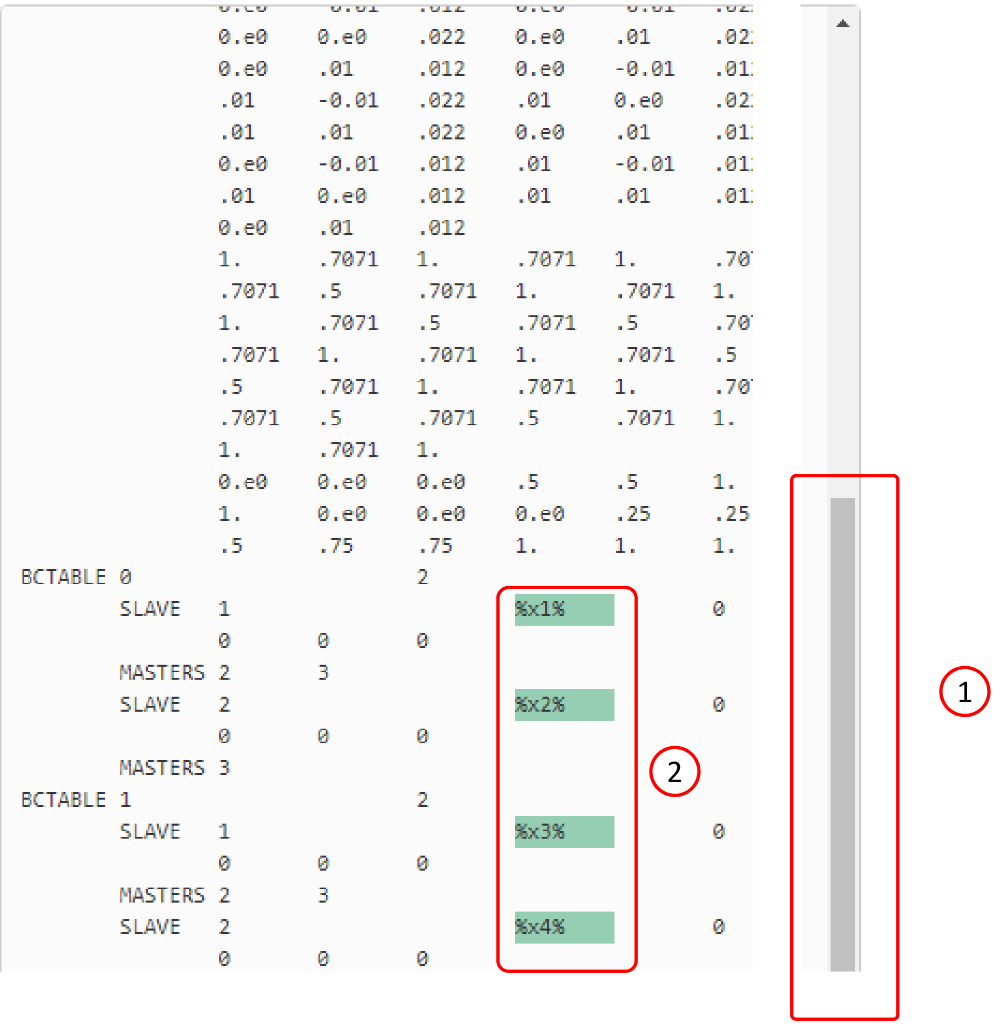


Parameters

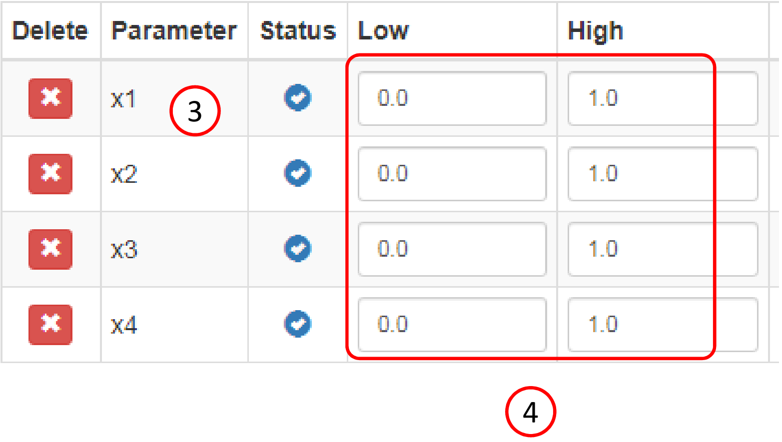
1. Move the scroll bar until the BCTABLE entries are visible
2. Set the following fields as parameters
   - x1: Friction coefficient of BCTABLE 0, SLAVE 1
   - x2: Friction coefficient of BCTABLE 0, SLAVE 2
   - x3: Friction coefficient of BCTABLE 1, SLAVE 1
   - x4: Friction coefficient of BCTABLE 1, SLAVE 2
3. Parameters have been created for the selected fields
4. For each parameter, use the following settings:
   - Low: 0.0
   - High: 1.0

- 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



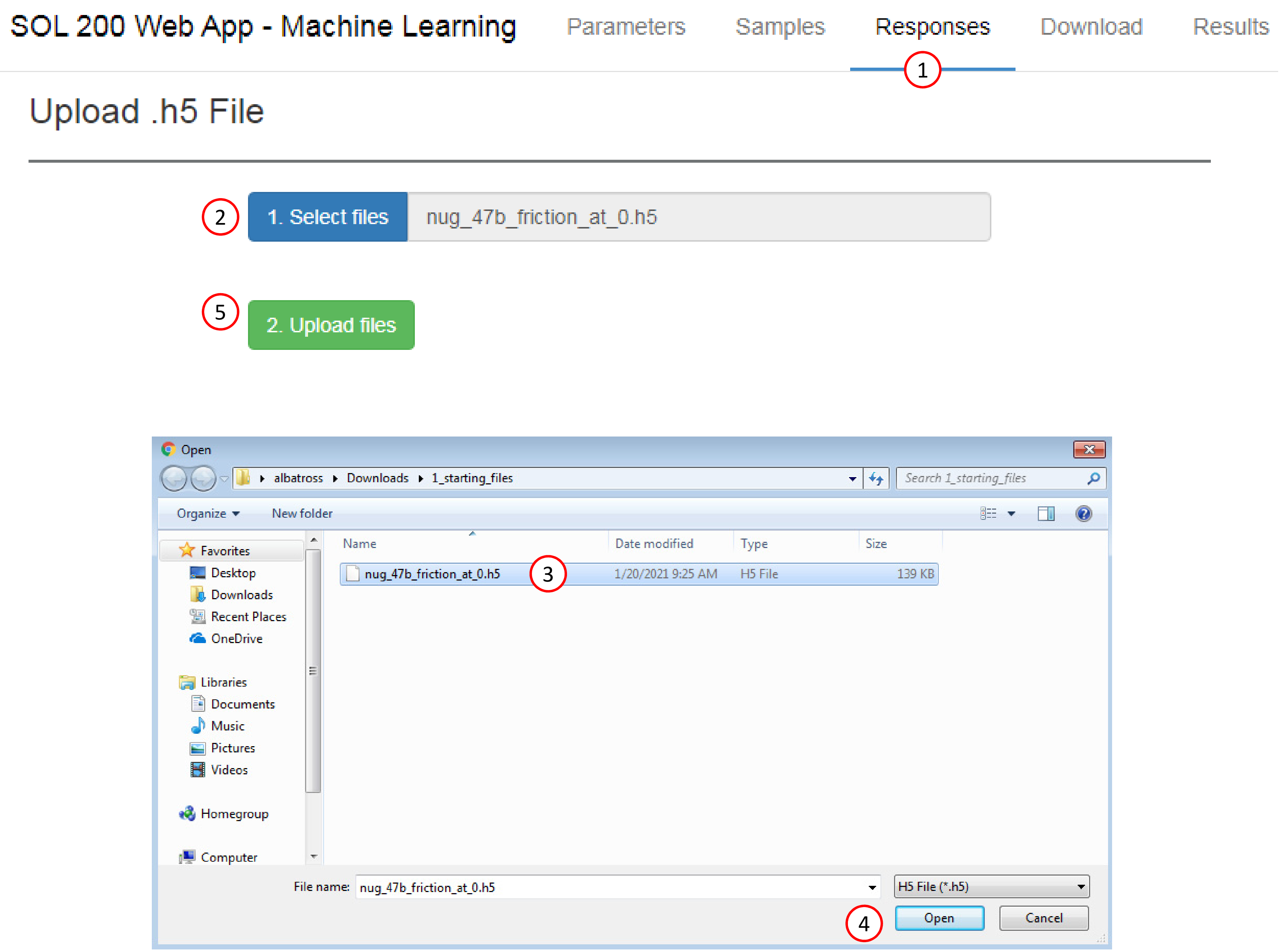
Configure Parameters



Responses

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

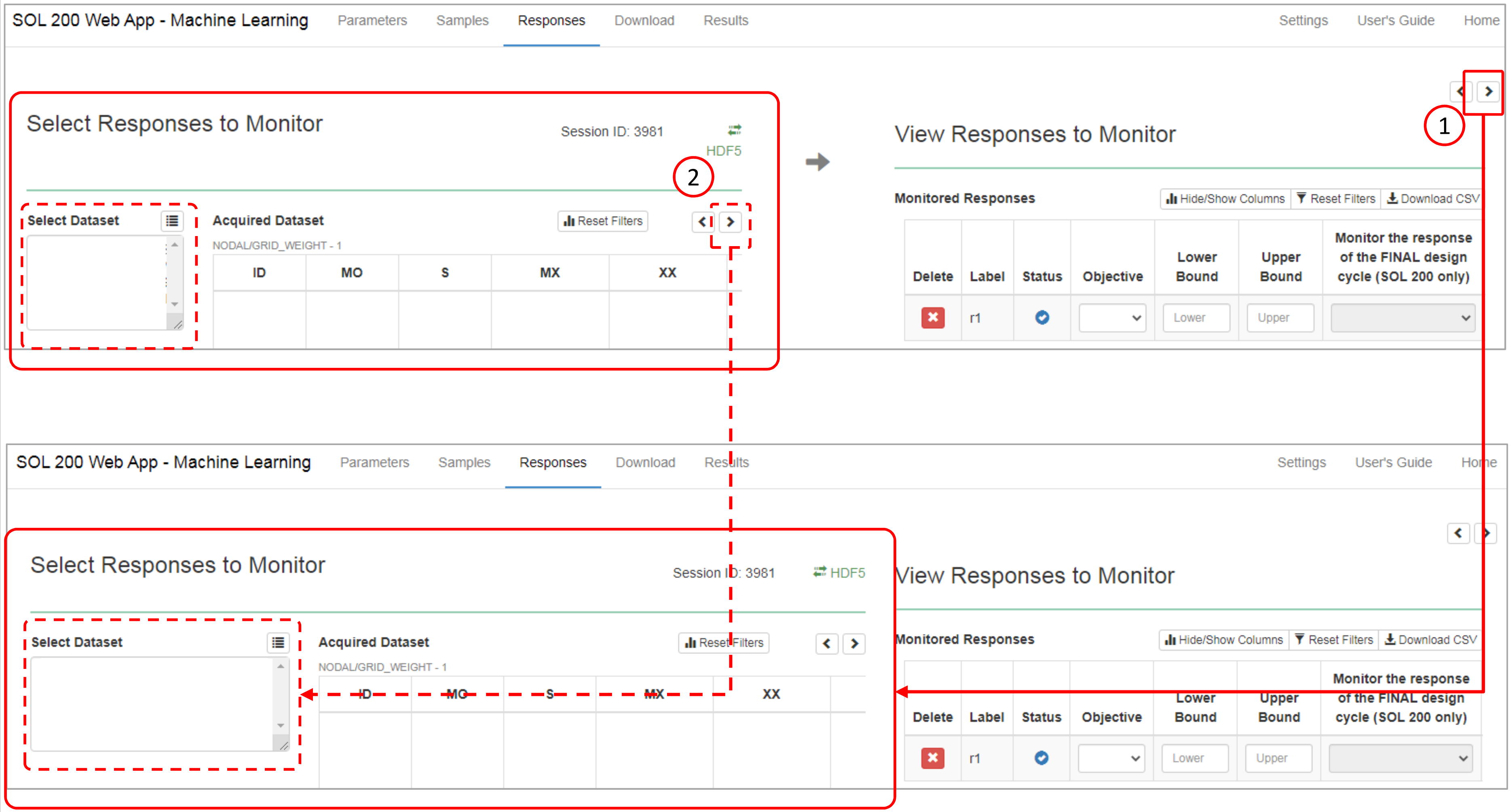
- On this page, the H5 file is uploaded to the web app.



Adjust the Column Width

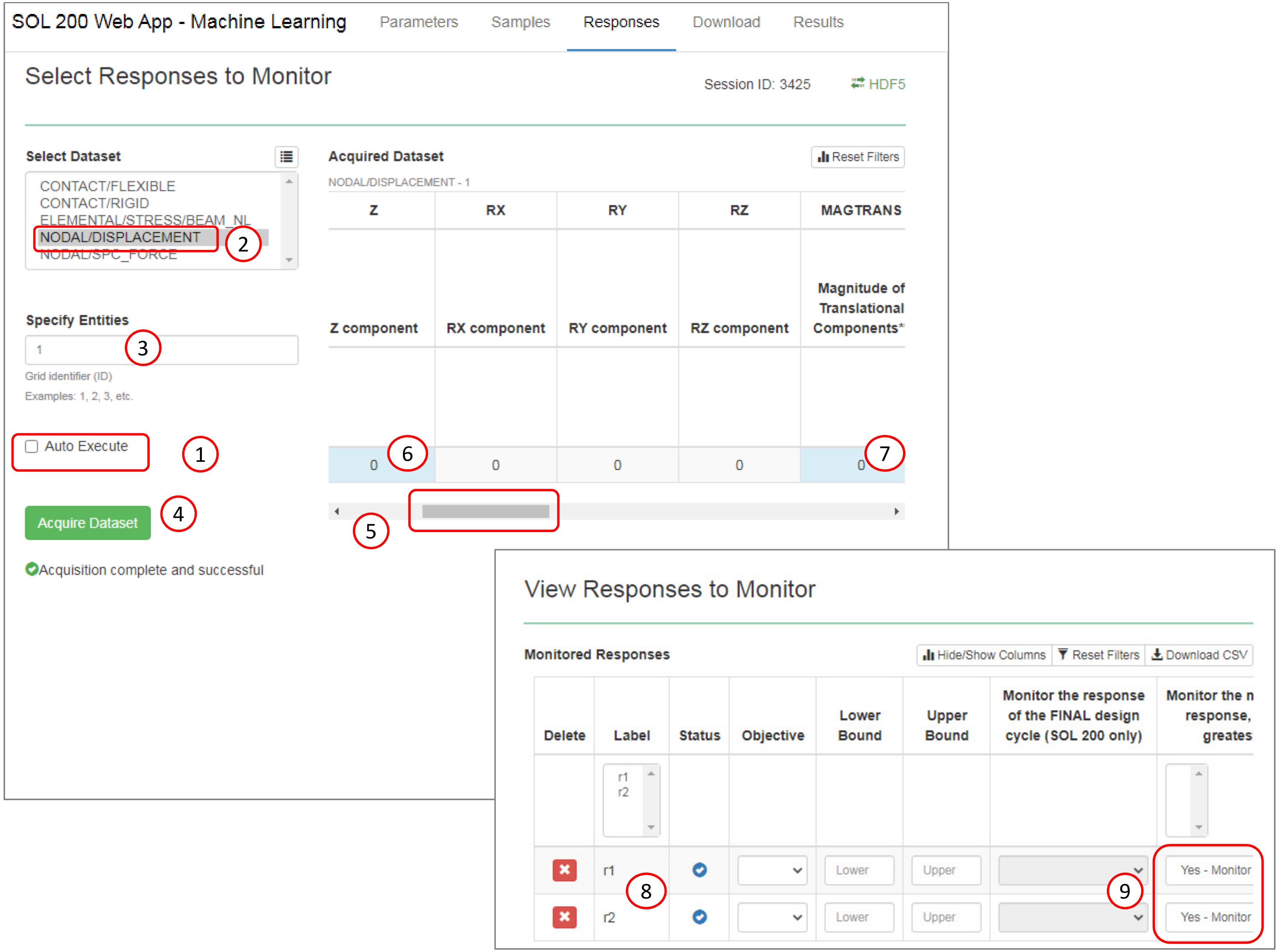
1. Optional - Use at your liking the buttons at the top right hand corner to adjust the width of the left and right columns
2. Optional – Use the indicated buttons to adjust the width of the column Select Dataset

- IMPORTANT! This image is not meant to match exactly what you see in your view. The text in this image is expected to be different from your view. The purpose of this page and image is to demonstrate how to increase the width of the indicated sections.



Select Responses

1. Uncheck the checkbox named Auto Execute
2. Select the following dataset: NODAL/DISPLACEMENT
3. Set Specify Entities to 1
4. Click Acquire Dataset
5. Use the horizontal scroll bar until the columns named Z and MAGTRANS are visible
6. Select the indicated cell
7. Select the indicated cell
8. New responses r1 and r2 are created
9. Configure the following setting for response r1 and r2
   - Monitor the maximum or minimum […]: Yes

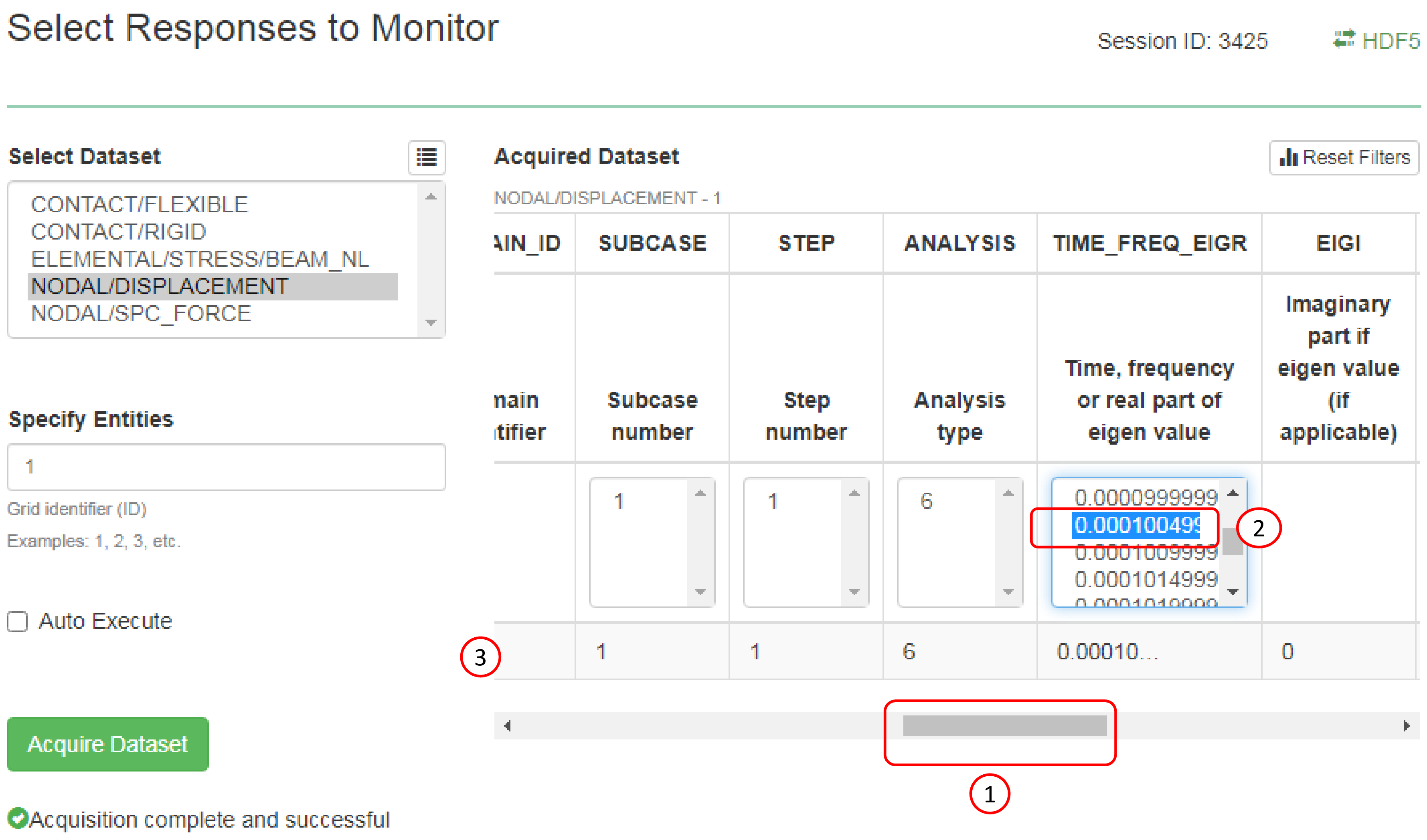


Questions? Email: christian@ the-engineering-lab.com

HEXAGON Technology Partner

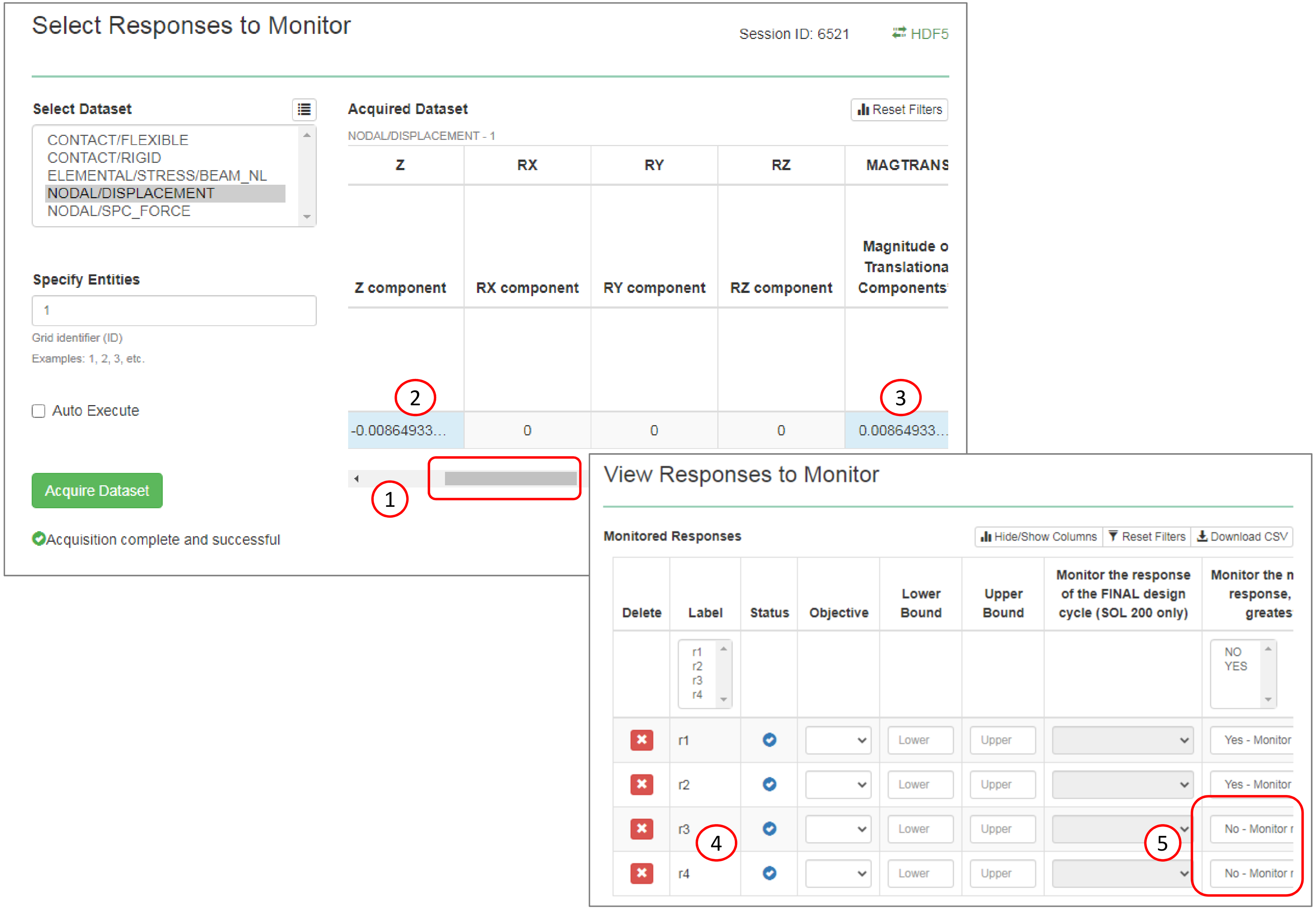
Select Responses

1. Use the horizontal scroll bar until this column is visible: TIME_FREQ_EIGR
2. Select the following time step: .000100499
3. The table has been updated to show only responses for the selected time step



Select Responses

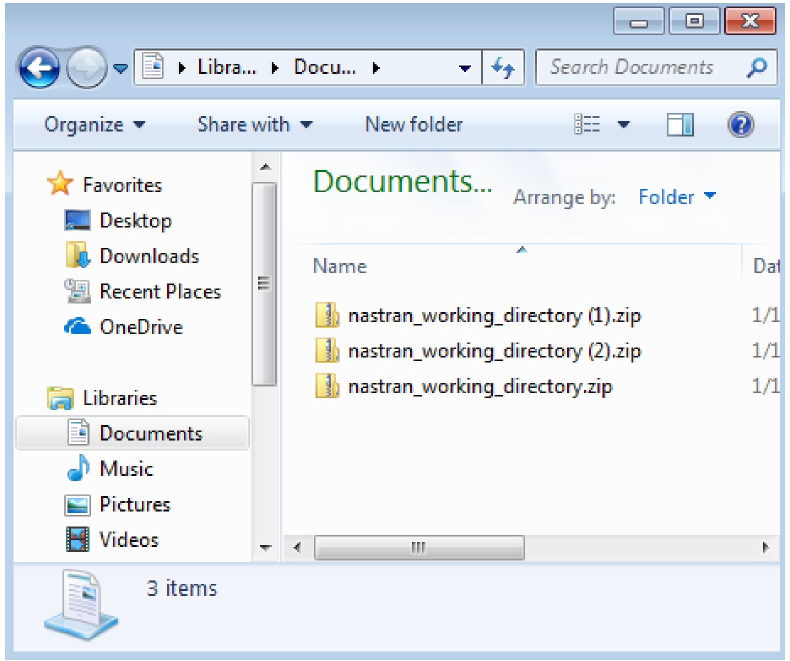
1. Use the horizontal scroll bar until the columns named Z and MAGTRANS are visible
2. Select the indicated cell
3. Select the indicated cell
4. New responses r3 and r4 are created
5. Configure the following setting for response r3 and r4
    - Monitor the maximum or minimum […]: No



Configuring Multiple Batch Runs

Samples

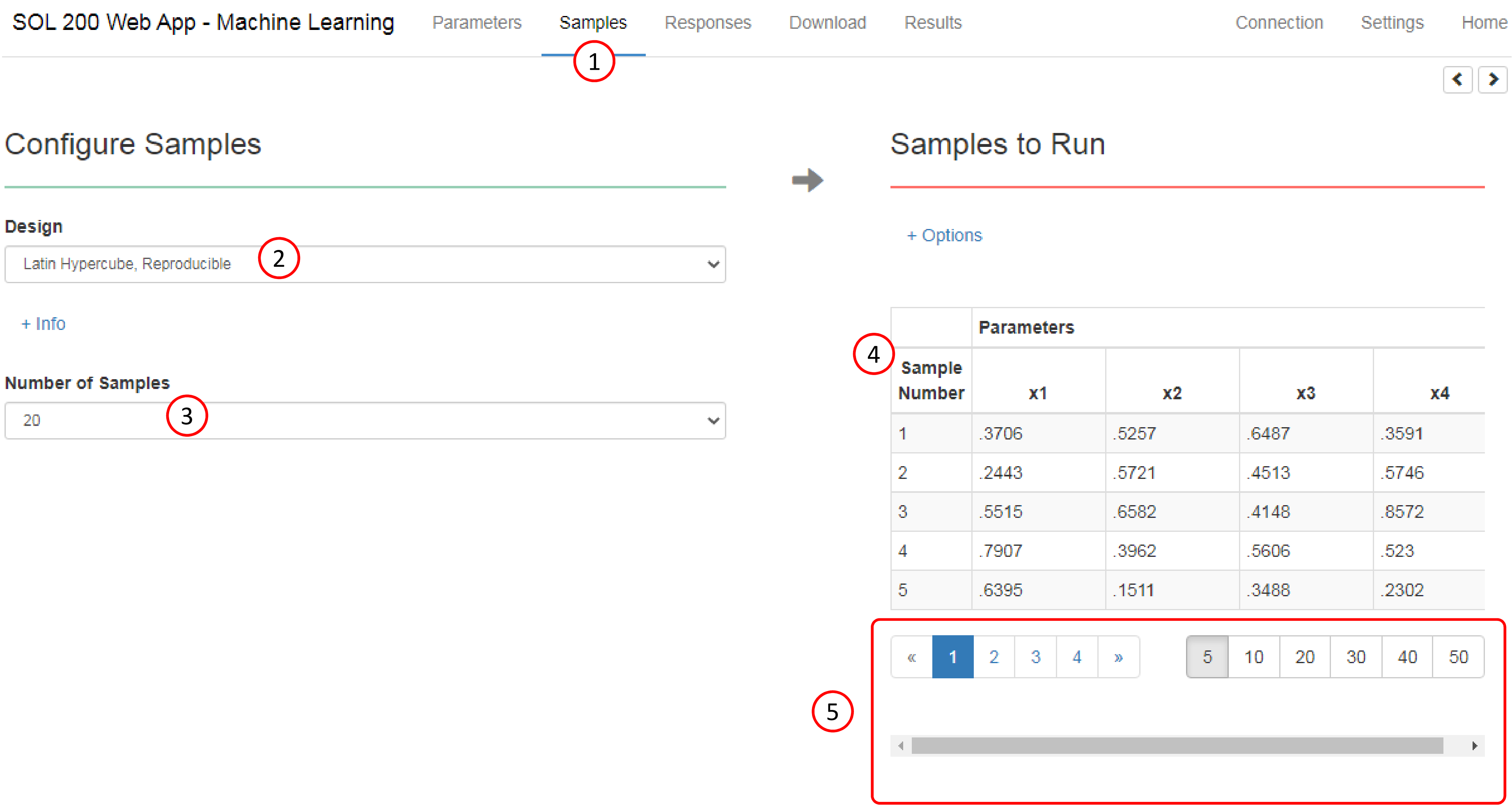
In the following slides, we will configure 3 batches to run.



Batch	File Name	Number of Runs	Purpose
1	nastran_working_directory.zip	20	The data from these 20 runs is used to train the surrogate model.
2	nastran_working_directory (1).zip	8	The data from these 8 runs is compared with the predictions from the surrogate model. The normalized root mean square error (NRMSE) is calculated based on these 8 runs.
3	nastran_working_directory (2).zip	3	This is a 3 run configuration. This set is used to compare the predicted responses with MSC Nastran responses.

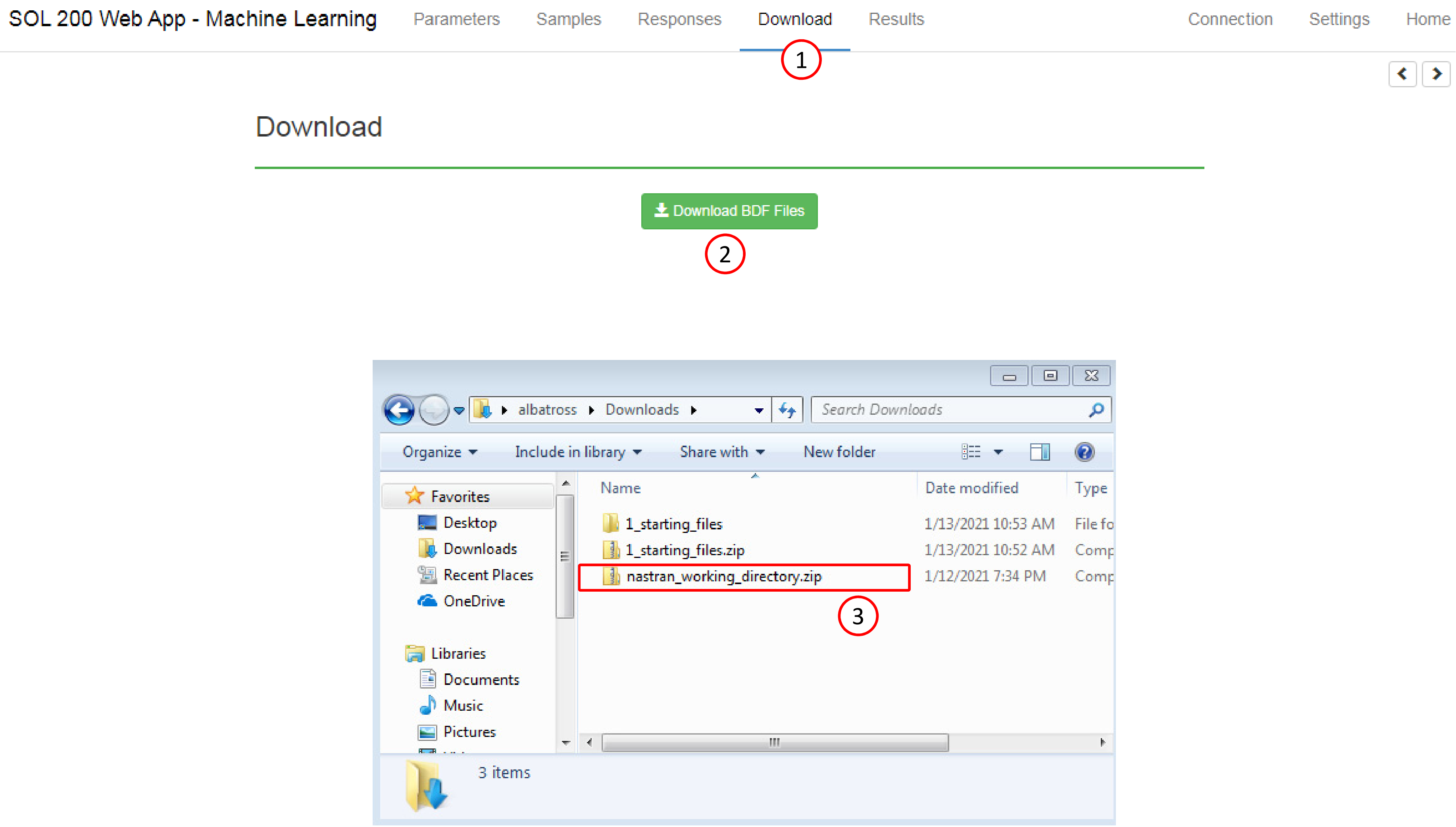
Samples

1. Click Samples
2. Ensure the following design is selected: Latin Hypercube, Reproducible
3. Set Number of Samples to 20
4. The samples have been updated, note that samples 1, 2, 3, …, 20 are contained in the table
5. The indicated controls can be used to display the other samples



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

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

Configure Samples

Design

Latin Hypercube, Reproducible

+ Info

Number of Samples

8

Samples to Run

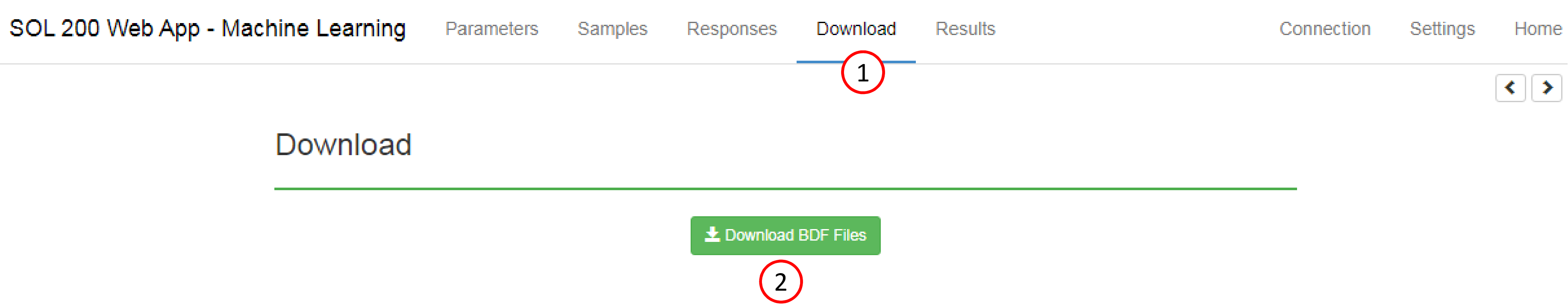
+ Options

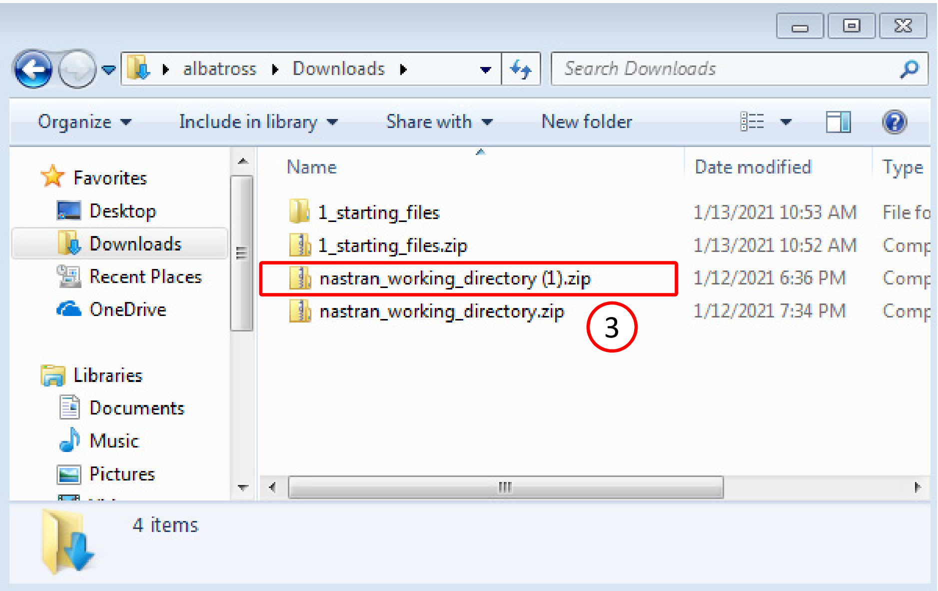
	Parameters			
Sample Number	**x1**	**x2**	**x3**	**x4**
1	.000000	.7143	.4286	.1429
2	.1429	.5714	.7143	1.
3	.2857	.000000	.1429	.5714
4	.4286	.1429	1.	.2857
5	.5714	.8571	.000000	.7143

« 1 2 »   5 10 20 30 40 50

Download

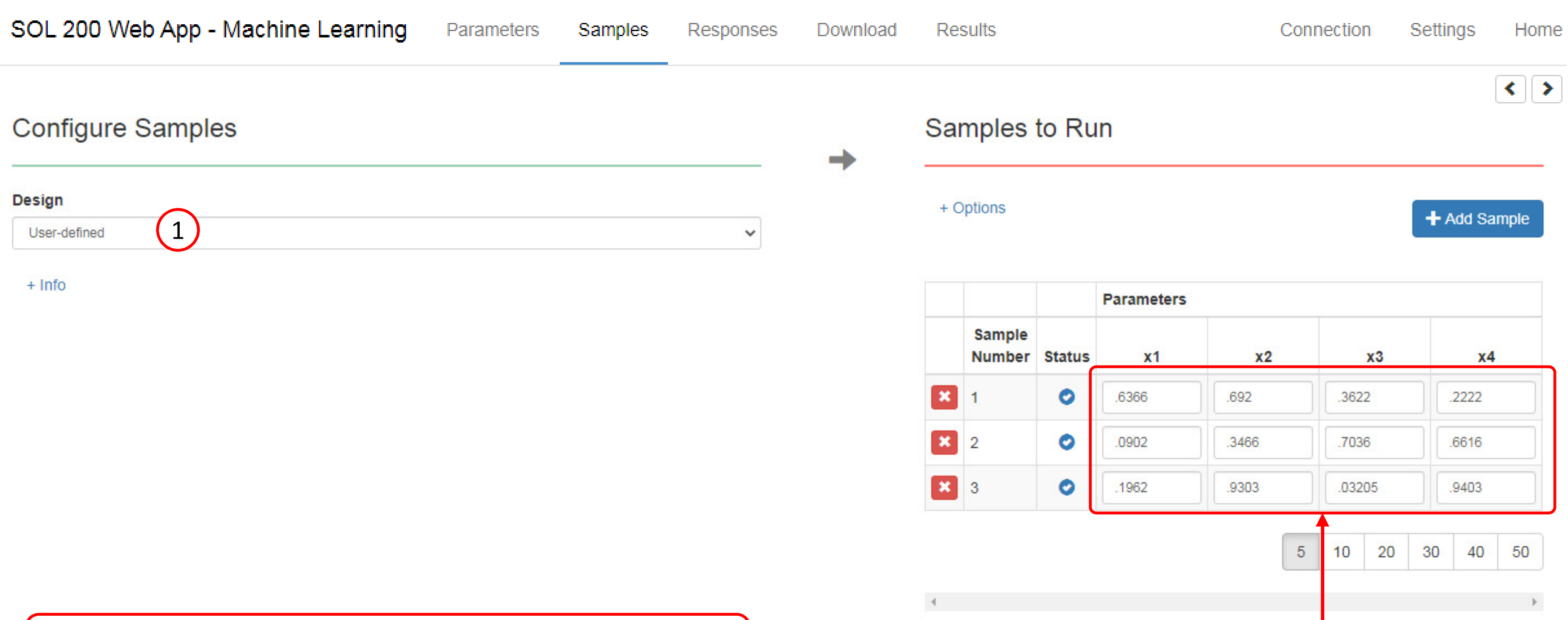
1. Click Download
2. Click Download BDF Files
3. A new ZIP file has been downloaded





Samples

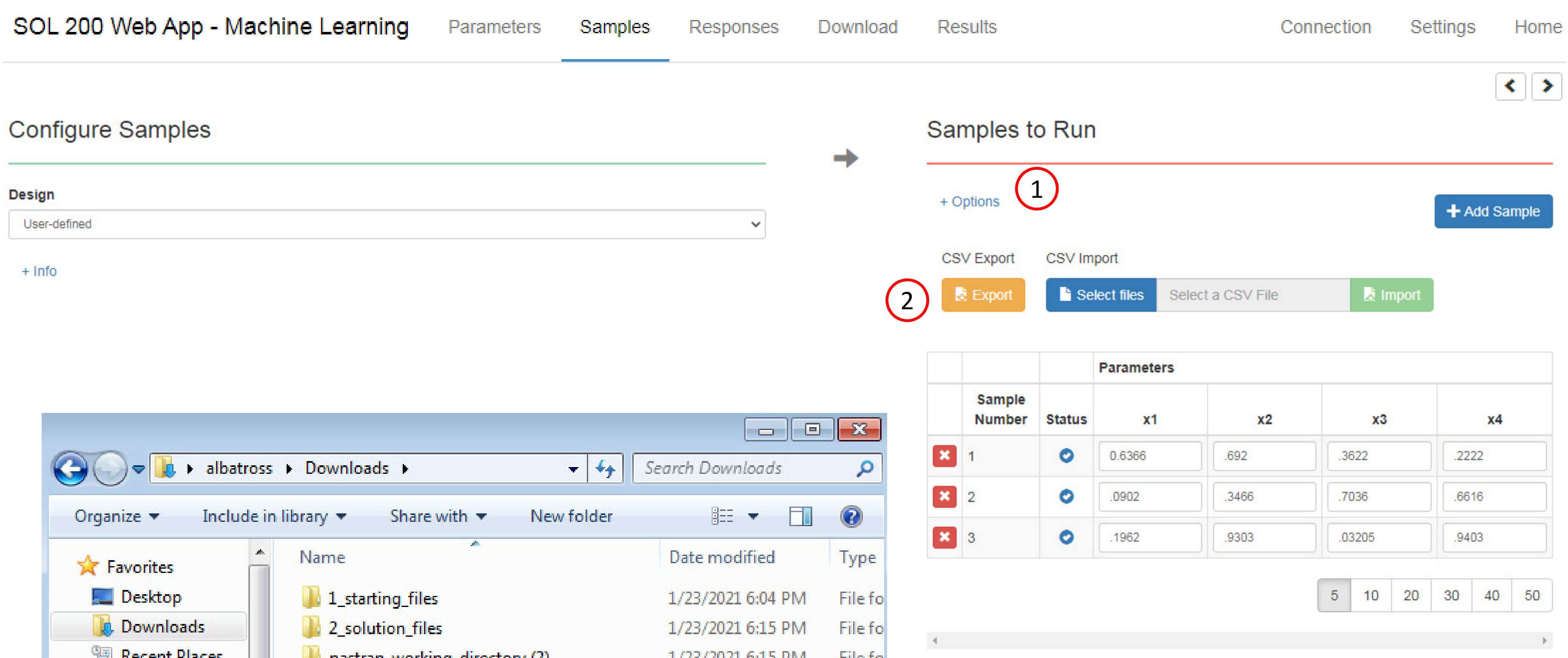
1. Set Design to user-defined
2. Use the sample values in the table and manually add 3 samples
   - Click the red x button to delete samples
   - Click Add Sample to create a new sample

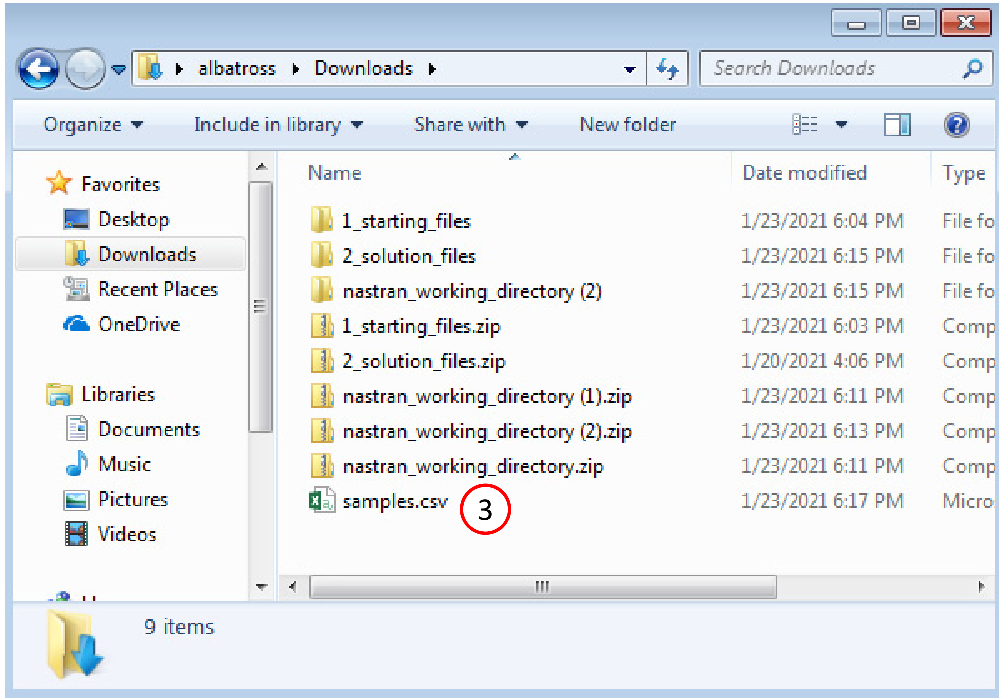


Sample	x1	x2	x3	x4
1	0.6366	0.692	0.3622	0.2222
2	0.0902	0.3466	0.7036	0.6616
3	0.1962	0.9303	0.03205	0.9403

Samples

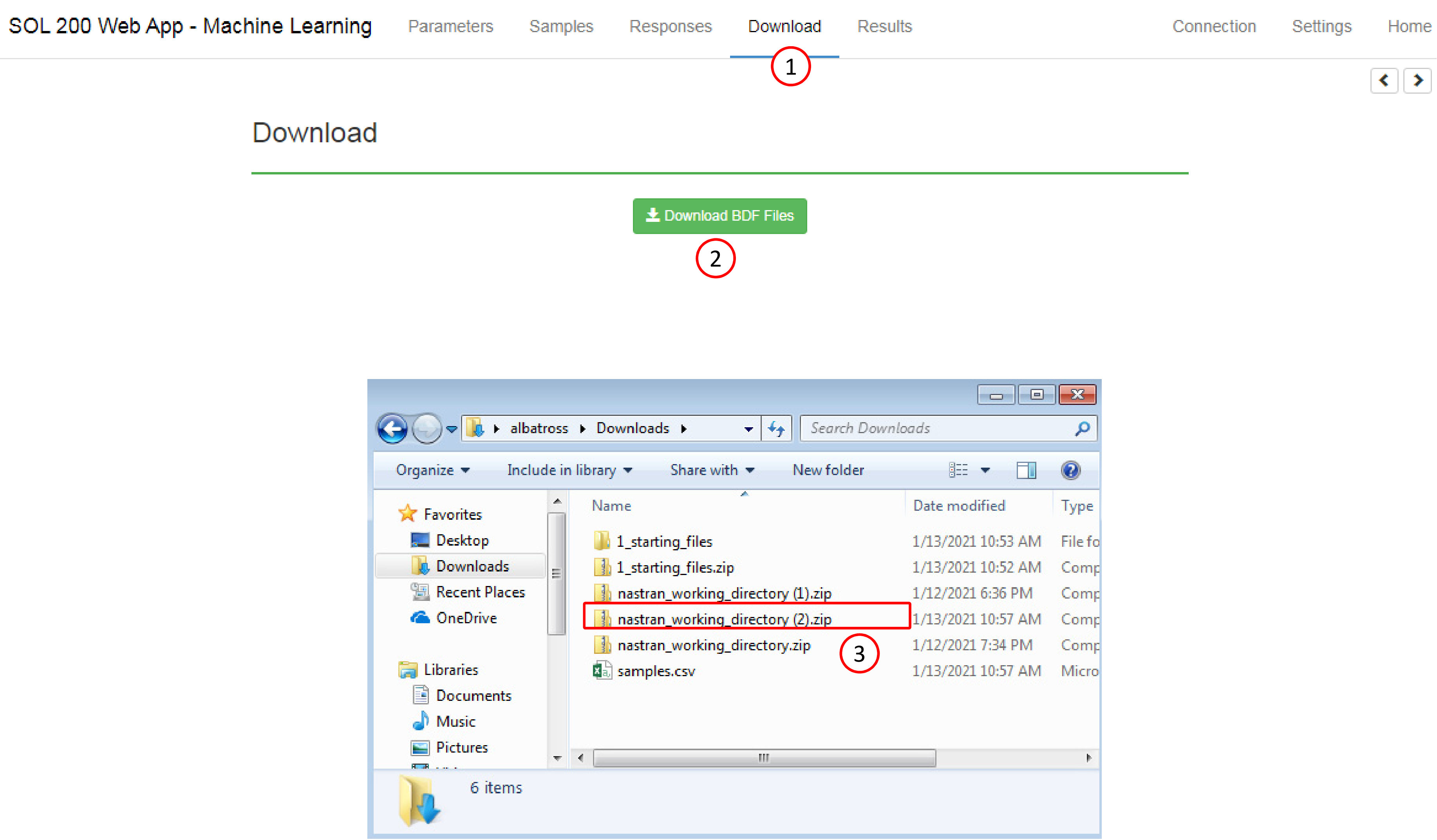
1. Click +Options
2. Click Export
3. The samples.csv file has been downloaded and contains the 3 samples. This file will be used later to make predictions.





Download

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

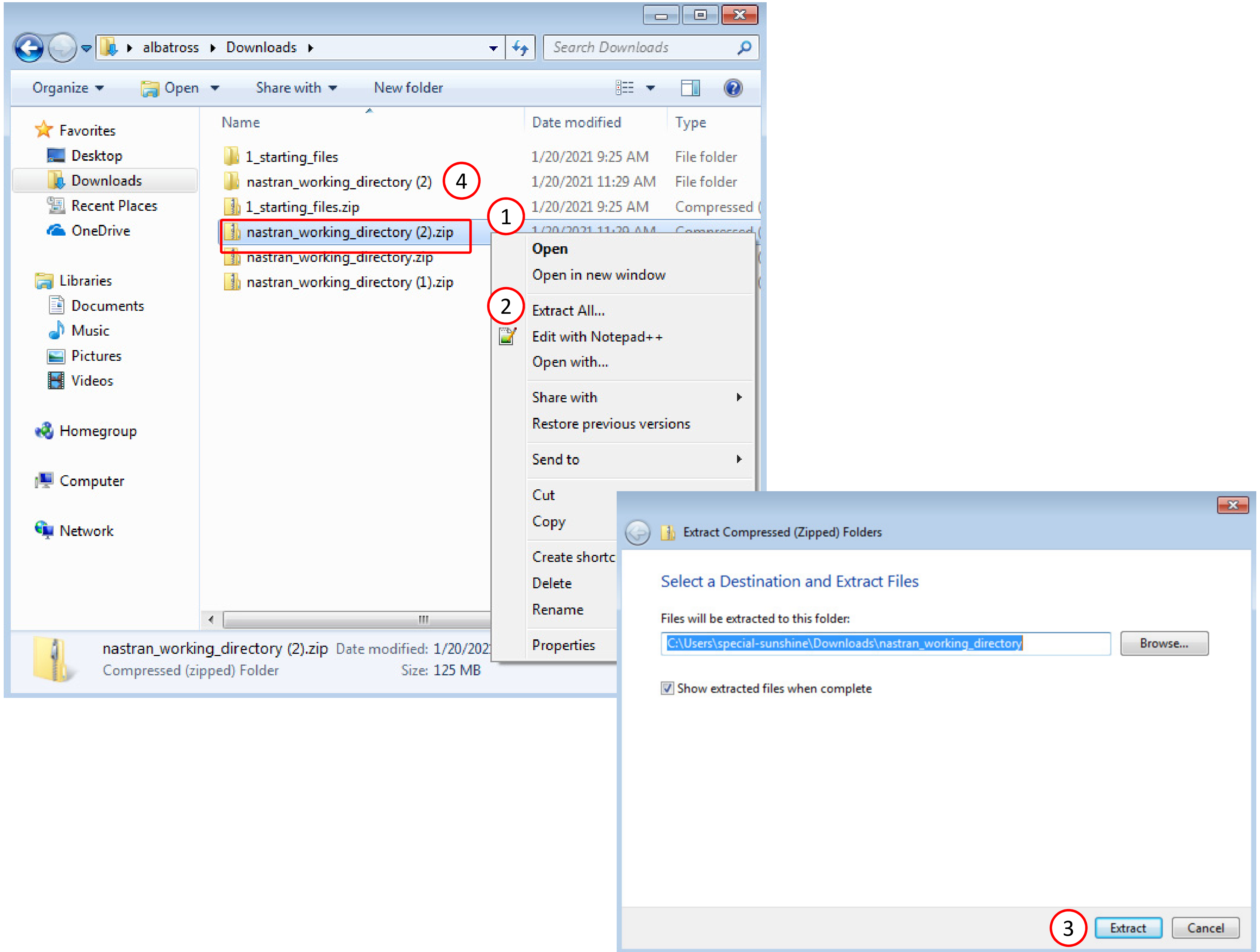


Start Desktop App

The batch with 3 runs will be executed.

1. Right click on the indicated file
2. Click Extract All
3. Click Extract on the following window

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



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

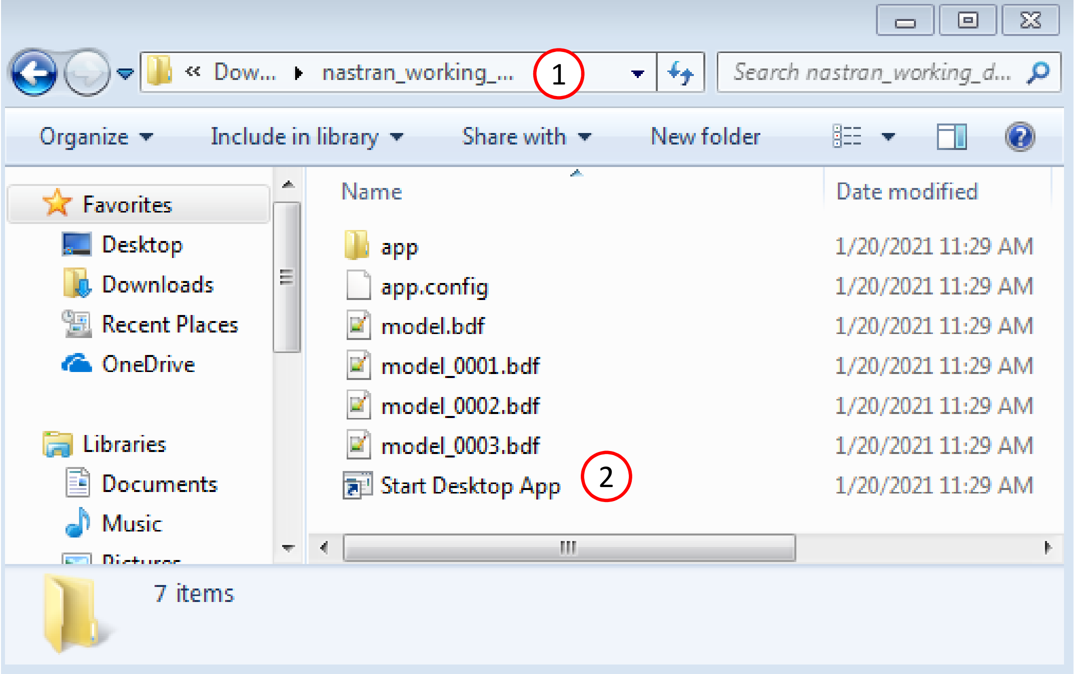
- One can run the Nastran job on a remote machine as follows:
  1) Copy the BDF files and the INCLUDE files to a remote machine. 2) Run the MSC Nastran job on the remote machine. 3) After completion, copy the BDF, F06, LOG, H5 files to the local machine. 4) Click “Start Desktop App” to display the results.

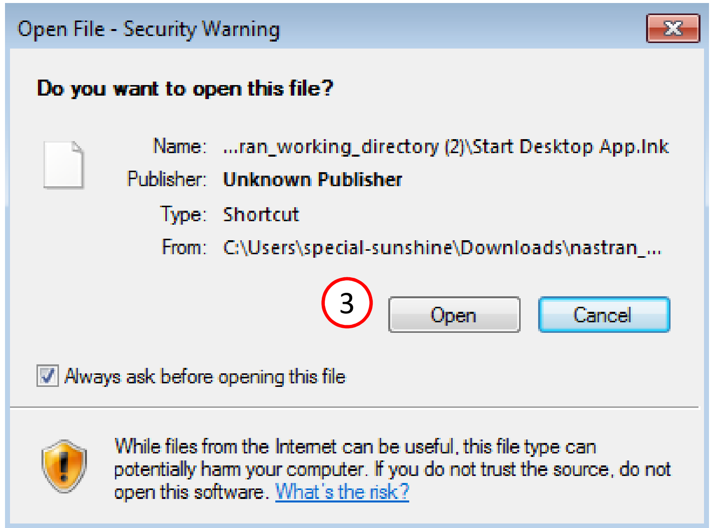
Using Linux?

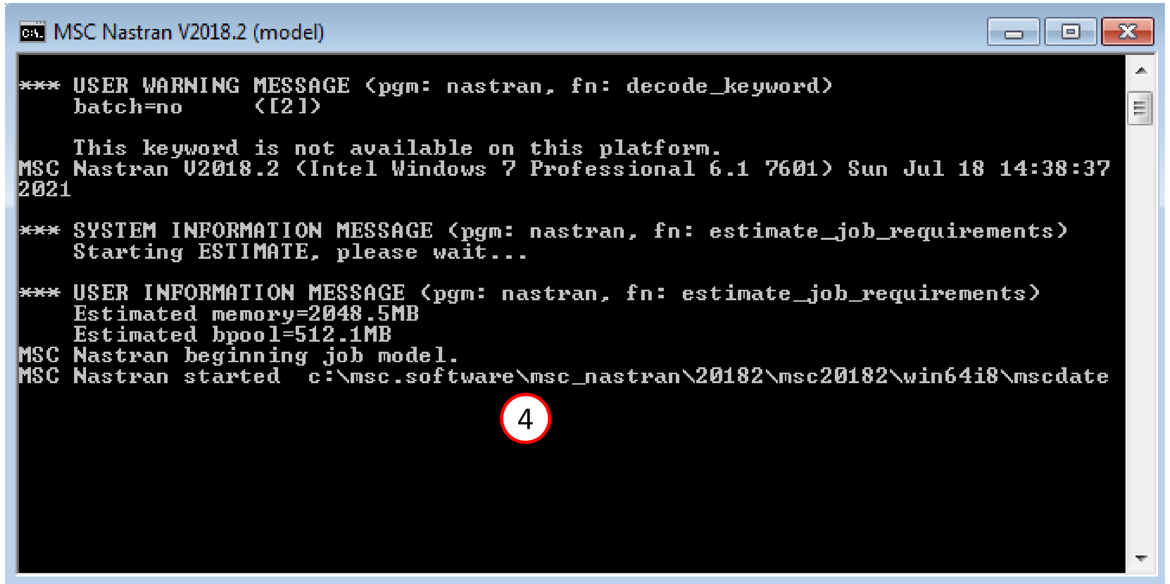
Follow these instructions:
1) Open Terminal
2) Navigate to the nastran_working_directory
cd ./nastran_working_directory
3) Use this command to start the process
./Start_MSC_Nastran.sh

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

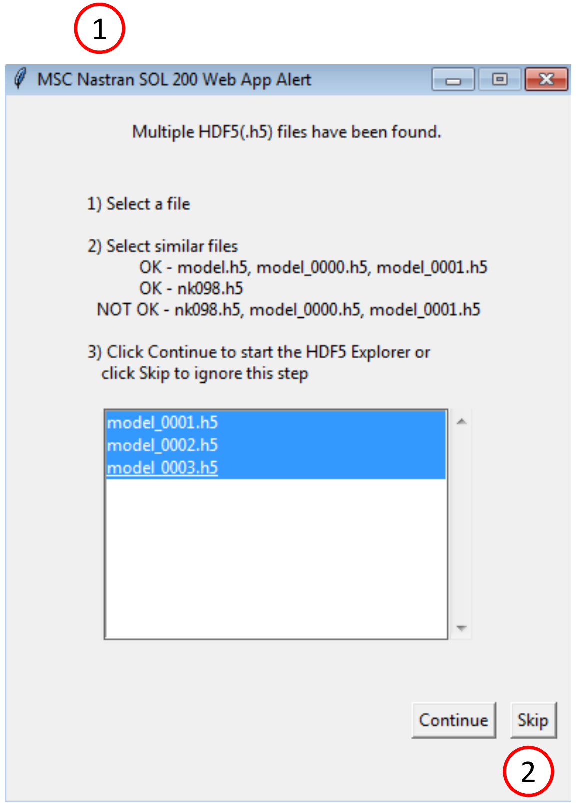
Python MSC Nastran

Status

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

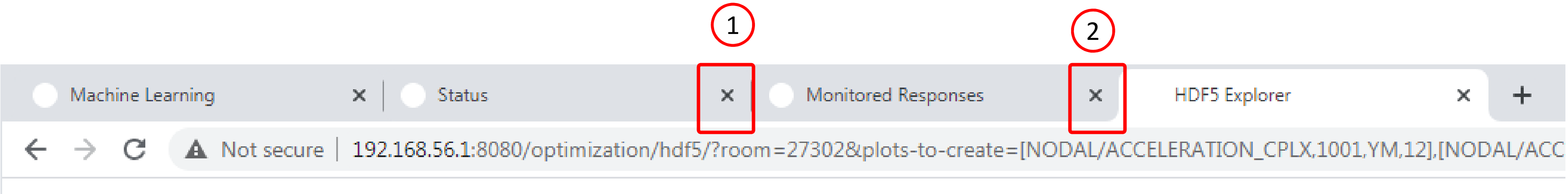
Review Results

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



Close Pages

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



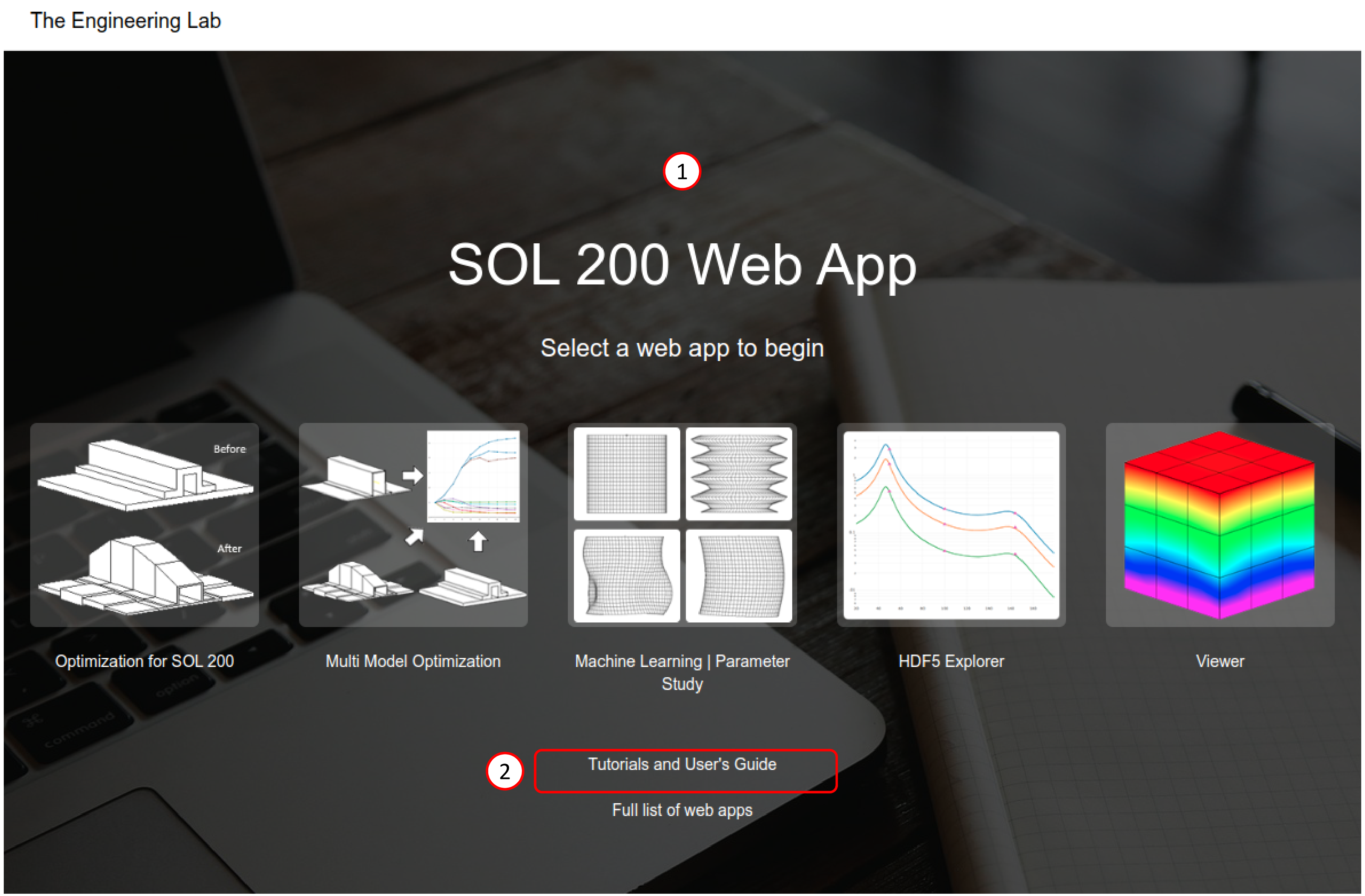
Go to the User's Guide

The following batches will take more than an hour to run

- nastran_working_directory
- nastran_working_directory (1)

These batches have already been executed and the solution files are available in the User's Guide.

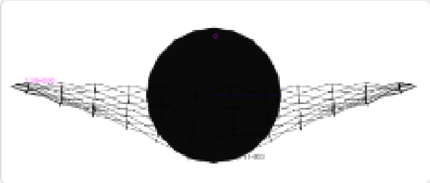
1. Go to the home page
2. Click on the indicated link



Obtain the Solution 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.

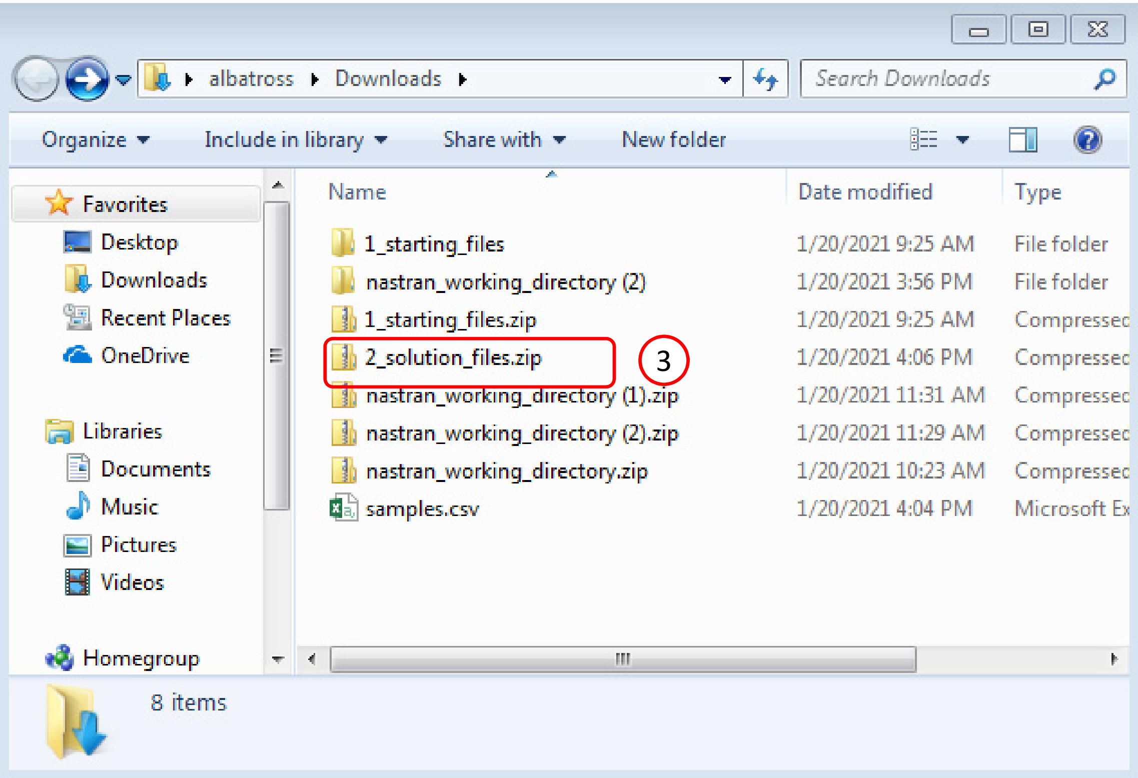


Parameter Study, Dynamic Impact of a Rigid Sphere on a Woven Fabric (1)

Consider a transient analysis of a rigid sphere impacting a woven fabric. The parameters allowed to vary include the friction coefficients. The response of interest are the displacements.

This tutorial describes how to configure multiple MSC Nastran runs to generate training data. Gaussian process regression is used to train a surrogate model and make predictions. The prediction performance of the surrogate model is also evaluated. Also discussed are instructions to create displacement vs. time plots .

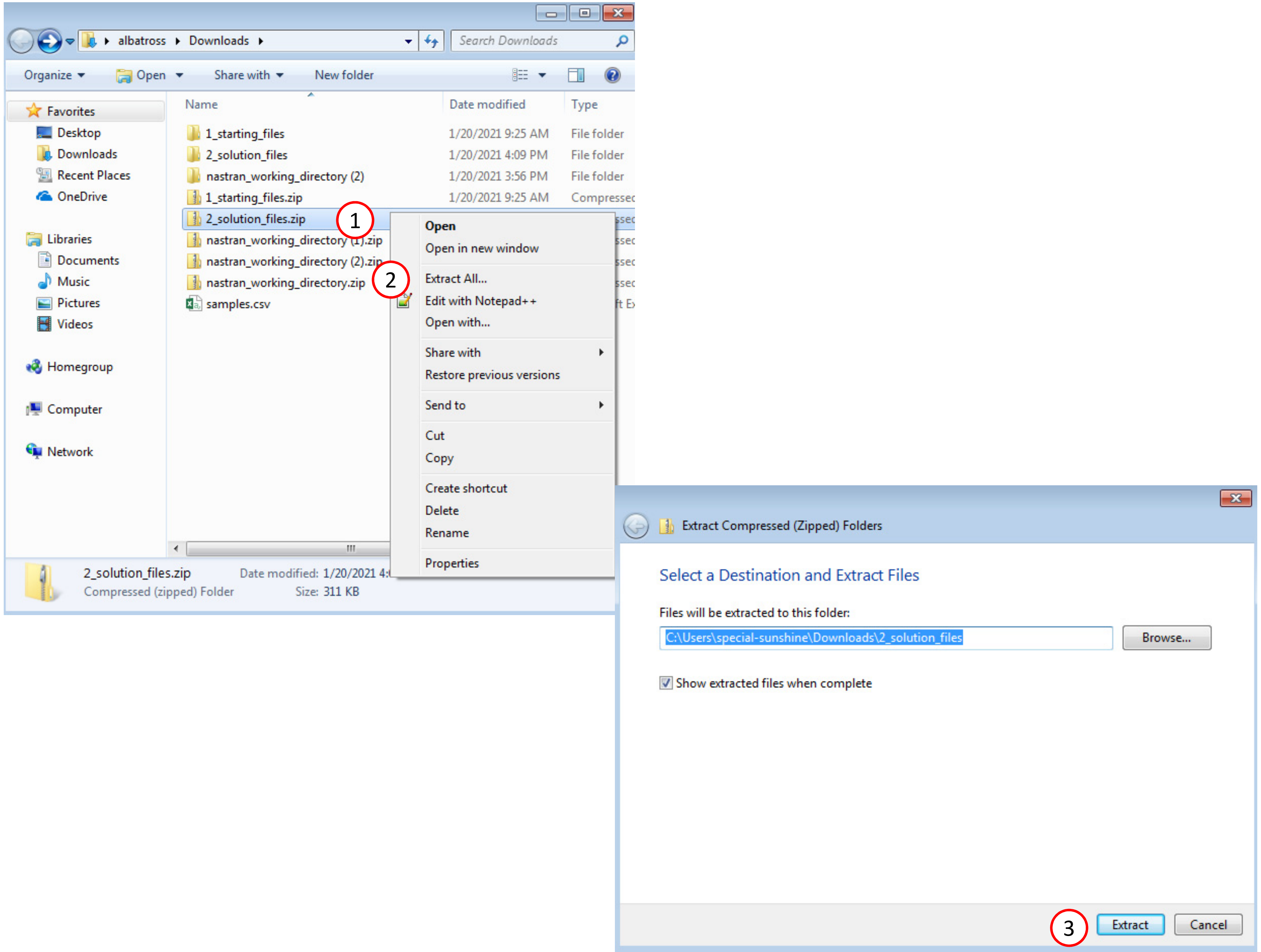
Starting Files: Link
Solution BDF Files: Link (2)



Obtain the Solution Files

1. Right click on the indicated file
2. Click Extract All
3. Click Extract on the following window

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

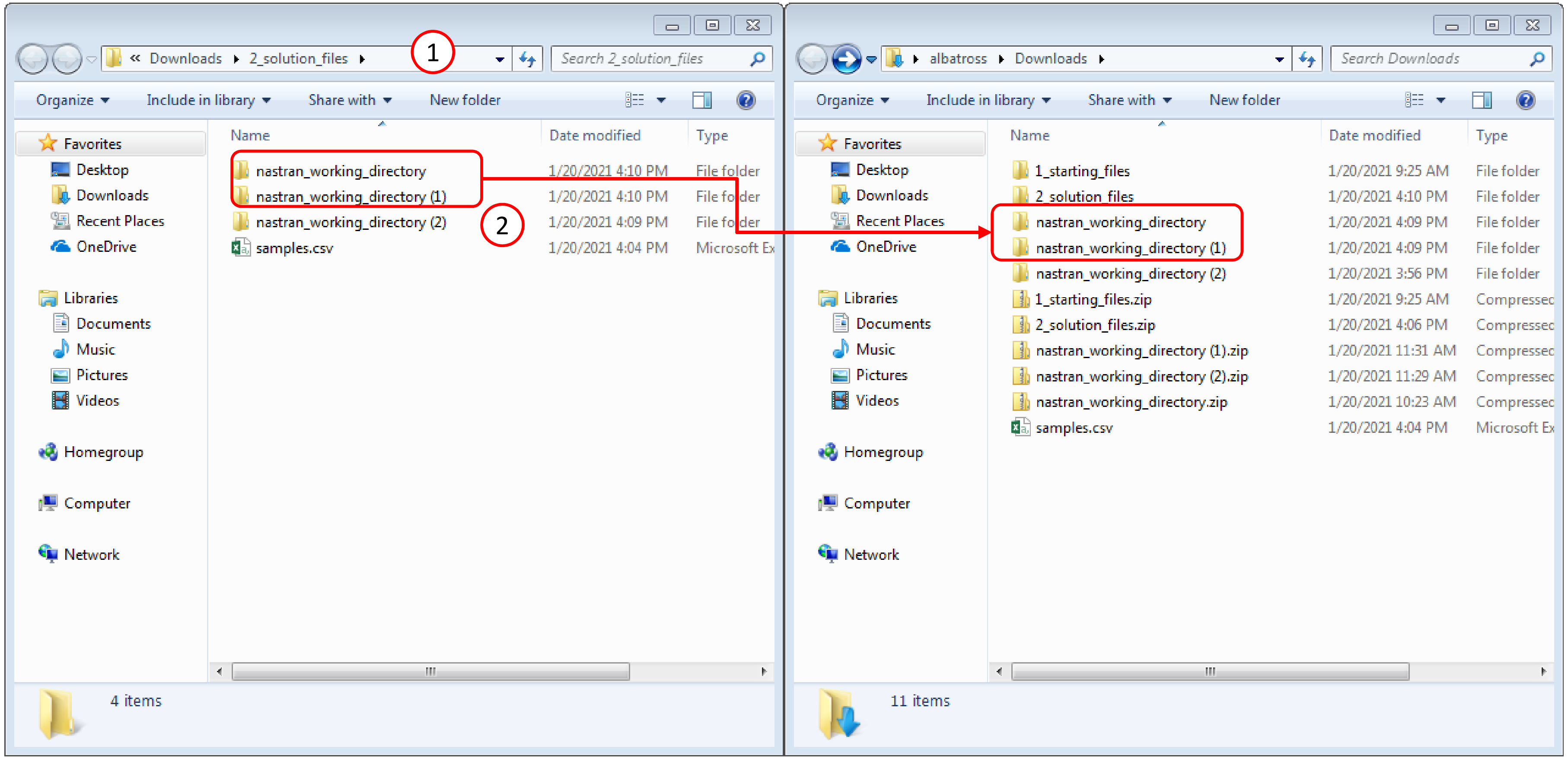


Obtain the Solution Files

1. Open the 2_solution_files folder
2. Copy the following files from the 2_solution_files folder to the Downloads folder
    - nastran_working_directory
    - nastran_working_directory (1)

2_solution_files

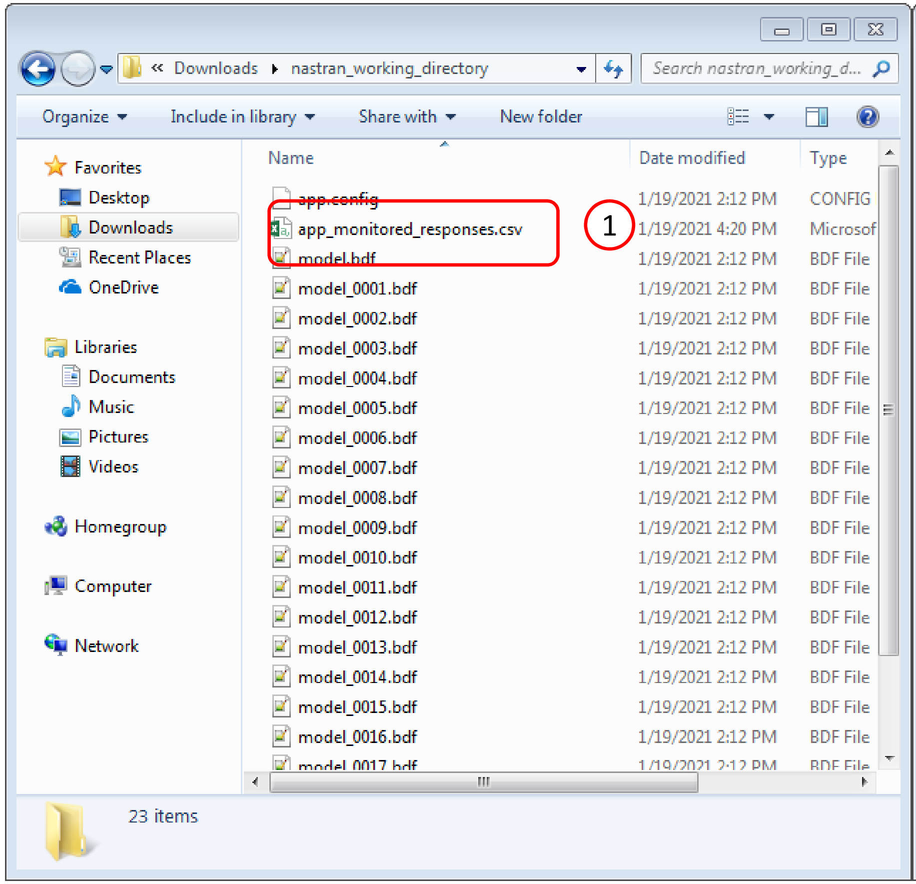
Downloads



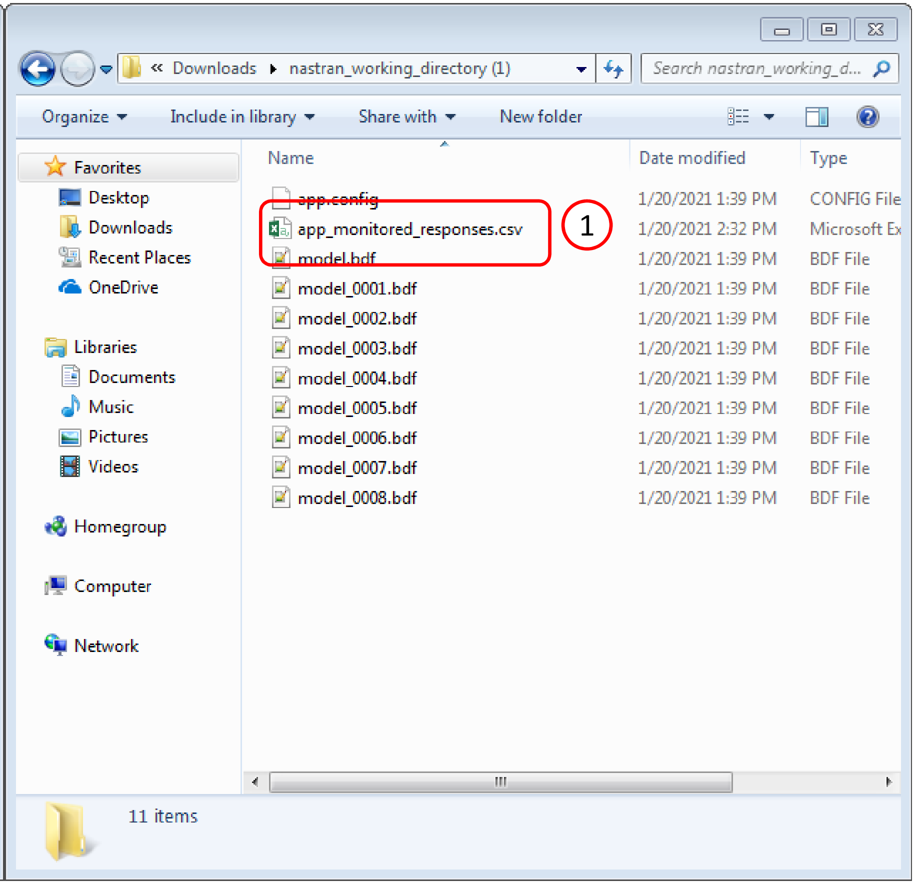
Obtain the Solution Files

1. Ensure the directories below have the file app_monitored_responses.csv. This file contains the outputs that are used to train the surrogate model
   - nastran_working_directory
   - nastran_working_directory (1)

nastran_working_directory



nastran_working_directory (1)



Creating Plots with the HDF5 Explorer

Start Desktop App

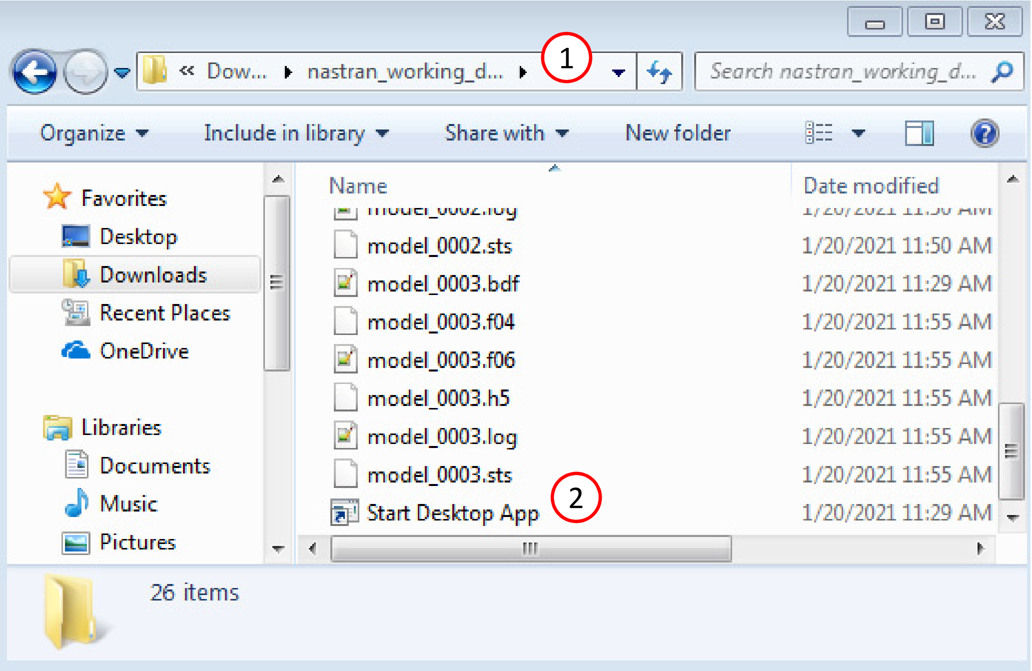
1. Open this folder: nastran_working_directory (2)
2. Inside of the new folder, double click on Start Desktop App
3. Click Open, Run or Allow Access on any subsequent windows

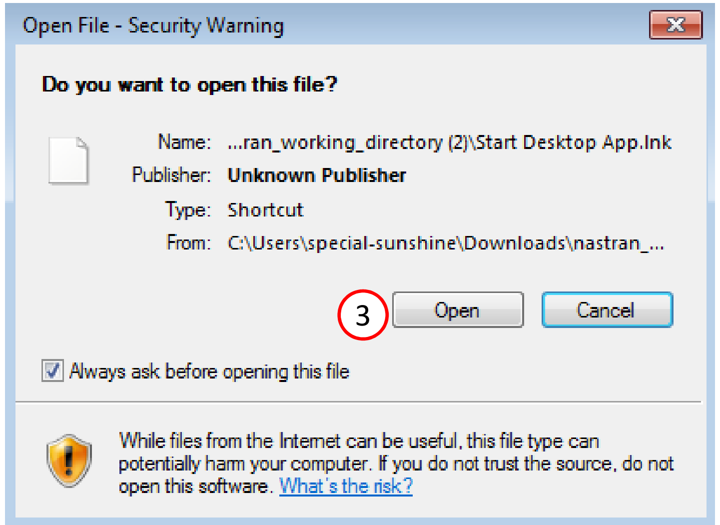
Using Linux?

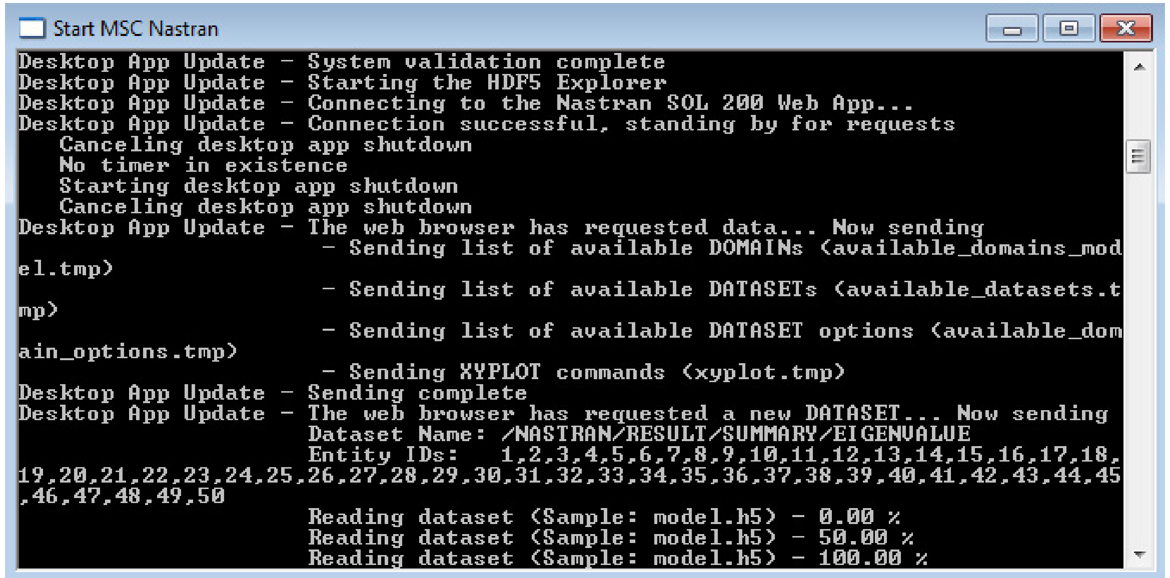
Follow these instructions:
1) Open Terminal
2) Navigate to the nastran_working_directory
cd ./nastran_working_directory
3) Use this command to start the process
./Start_MSC_Nastran.sh

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



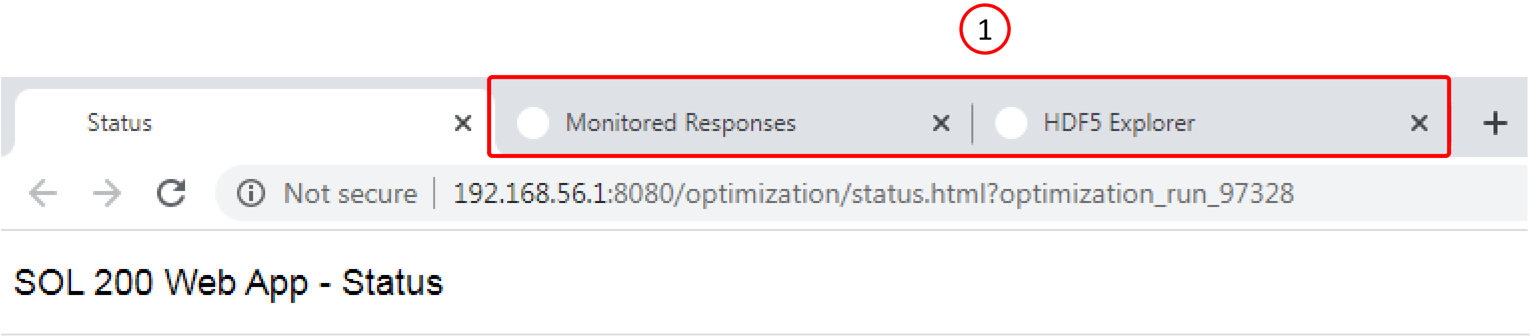




Results

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

After MSC Nastran is finished, the results will be automatically uploaded.

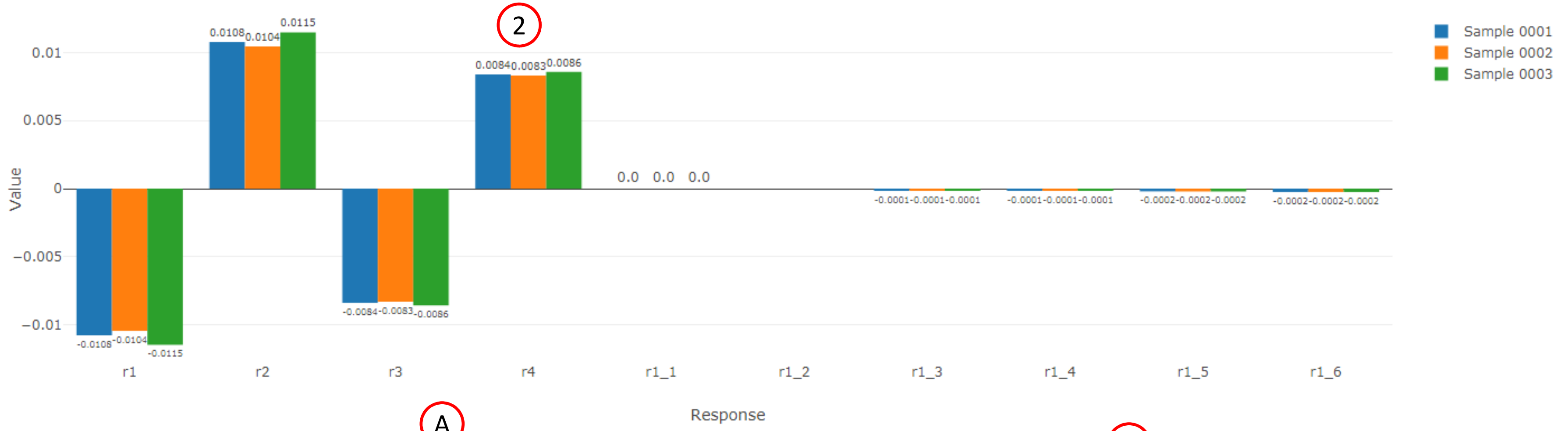
1. On this page, the Monitored Responses web app is opened.
2. The value of each response and for each sample is displayed in a bar chart
3. A table lists the values for each response and sample.

A. 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

(2)



(A)

Monitored Responses

Display MAX and MIN | Download CSV | Reset Filters

Label	Dataset Name	Field	Field Description
r1 r1_1 r1_2 r1_3	NODAL/DISPLACEMENT	MAGTRANS Z	Magnitude of Translational Components** Z component
r1	NODAL/DISPLACEMENT	Z	Z component
r2	NODAL/DISPLACEMENT	MAGTRANS	Magnitude of Translational Component
r3	NODAL/DISPLACEMENT	Z	Z component
r4	NODAL/DISPLACEMENT	MAGTRANS	Magnitude of Translational Component

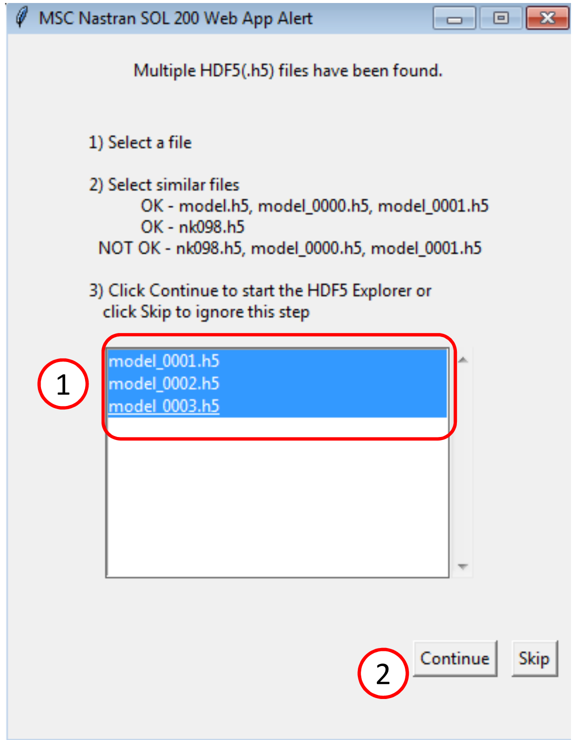
Monitored Responses from Each Sample (3)

0001	0002
-0.010760165764037181	-0.010449259269352605
0.010760165764037181	0.010449259269352605
-0.008387852952825688	-0.008301875773497372
0.008387852952825688	0.008301875773497372

Review Results

On this page, the HDF5 Explorer is opened.

1. Select all the H5 files
2. Click Continue
3. The HDF5 Explorer is automatically opened.
4. Click on the indicated plot



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

1. A history plot of the z displacement of the rigid sphere has been created

Later in this tutorial, a surrogate model will be created for response r1 and corresponds to the Z component displacement.

Review Results

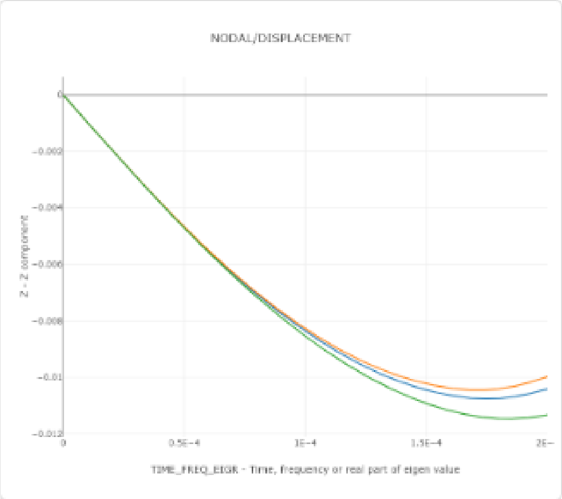
1. Click Plots Browser
2. Click Plot # 2

SOL 200 Web App - HDF5 Explorer Acquire Dataset | Plots Browser | Combine Plots | Last Plot Added

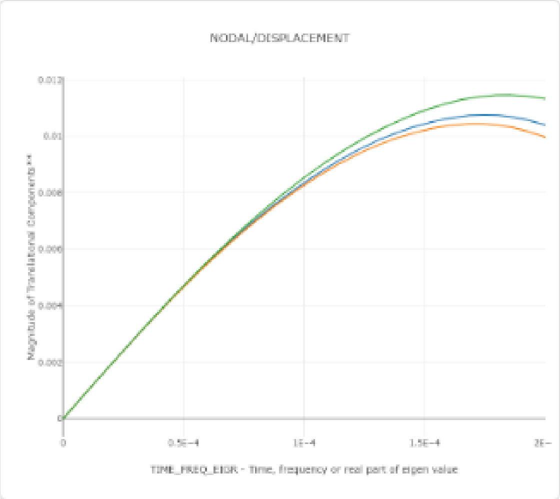
1

Plots Browser

NODAL/DISPLACEMENT



Plot #: 1 - ID: 1 | SAMPLE: model_0001, model_0002, model_0003 | SUBCASE: 1 | STEP: 1 | Z vs. TIME_FREQ_EIGR



Plot #: 2 - ID: 1 | SAMPLE: model_0001, model_0002, model_0003 | SUBCASE: 1 | STEP: 1 | MAGTRANS vs. TIME_FREQ_EIGR

2

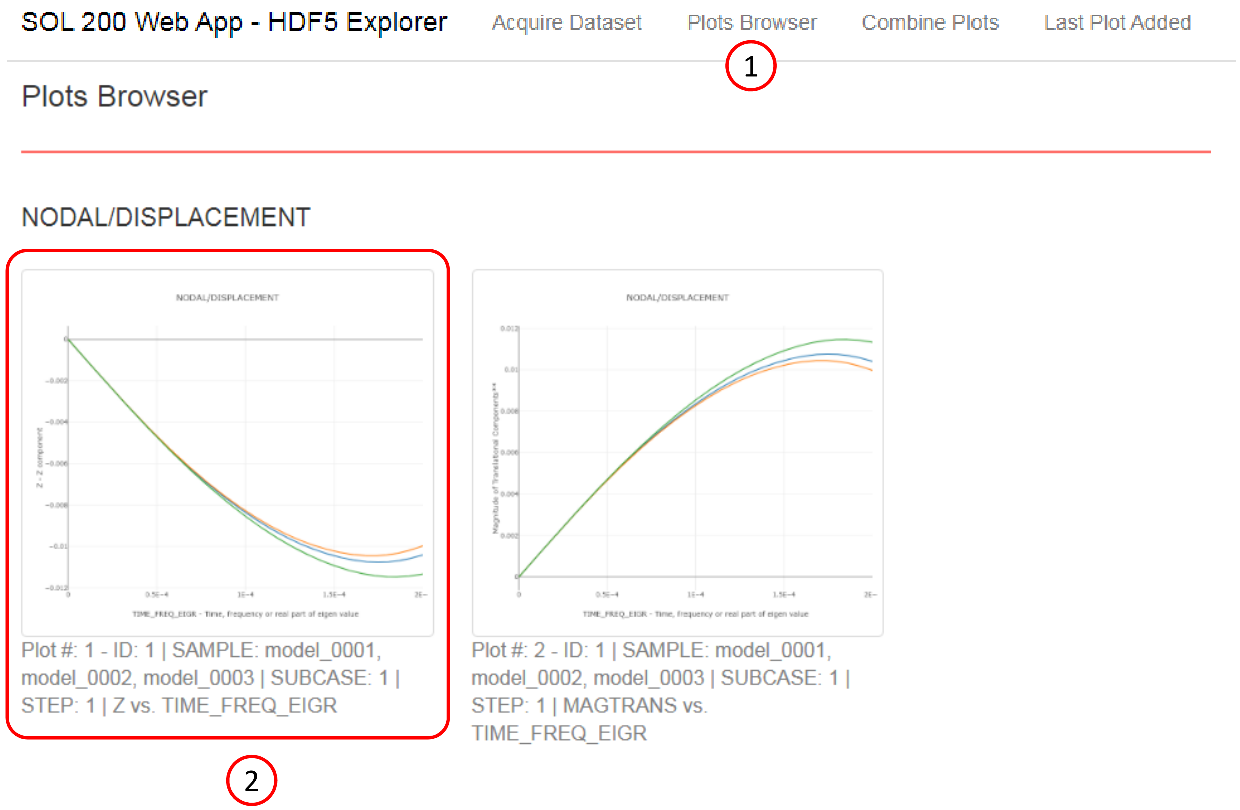
Review Results

1. A history plot of the magnitude of displacement of the rigid sphere has been created

Later in this tutorial, a surrogate model will be created for response r2 and corresponds to the magnitude of displacement.

Review Results

1. Click Plots Browser
2. Click on the indicated plot



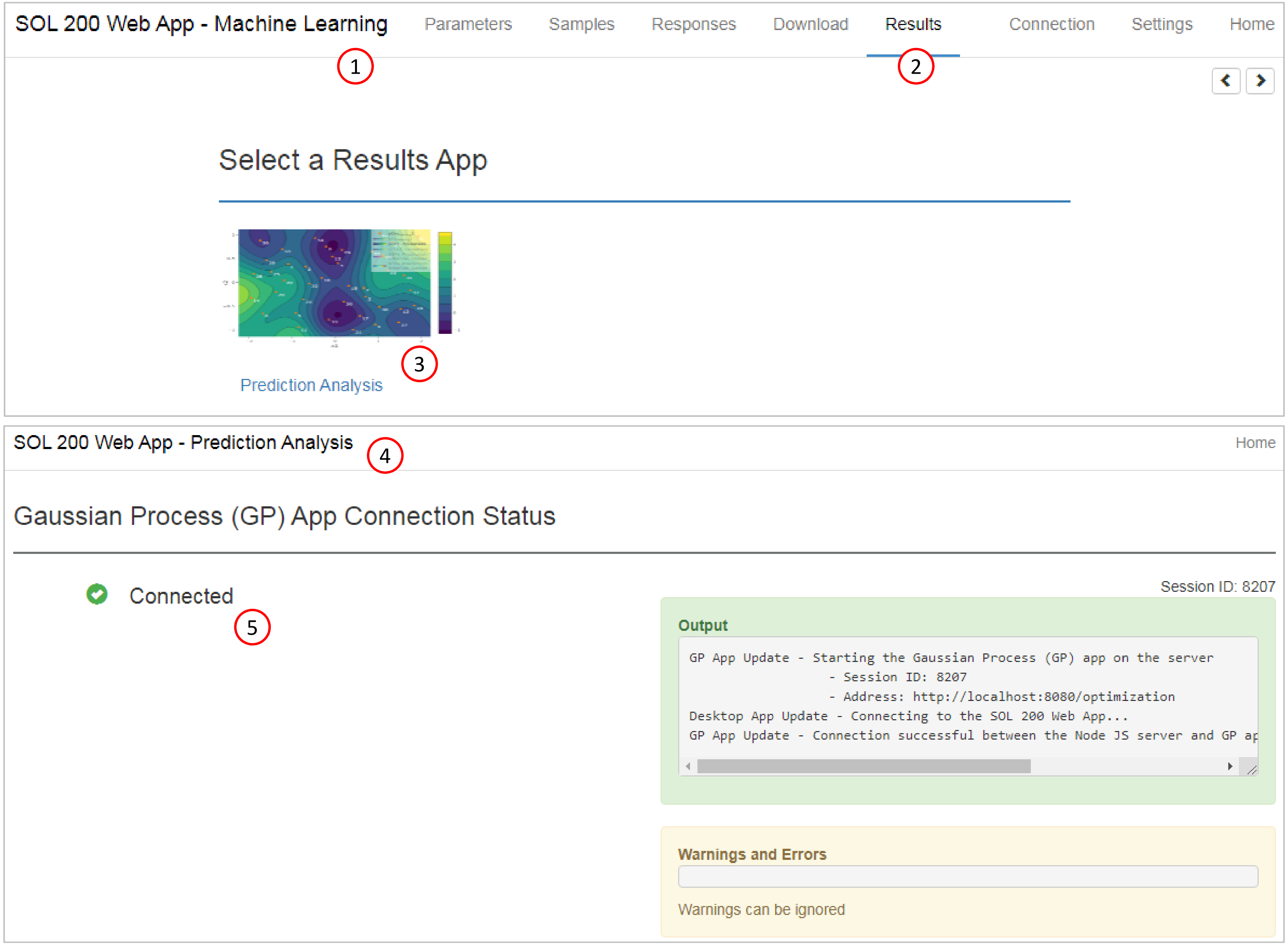
Review Results

1. This plot will be used later in this tutorial

Performing Predictions

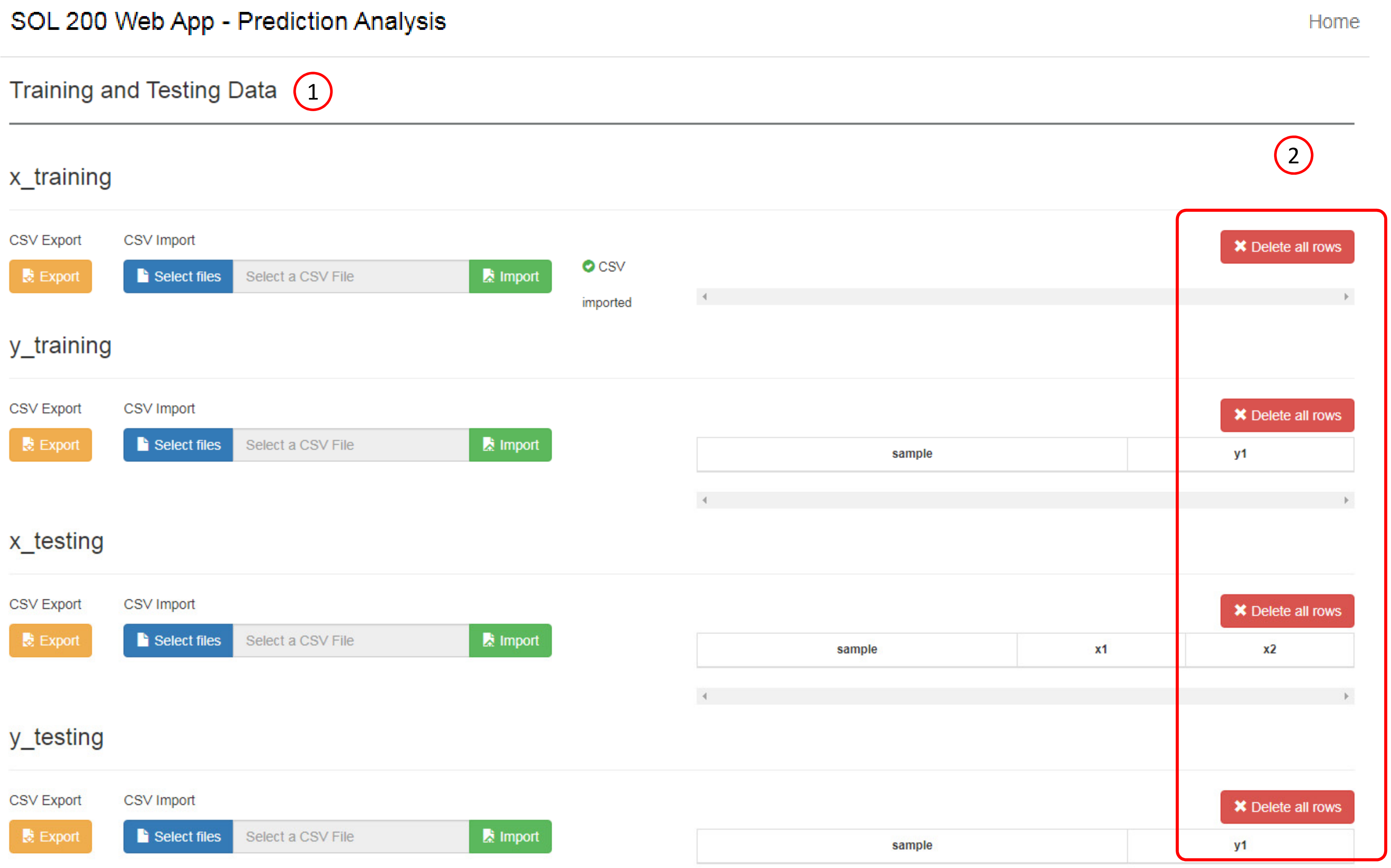
Prediction Analysis Web App

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

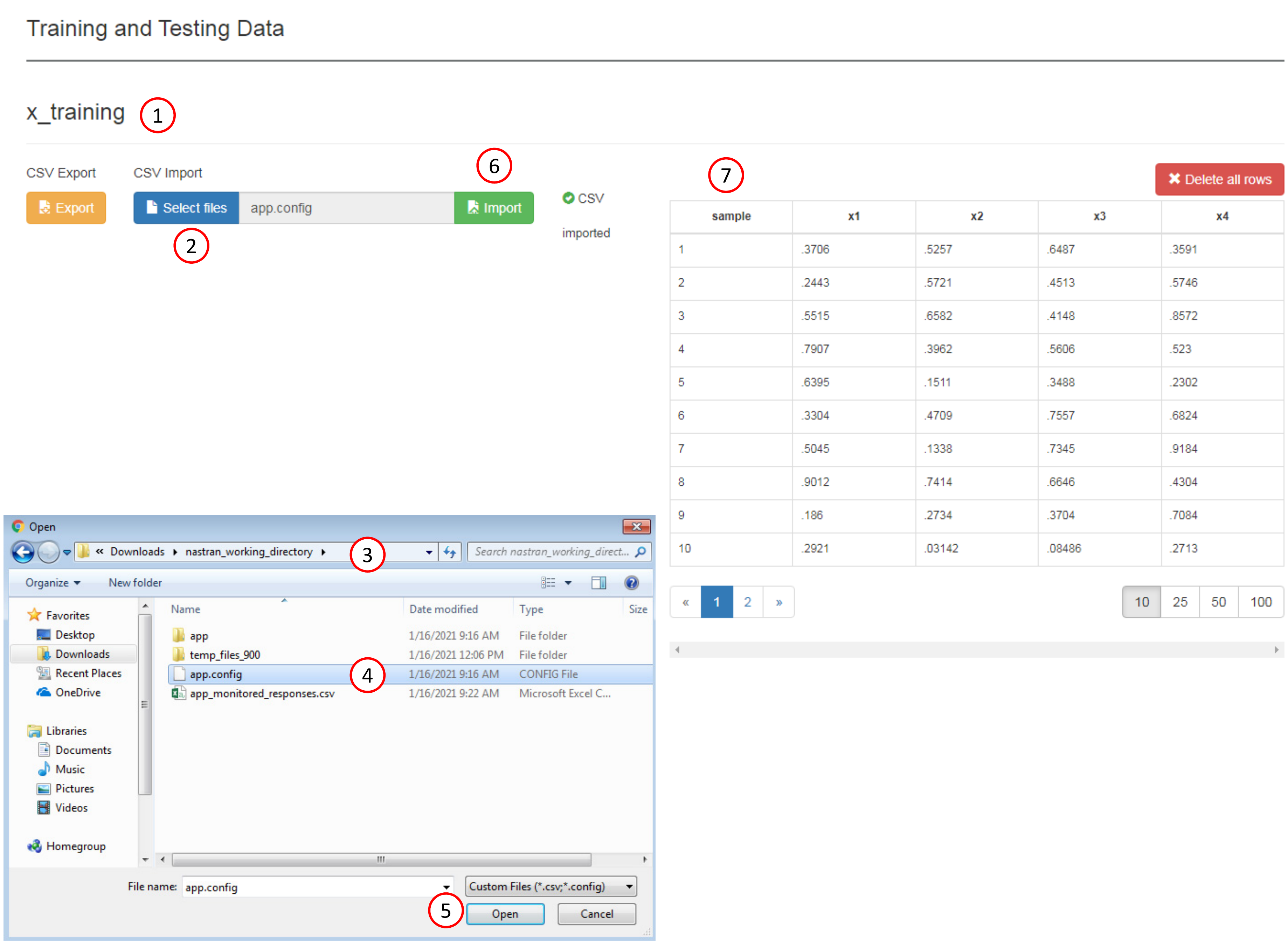
1. Navigate to the Training and Testing Data section
2. Delete any previous table data by clicking the four (4) buttons named Delete all rows



- **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

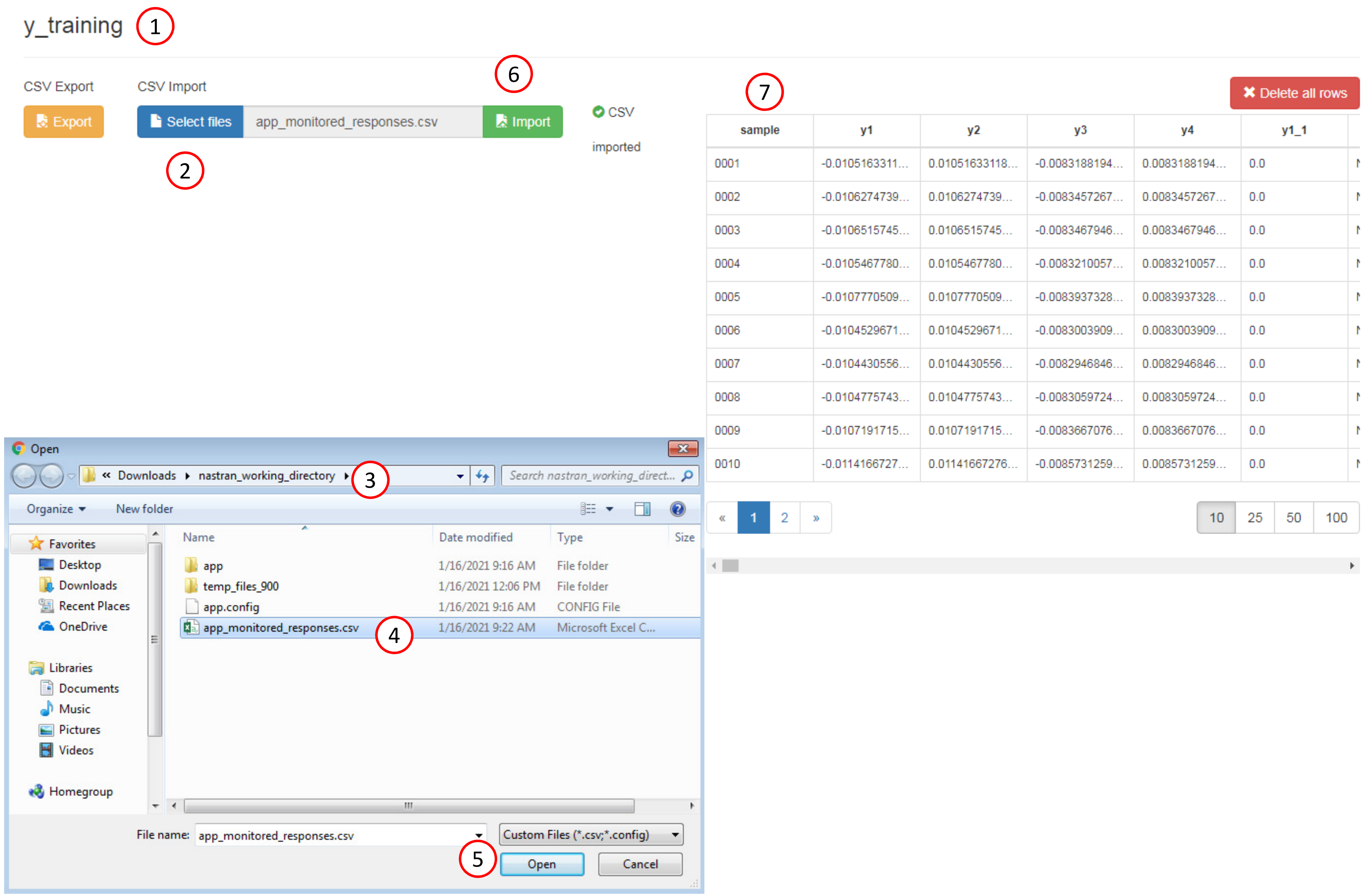
1. Navigate to the section titled x_training
2. Click Select files
3. Navigate to the folder named nastran_working_directory which contains data for 20 runs
4. Select the file app.config
5. Click Open
6. Click Import
7. The table is now loaded with the x inputs for all 20 runs



sample	x1	x2	x3	x4
1	.3706	.5257	.6487	.3591
2	.2443	.5721	.4513	.5746
3	.5515	.6582	.4148	.8572
4	.7907	.3962	.5606	.523
5	.6395	.1511	.3488	.2302
6	.3304	.4709	.7557	.6824
7	.5045	.1338	.7345	.9184
8	.9012	.7414	.6646	.4304
9	.186	.2734	.3704	.7084
10	.2921	.03142	.08486	.2713

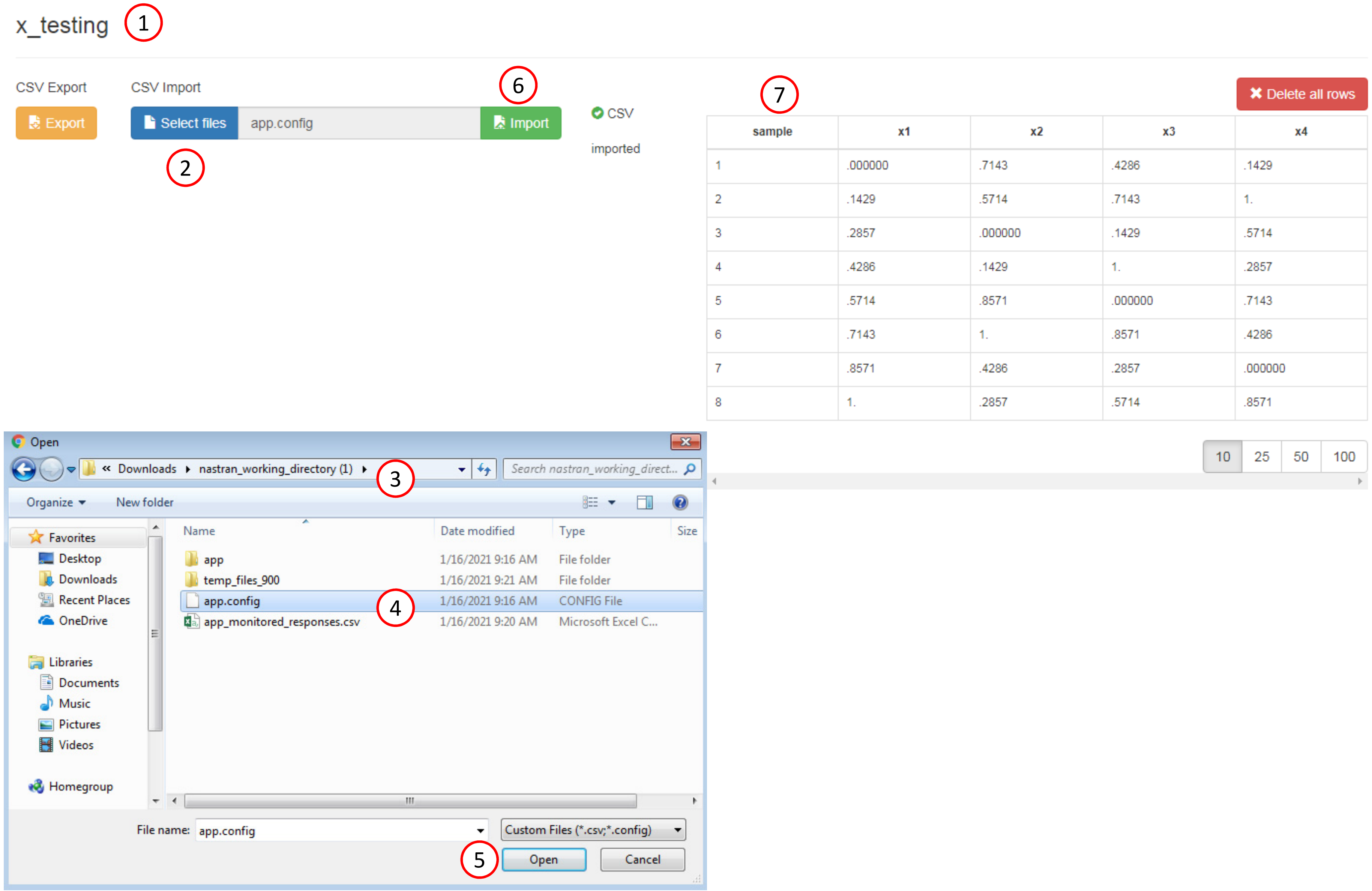
Training Data

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 20 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 20 runs



Testing Data

1. Navigate to the section titled x_testing
2. Click Select files
3. Navigate to the folder named nastran_working_directory (1) which contains data for 8 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 8 runs

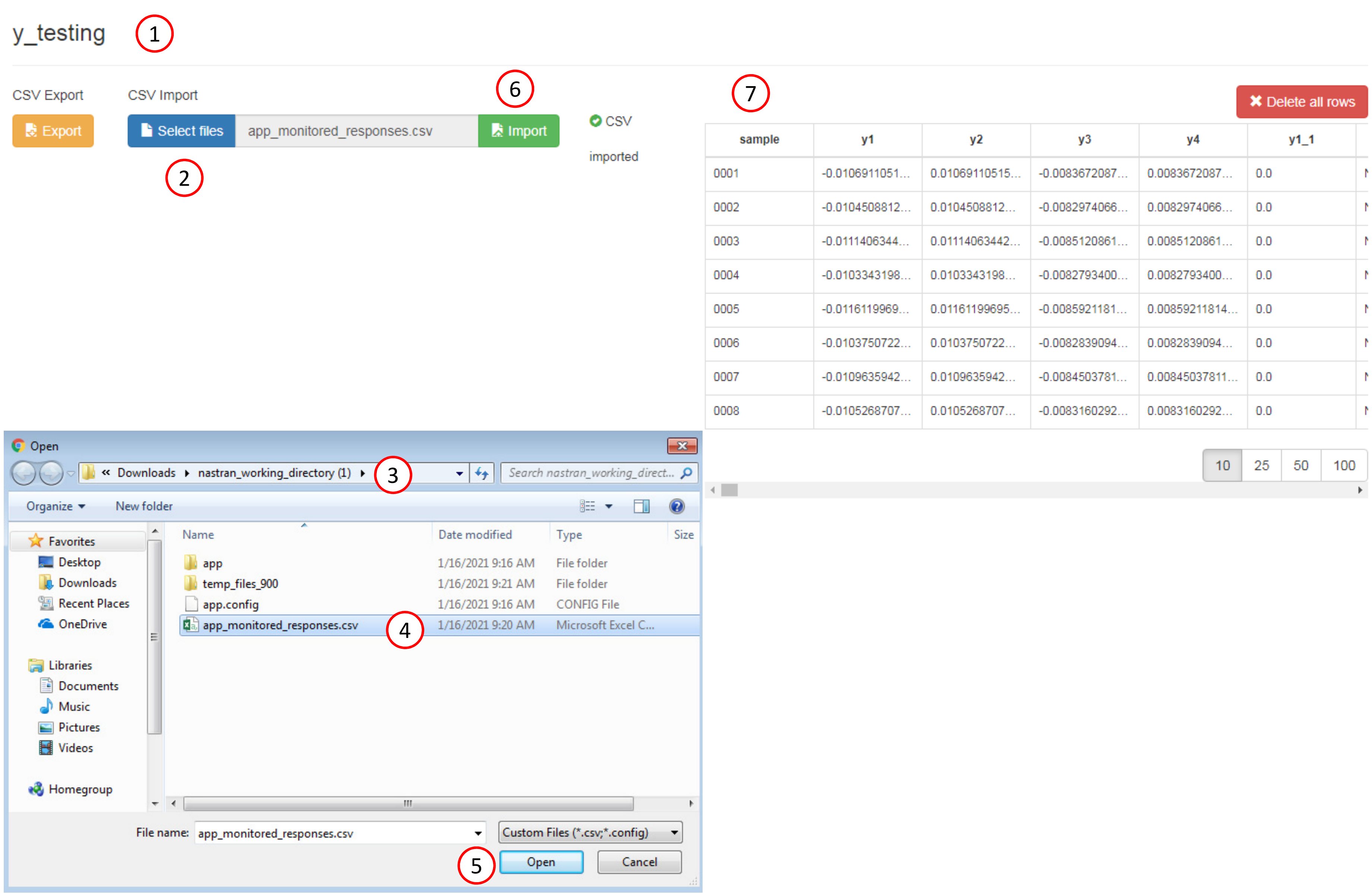


Questions? Email: christian@ the-engineering-lab.com

HEXAGON Technology Partner

Testing Data

1. Navigate to the section titled y_testing
2. Click Select files
3. Navigate to the folder named nastran_working_directory (1) which contains data for 8 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 8 runs



Perform Regression

1. Click Perform Regression
2. An error is immediately detected with the training data. This error is corrected 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 encountered errors, review the Warnings and Errors

Output

```
GP App Update - The web browser has requested a regression
```

Warnings and Errors

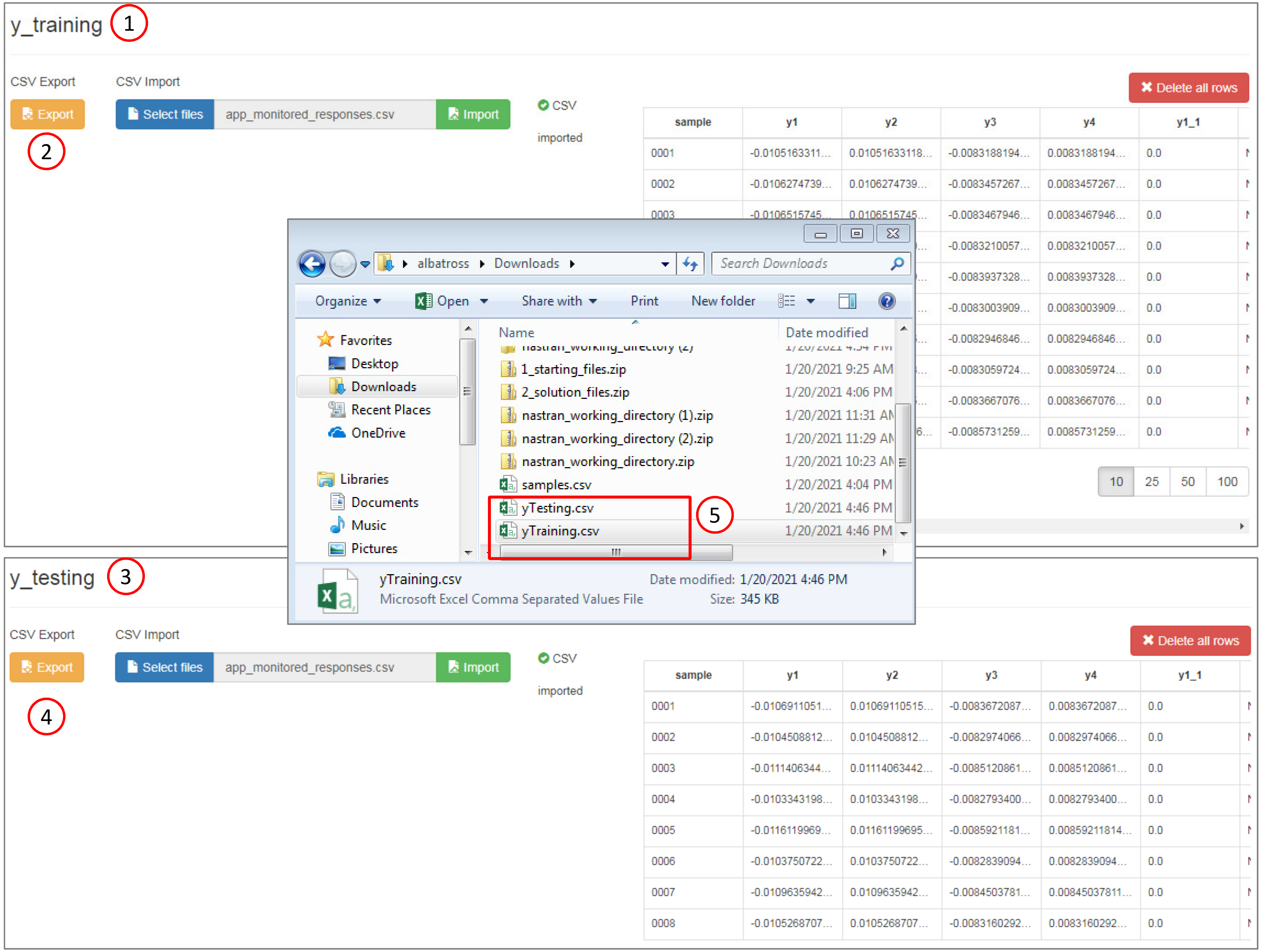
```
Traceback (most recent call last):
  File "/home/apricot/PycharmProjects/python-app/optimization_working_directory/sandbox-ap
    self.function_a_perform_initial_regression_and_predictions(incoming_csv_string)
  File "/home/apricot/PycharmProjects/python-app/optimization_working_directory/sandbox-ap
    x_train_with_samples_column, y_train_with_samples_column, x_test_with_samples_column,
  File "/home/apricot/PycharmProjects/python-app/optimization_working_directory/sandbox-ap
    x_training, y_training = recover_x_and_y_in_numpy_form_2(elements_in_string[1], elemen
  File "/home/apricot/PycharmProjects/python-app/optimization_working_directory/sandbox-ap
    y_train_new = convert_list_to_numpy_array(y_train_new)
  File "/home/apricot/PycharmProjects/python-app/optimization_working_directory/sandbox-ap
    x_train = x_train.astype(np.float)
ValueError: could not convert string to float: 'None-TheresponsecouldnotbefoundintheH5file
GP App Update - IMPORTANT! The last operation could not be completed.
```

(2)

Warnings can be ignored

Updating the Y Outputs

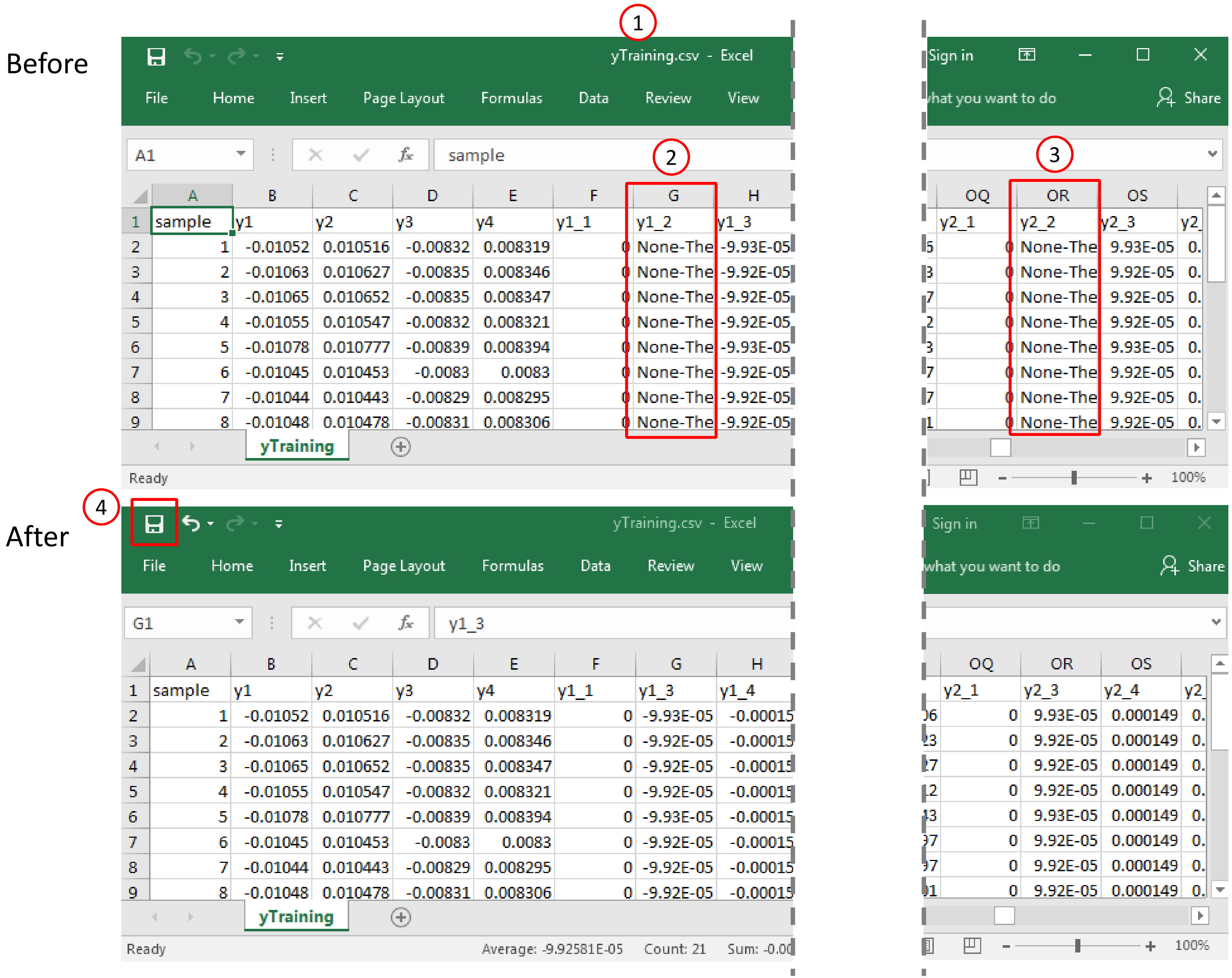
1. Navigate to the section titled y_training
2. Click Export
3. Navigate to the section titled y_testing
4. Click Export
5. Two CSV files have been downloaded and are named:
    - yTraining.csv
    - yTesting.csv



Updating the Y Outputs

Some of the columns contains words instead of number values. These words are causing the previous error. The columns with the words are removed to resolve the error.

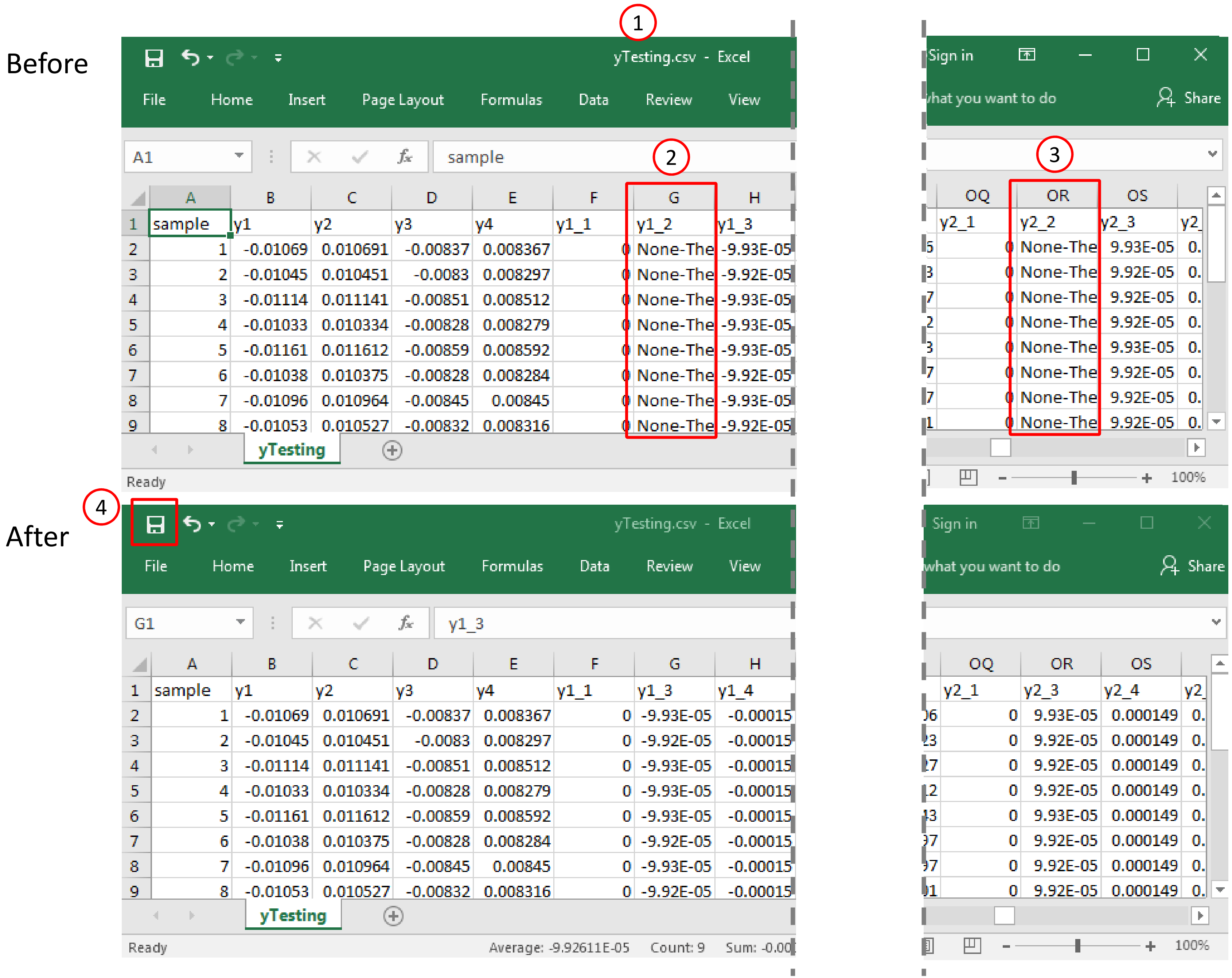
1. Open this file in Excel: yTraining.csv
2. Delete the column for response y1_2
3. Delete the column for response y2_2
4. Click Save



Updating the Y Outputs

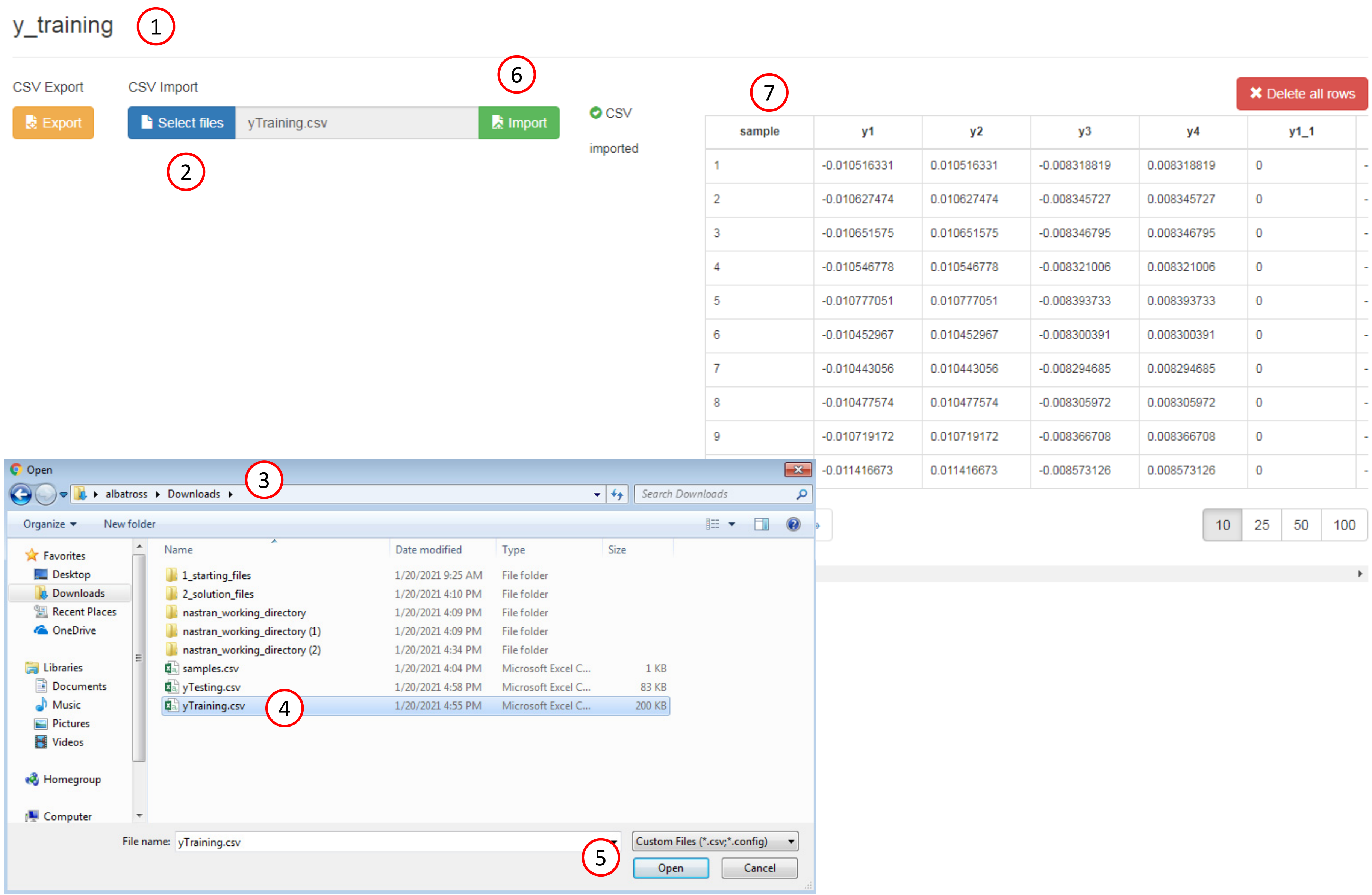
Some of the columns contains words instead of number values. These words are causing the previous error. The columns with the words are removed to resolve the error.

1. Open this file in Excel: yTesting.csv
2. Delete the column for response y1_2
3. Delete the column for response y2_2
4. Click Save



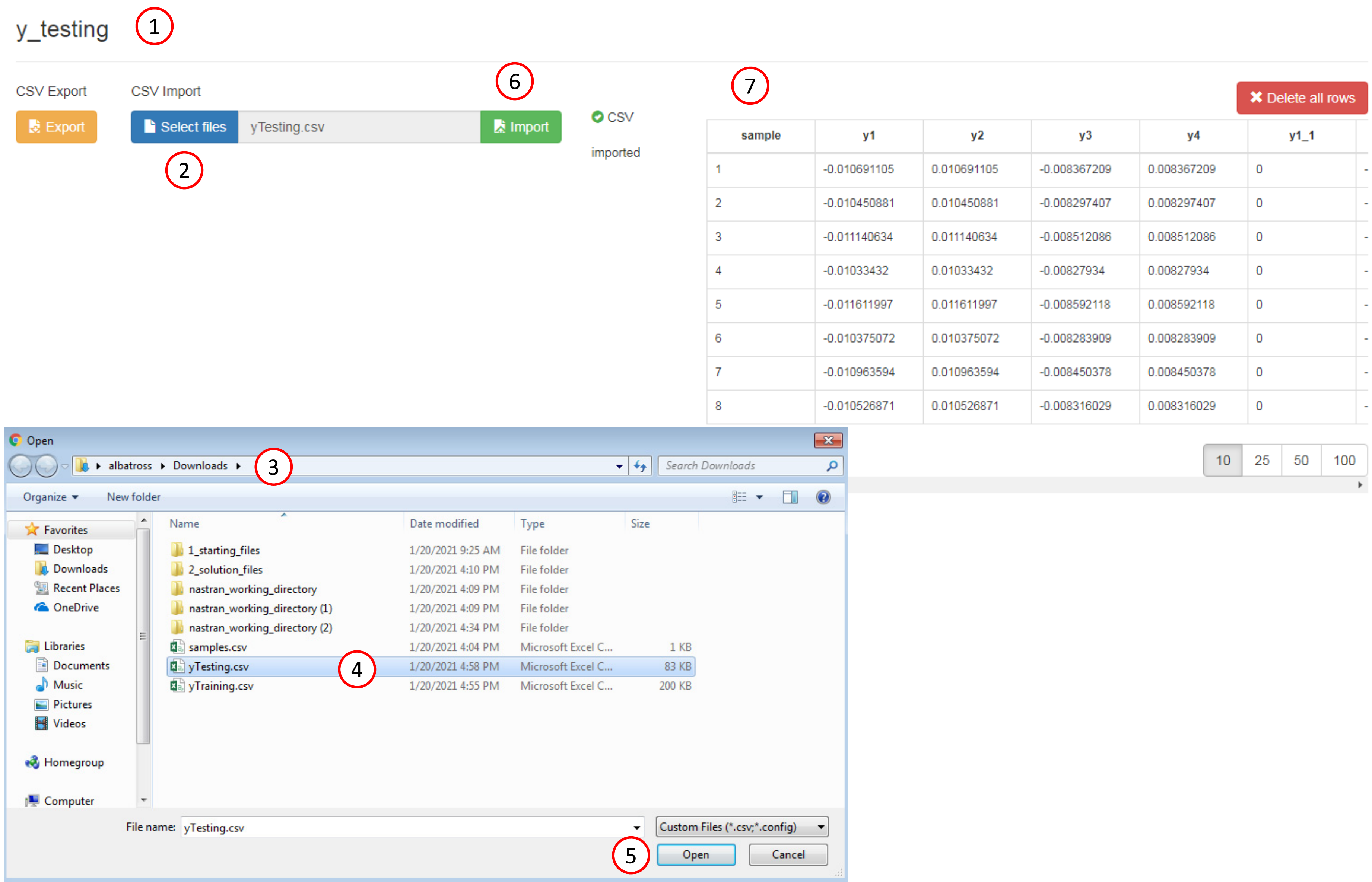
Training Data, Updated

1. Navigate to the section titled y_training
2. Click Select files
3. Navigate to the folder which contains the yTraining.csv file
4. Select the file yTraining.csv
5. Click Open
6. Click Import
7. The table is now loaded with the y outputs (monitored responses) for all 20 runs



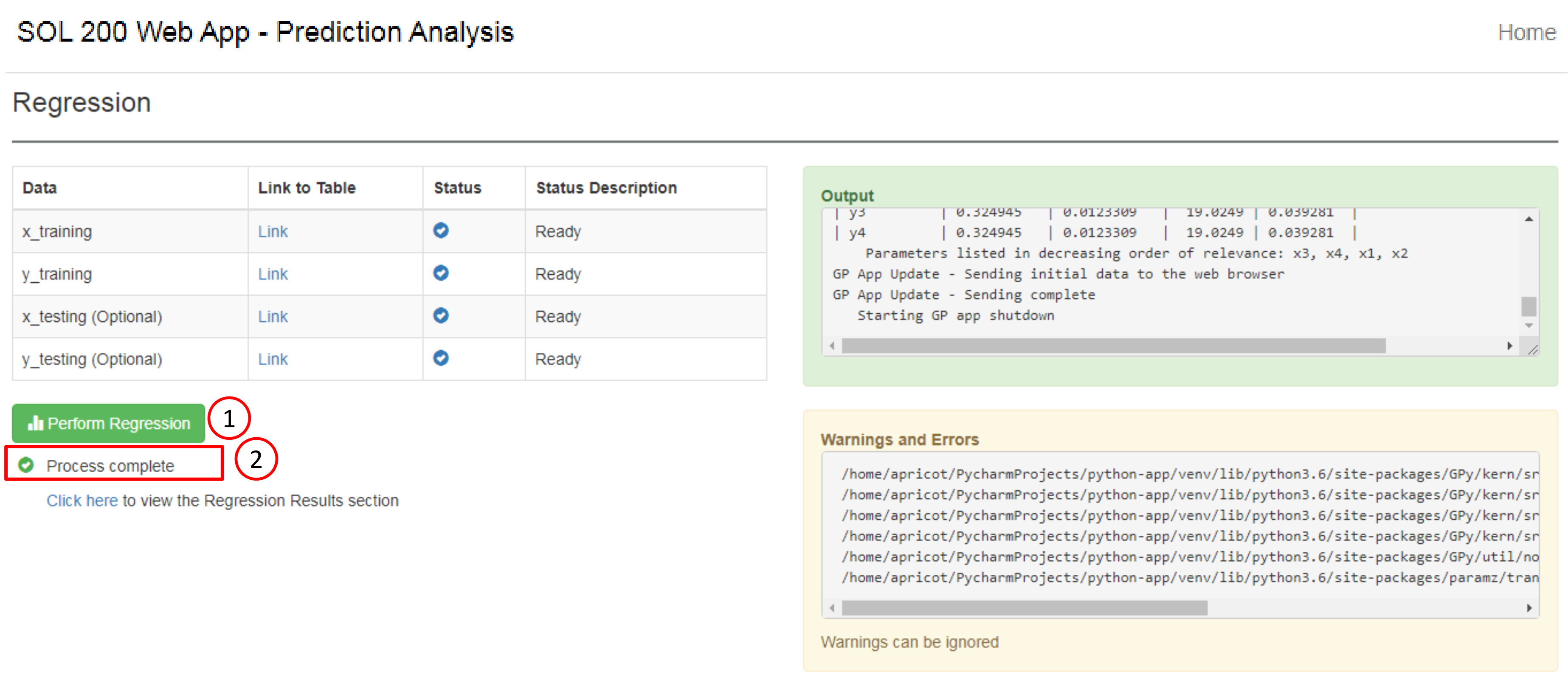
Testing Data, Updated

1. Navigate to the section titled y_testing
2. Click Select files
3. Navigate to the folder which contains the yTesting.csv file
4. Select the file yTesting.csv
5. Click Open
6. Click Import
7. The table is now loaded with the y outputs (monitored responses) for all 8 runs



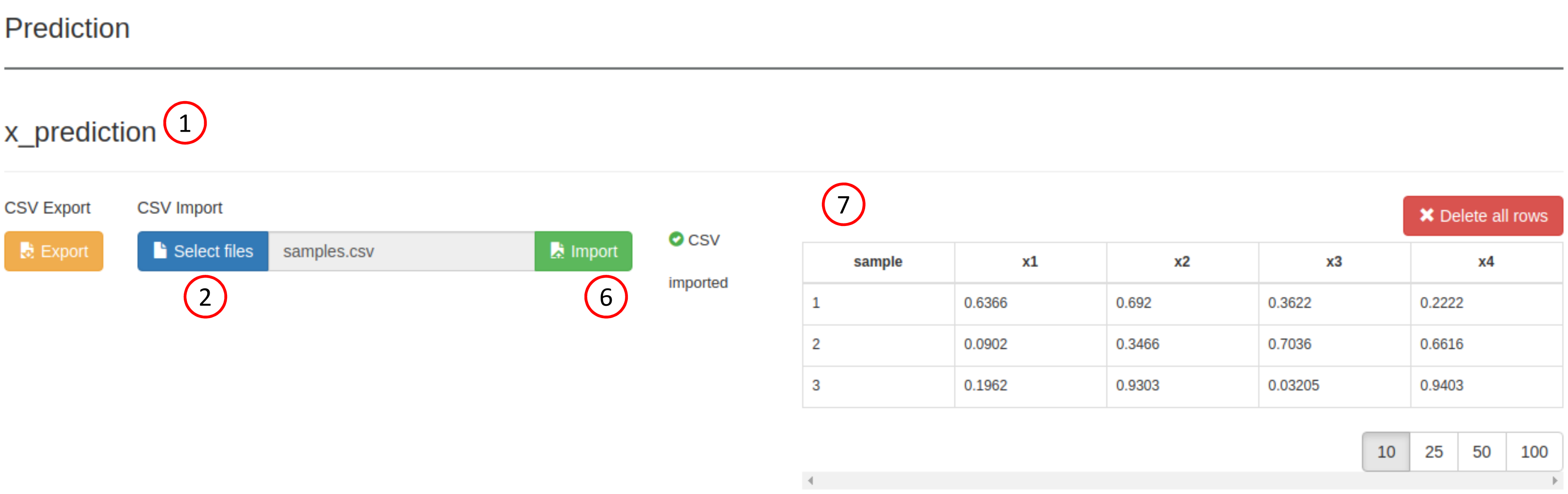
Perform Regression

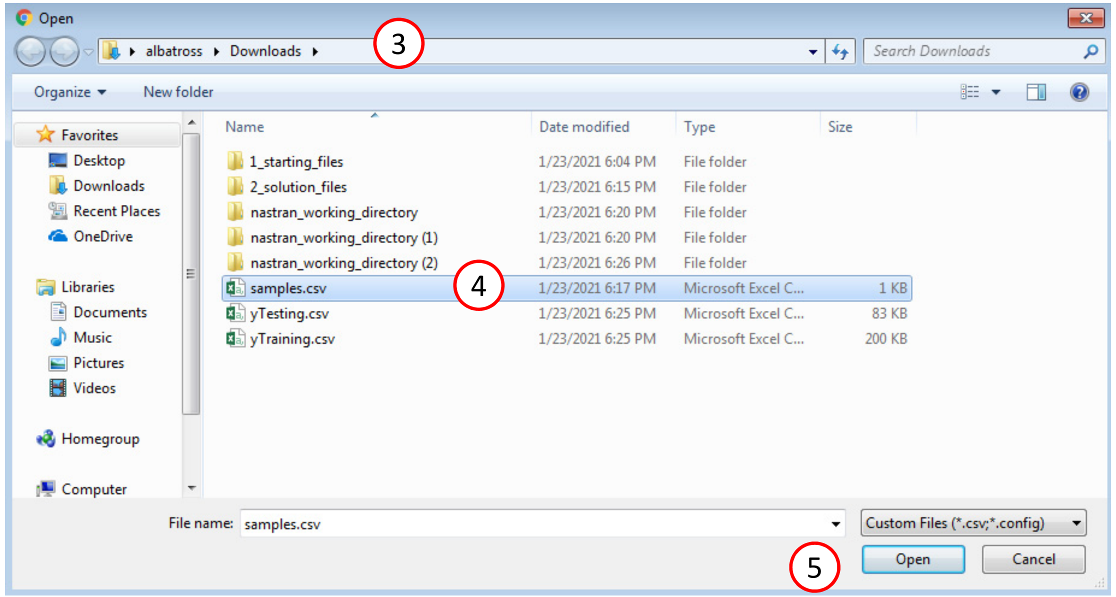
1. Click Perform Regression and the surrogate model will be fitted
2. The regression is complete when the following status message is visible:
   - Process complete



Perform Prediction

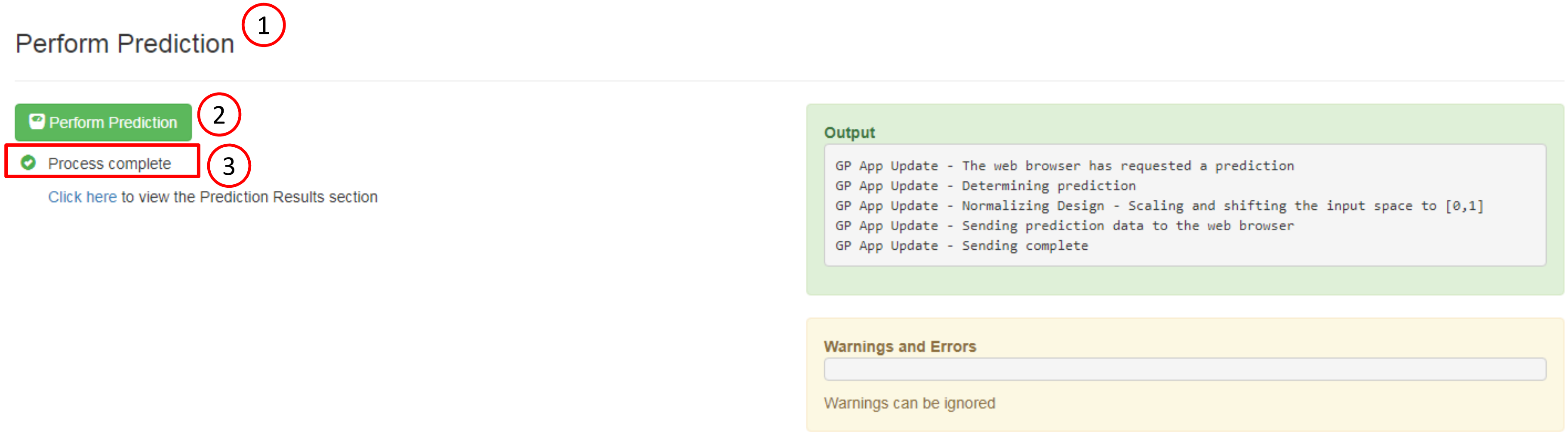
1. Navigate to the section titled x_prediction
2. Click Select files
3. Navigate to the location of the file named samples.csv
4. Select the file samples.csv
5. Click Open
6. Click Import
7. The table is now loaded with the x inputs for 3 runs





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

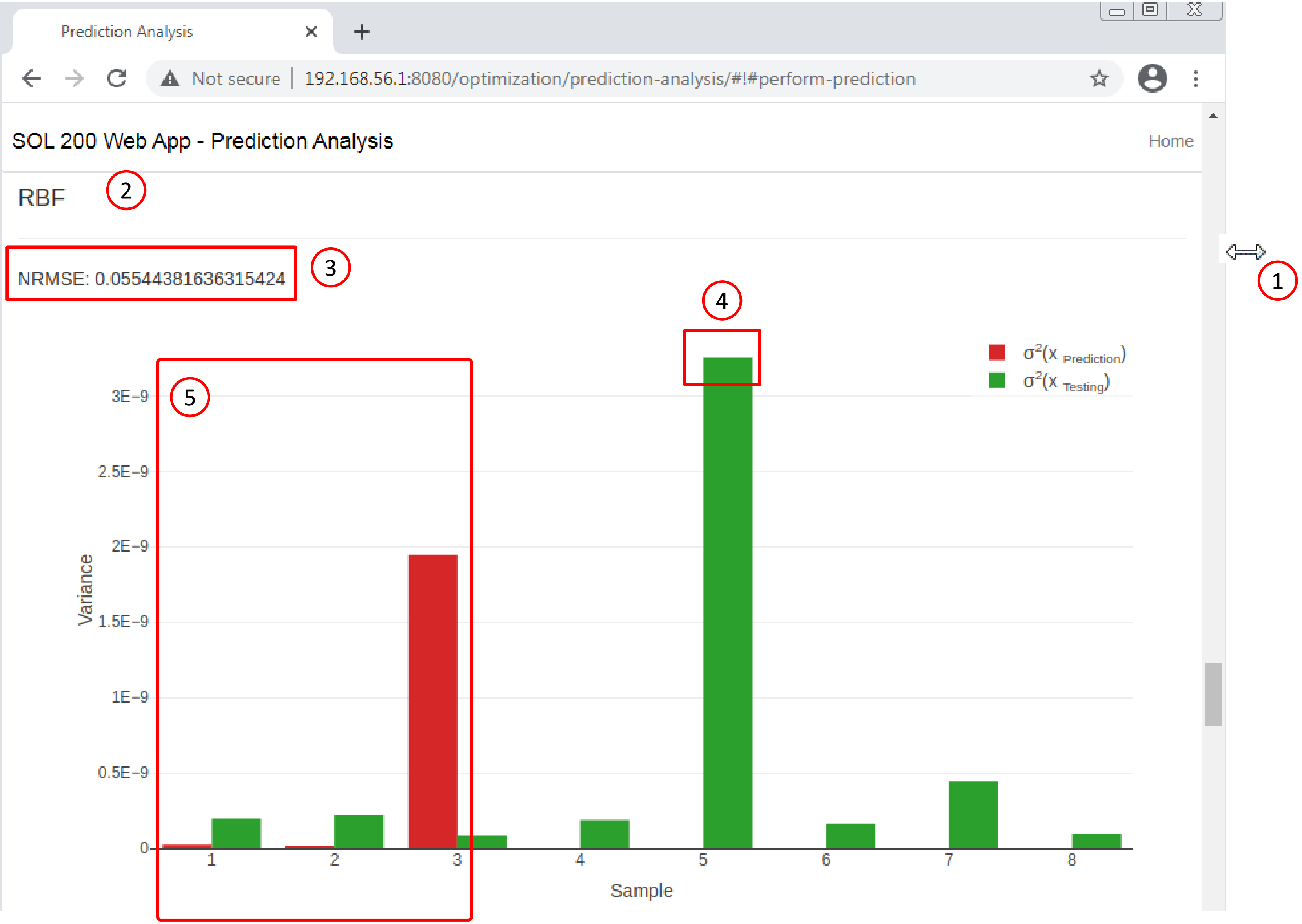
Variance

1. Navigate to the section titled Variance

Variance

1. Resize the window to fit half the screen, this causes the plot to be increased in size
2. The variance values shown are based on the RBF kernel
3. Note the normalized root mean square error (NRMSE)
   - NRMSE values are only calculated if x_testing and y_testing are provided
   - NRMSE values less than .15 indicate the surrogate model has good prediction performance
4. 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.
5. Predictions have been made at 3 samples and are indicated by 3 red bars
   - When making predictions, the prediction uncertainty should ideally be low, like in this example
   - Note that samples 1 and 2 have a low variance (prediction uncertainty). Sample 3 has a high variance. The predicted values for samples 1 and 2 are more reliable than sample 3.

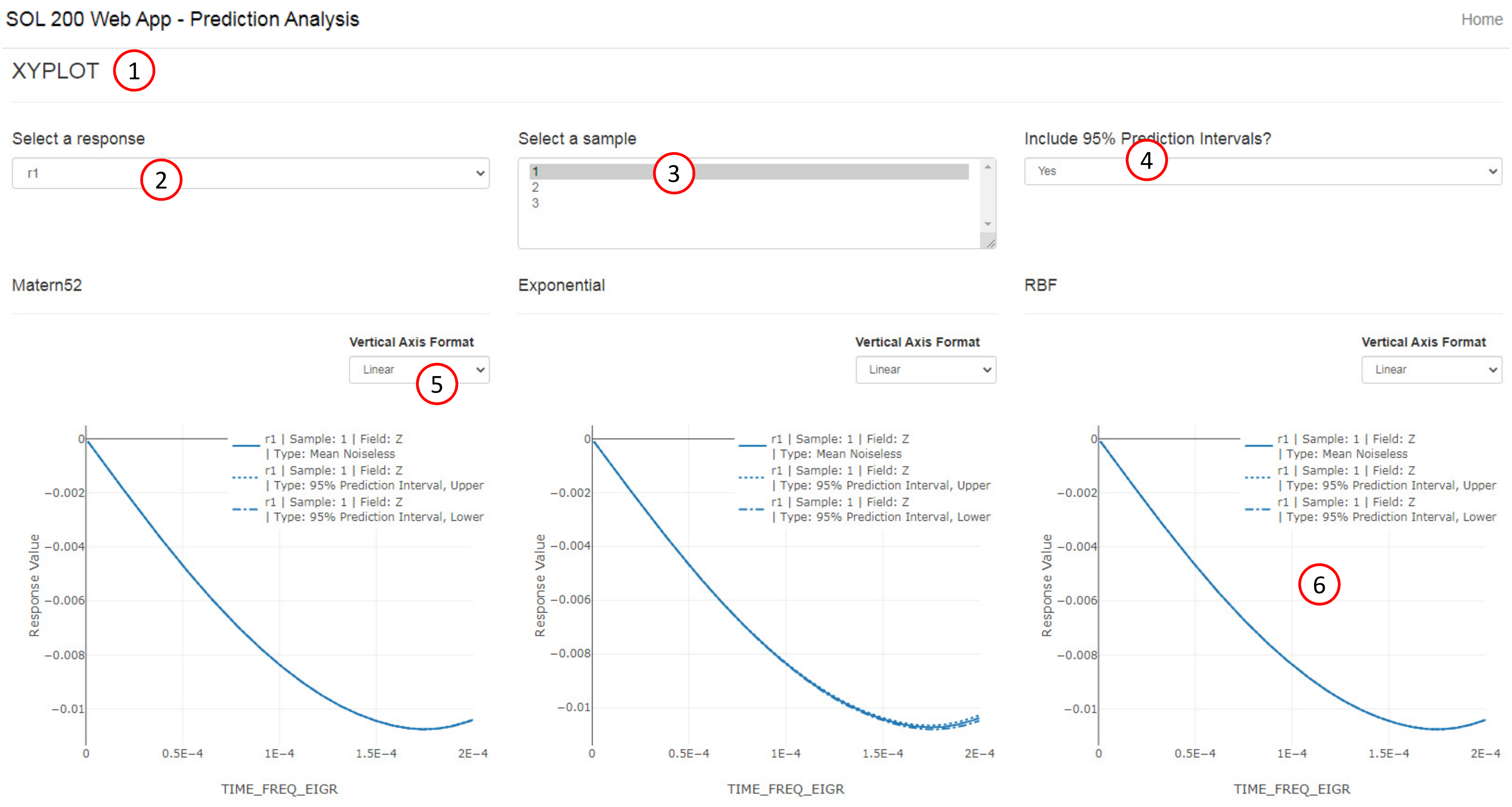
- In this tutorial, variance (σ^2) is used to gauge the prediction uncertainty. Sometimes, you will see this prediction uncertainty expressed as the standard deviation (σ).



Displacement vs. Time

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

1. Navigate to the section titled XYPLOT
2. Set Select a response to r1
3. Set Select a sample to 1
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

1. Recall that batch 1 was used to produce the training data, fit the surrogate model, and produce the indicated prediction
2. Batch 2 was used to calculate the NRMSE, which is an indication of the surrogate model's prediction performance (Not shown)
3. Batch 3 was opened in the HDF5 Explorer

In the HDF5 Explorer

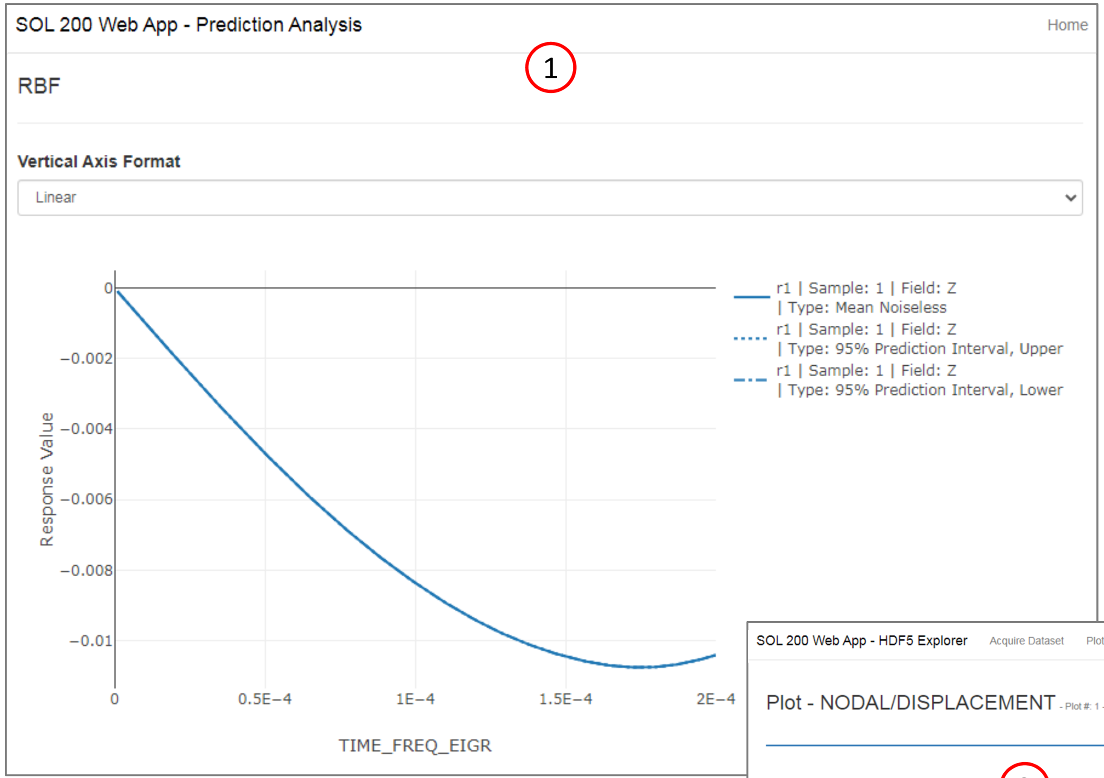
4. Click Display None
5. Mark the checkbox for sample 1

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

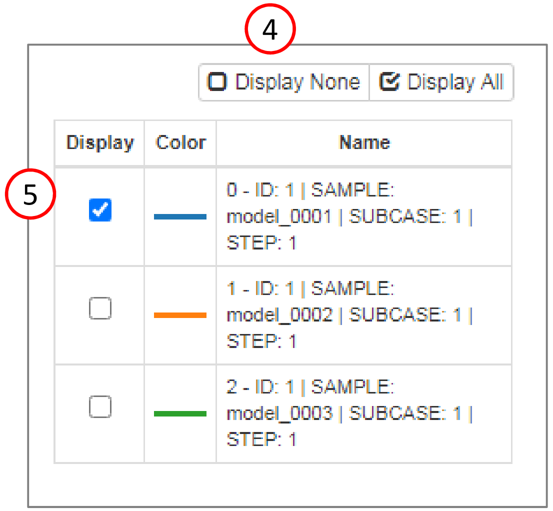
- In this tutorial, variance (σ^2) is used to gauge the prediction uncertainty. Sometimes, you will see this prediction uncertainty expressed as the standard deviation (σ).

Predicted response

95% prediction interval

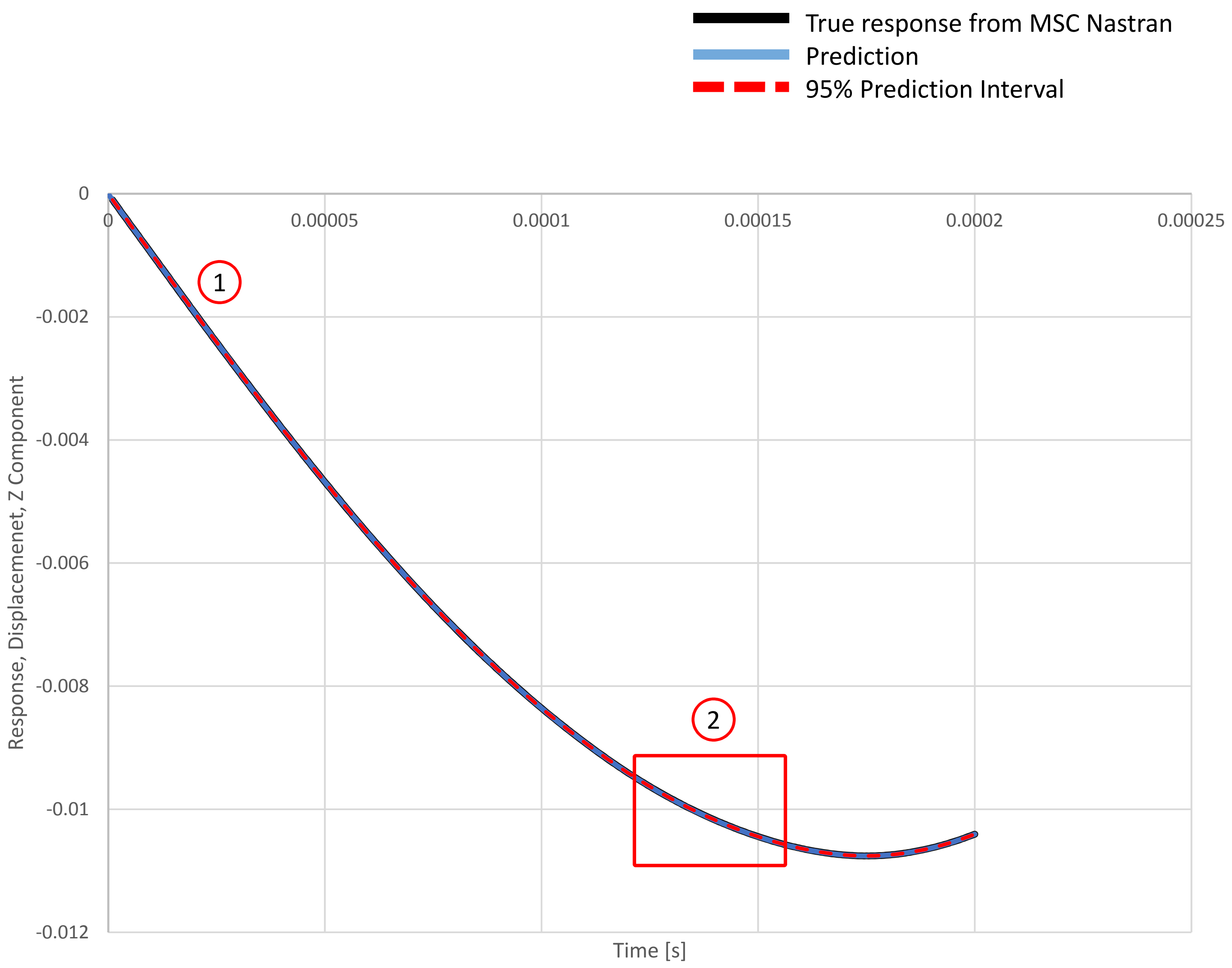


True response from MSC Nastran



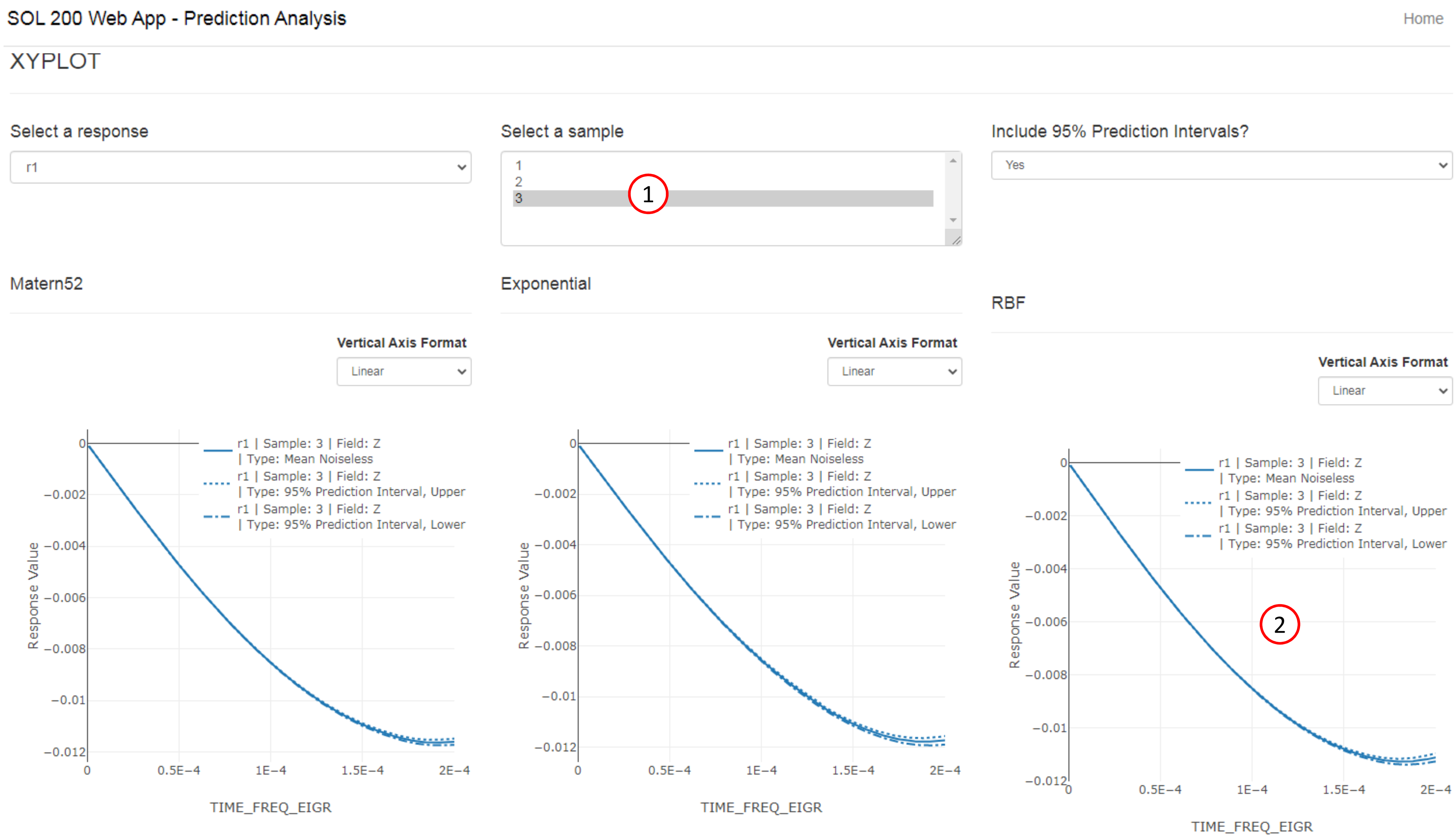
Comparison of Prediction with MSC Nastran

1. Optional - Excel was used to overlap the MSC Nastran output over the predicted response
2. The predicted value and MSC Nastran response are overlapping, indicating the surrogate model has yielded a good prediction.



Displacement vs. Time

1. Set Select a sample to 3
2. The plots have been updated and are the predicted values for sample 3



Comparison of Prediction with MSC Nastran

1. Recall that batch 1 was used to produce the training data, fit the surrogate model, and produce the indicated prediction
2. Batch 2 was used to calculate the NRMSE, which is an indication of the surrogate model's prediction performance (Not shown)
3. Batch 3 was opened in the HDF5 Explorer

In the HDF5 Explorer

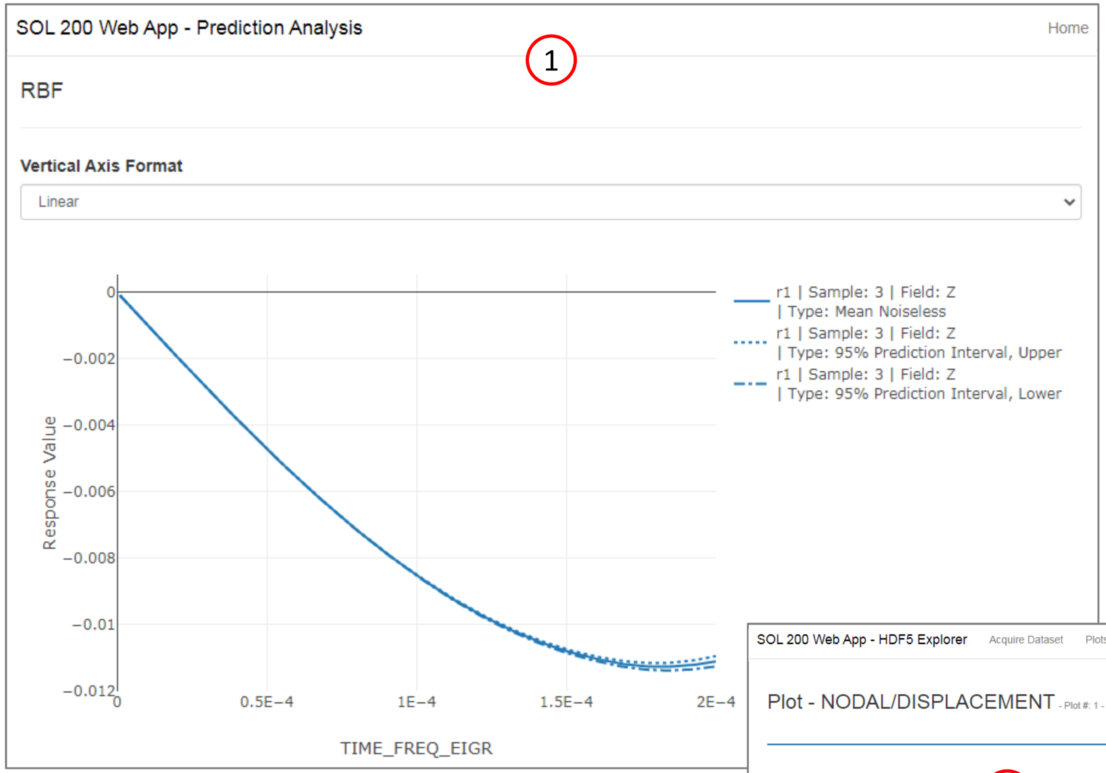
4. Click Display None
5. Mark the checkbox for sample 3

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

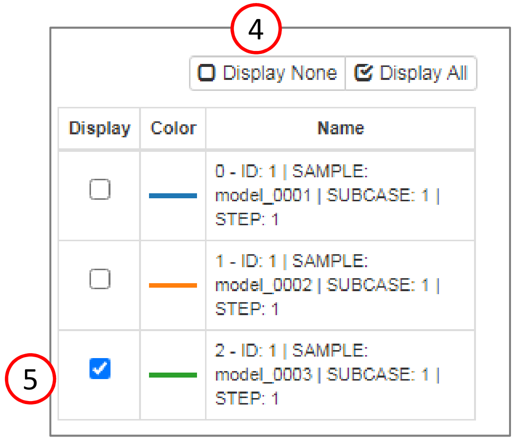
- In this tutorial, variance (σ^2) is used to gauge the prediction uncertainty. Sometimes, you will see this prediction uncertainty expressed as the standard deviation (σ).

Predicted response

95% prediction interval



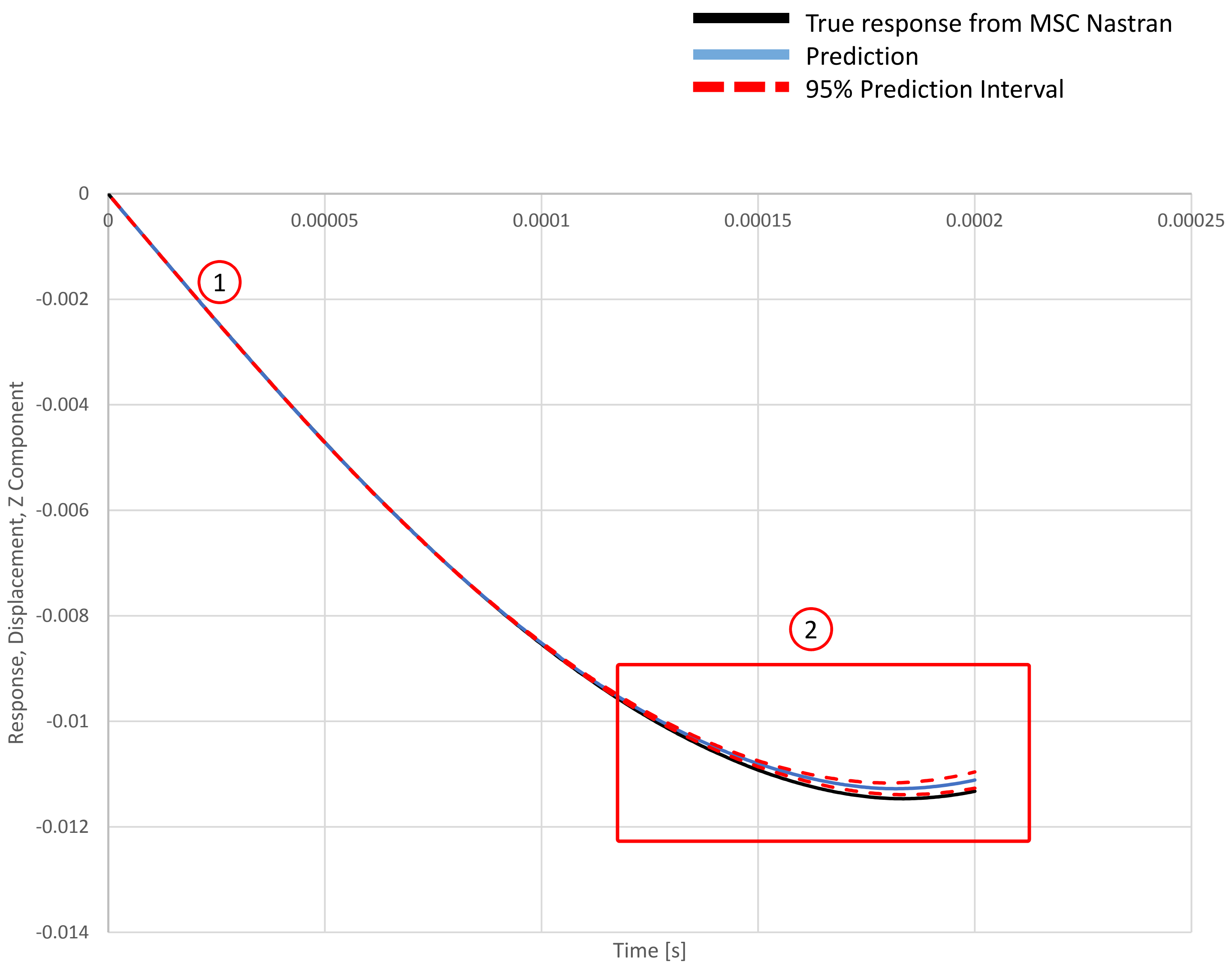
True response from MSC Nastran



Comparison of Prediction with MSC Nastran

1. Optional - Excel was used to overlap the MSC Nastran output over the predicted response

2. Towards the second half of the time steps, the predicted values do not align well with the true responses from MSC Nastran. Recall that the variance for sample 3 was relatively high and is reflected in this plot where the MSC Nastran response (black line) is outside of the 95% prediction interval (red dotted lines).



End of Tutorial

Appendix

Appendix Contents

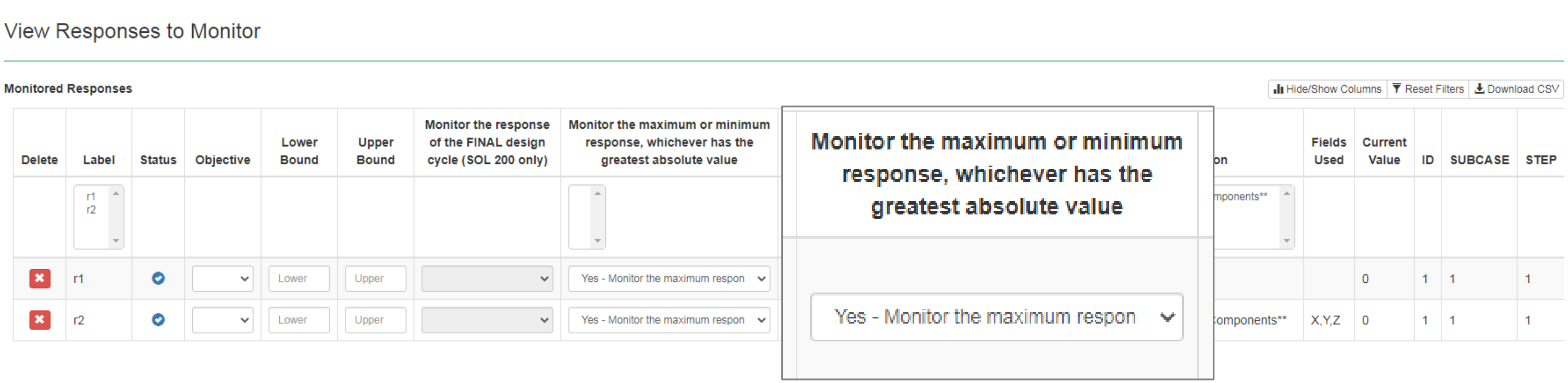
- Response Configuration
  - Monitor the maximum or minimum response, whichever has the greatest absolute value: Yes, No or blank
- How to import and edit previous files
- What is Gaussian Process Regression?

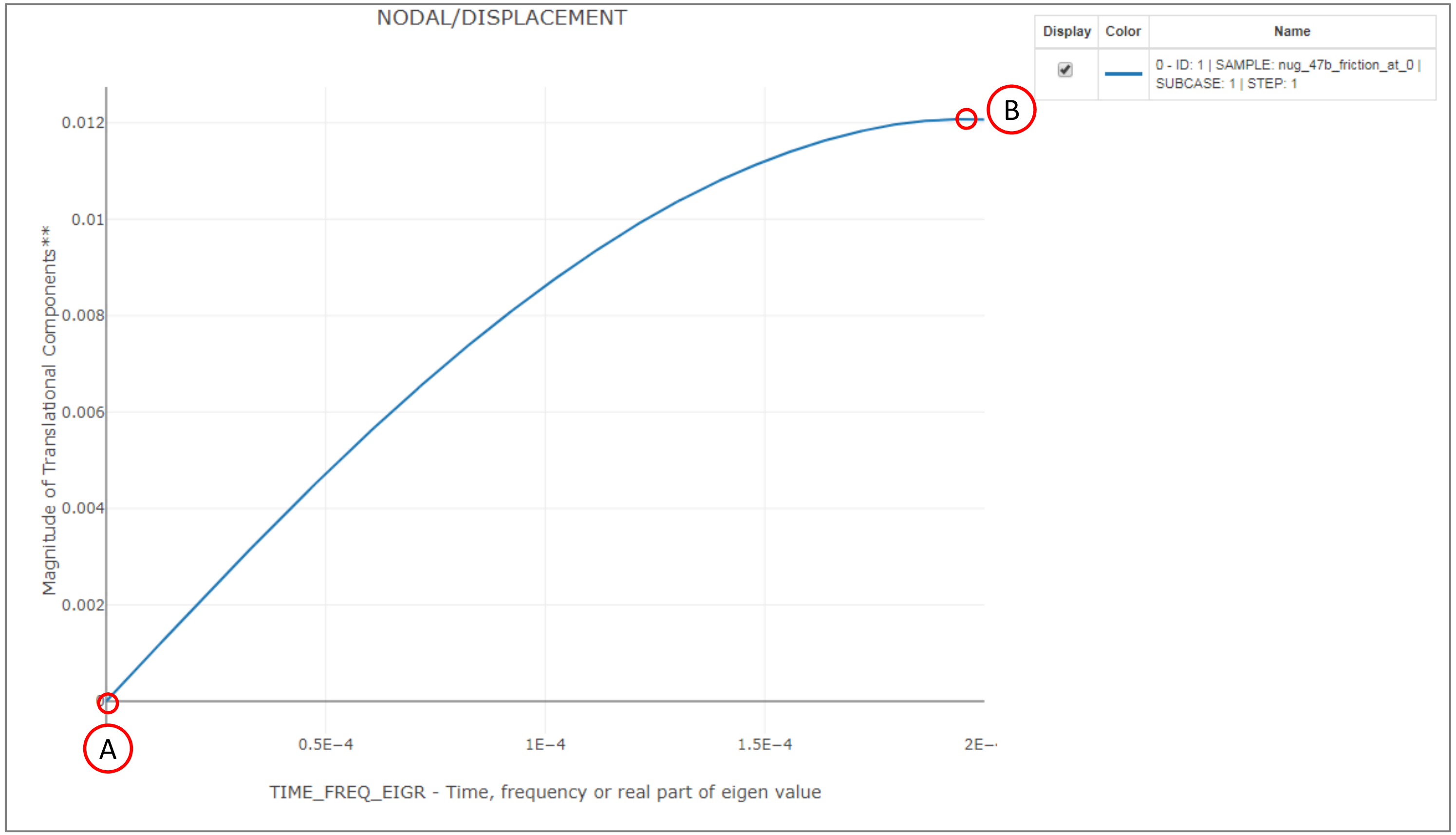
Response Configuration

During this tutorial, this option was used:

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

Suppose response r2 is configured for 0 seconds and corresponds to point A on the plot. When Yes is used for the option, the absolute value of each point is taken and the maximum point is used. Point B is the maximum and is the value used for response r2.





How to import and edit previous files

How to import and edit previous files

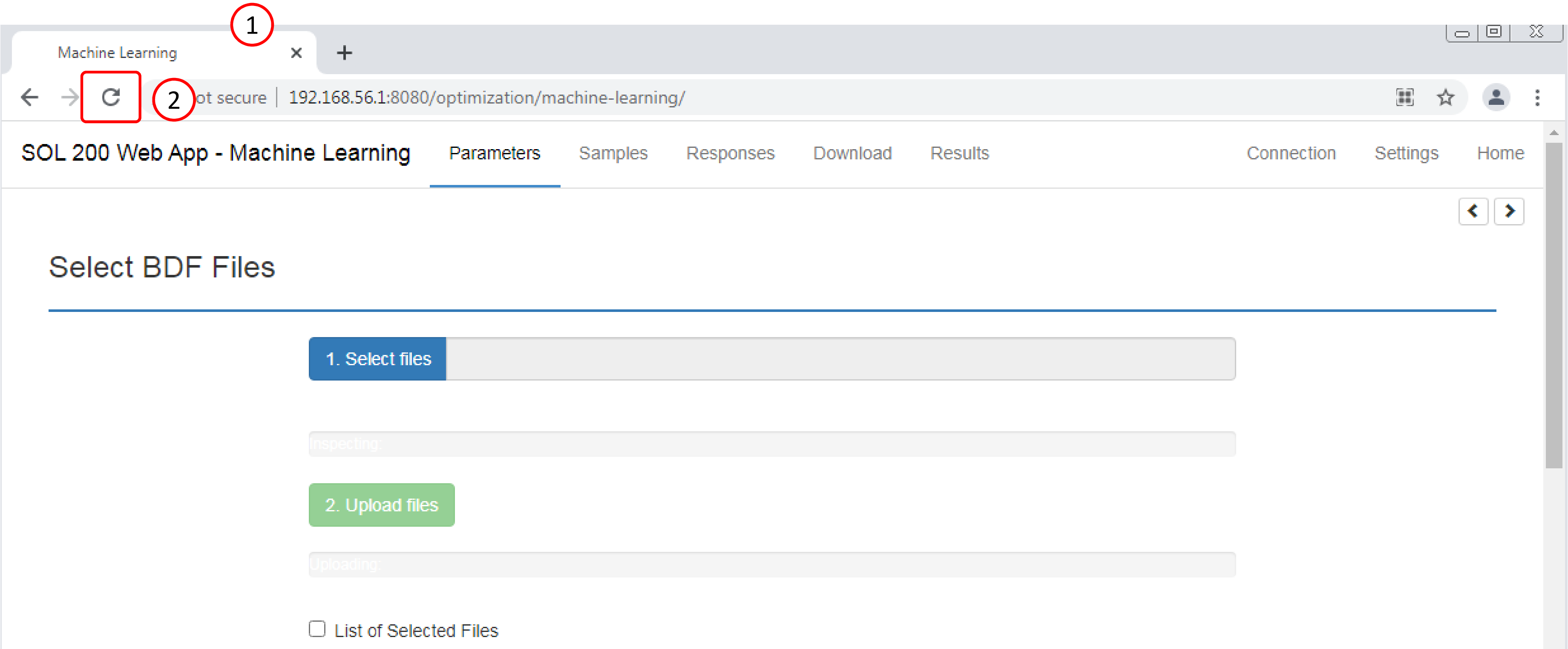
The parameters, samples and responses are contained in the following files

- 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

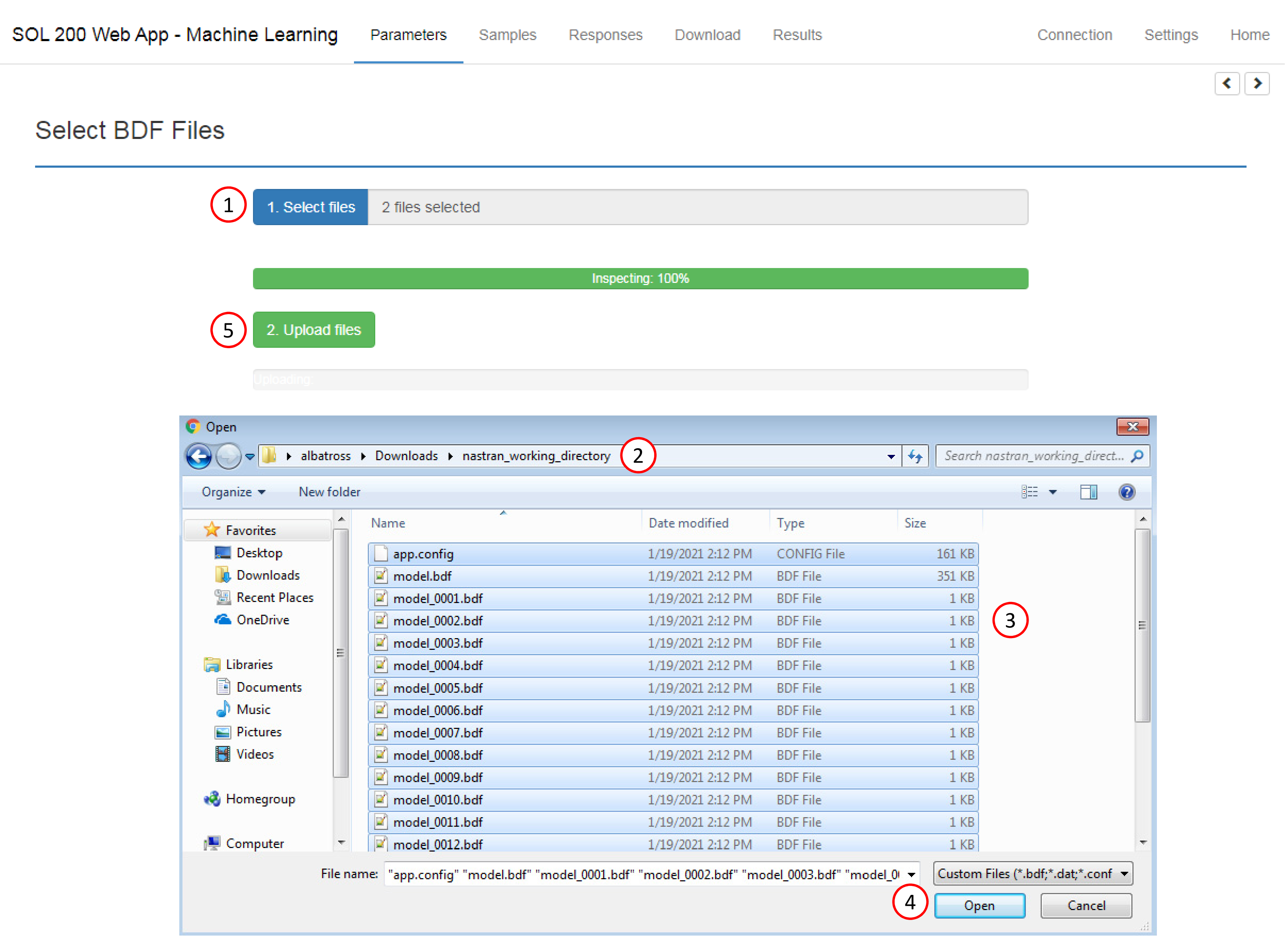


- Refreshing the page is only required when the *Select files* button is disabled.

Import

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

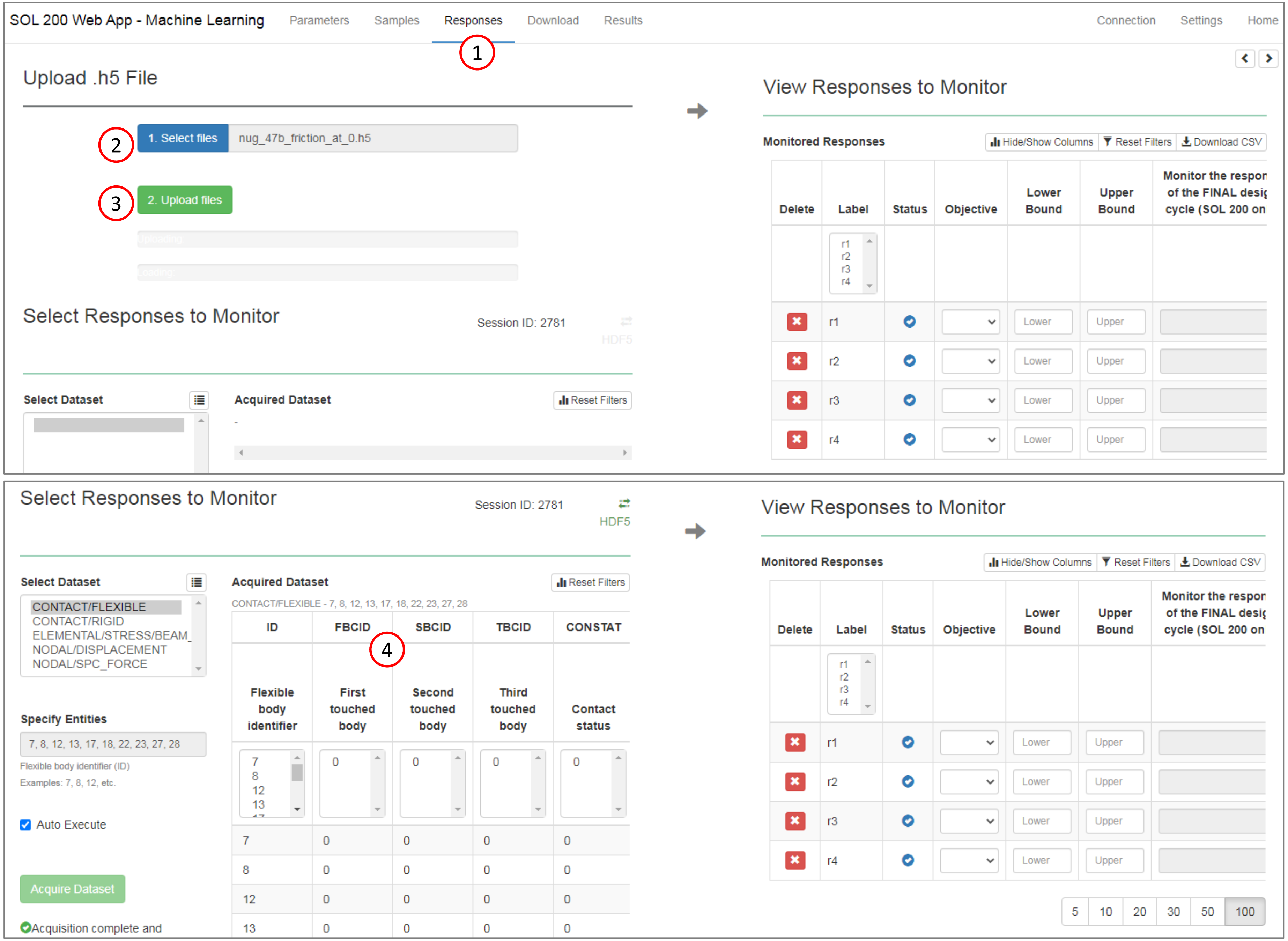
- All imports require the app.config file to be selected.



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 | 2 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__|


BCBODY  3       3D      RIGID   0       0       0.e0    0       1
        0       0.e0    0.e0    0.e0    1.
        RIGID   1       1       sphere
        APPROV                                  0.e0    0.e0    -0.01
        NURBS   -5      9       3       3       24      48      0
                0.e0    -0.01   .012    .01     -0.01   .012
                .01     0.e0    .012    .01     .01     .012
                0.e0    .01     .012    0.e0    -0.01   .012
                .01     -0.01   .002    .01     0.e0    .002
                .01     .01     .002    0.e0    .01     .012
                0.e0    -0.01   .012    0.e0    -0.01   .002
                0.e0    0.e0    .002    0.e0    .01     .002
                0.e0    .01     .012    0.e0    -0.01   .012
                -0.01   -0.01   .002    -0.01   0.e0    .002
```

Configure Parameters

Delete	Parameter	Status	Low	High	Comments
✖	x1	✔	0.0	1.0	Field 16 of BCT
✖	x2	✔	0.0	1.0	Field 46 of BCT
✖	x3	✔	0.0	1.0	Field 16 of BCT
✖	x4	✔	0.0	1.0	Field 46 of BCT

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

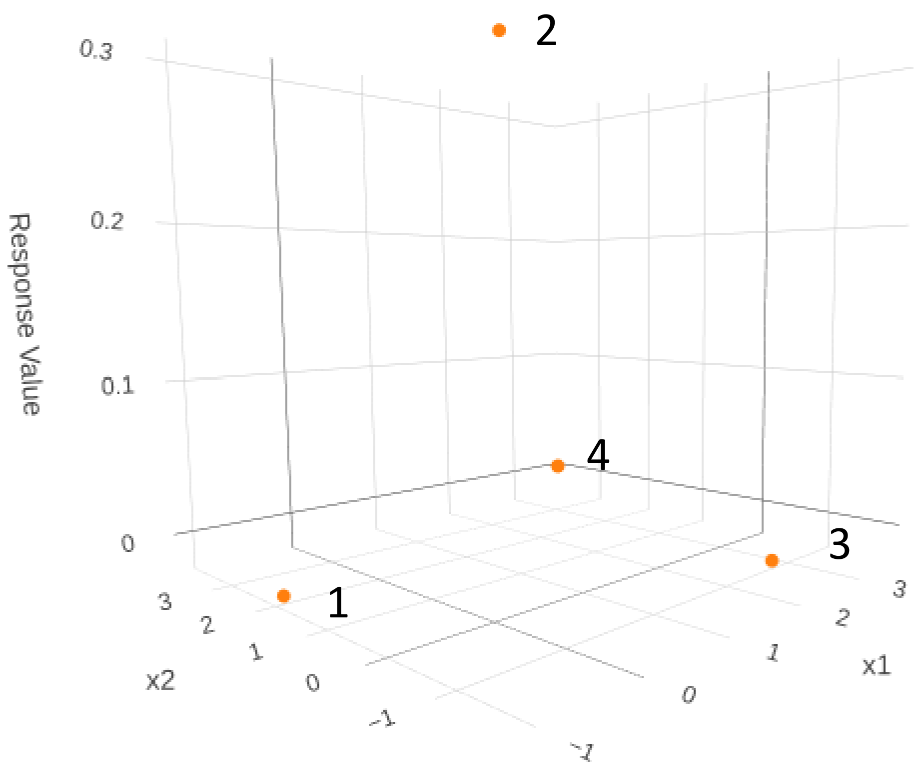
Example 1

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

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

Calculation of Σ

$\Sigma =$

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

Calculation of Σ

$$\Sigma = \left[\begin{array}{cc|cccc}
e^{0} = 1 & e^{-.1429} = .8668 & e^{-3.0493} = .0474 & e^{-.0596} = .9421 & e^{-8.068} = .0003 & e^{-20.1178} = 1.832\text{e-}9 \\
.8668 & e^{0} = 1 & e^{-4.5124} = .0110 & e^{-.0265} = .9738 & e^{-6.\text{[illegible]}273} = .0020 & e^{-19.7109} = 2.8\text{e-}9 \\
\hline
.0474 & .0110 & e^{0} = 1 & e^{-3.9233} = .0198 & e^{-20.3009} = 1.5\text{e-}9 & e^{-25.6225} = 7.5e-12 \\
.9421 & .9738 & .0198 & e^{0} = 1 & e^{-6.746} = .0012 & e^{-20.4898} = 1.263\text{e-}9 \\
.0003 & .0020 & 1.5\text{e-}9 & .0012 & e^{0} = 1 & e^{-34.0034} = 1.7e-15 \\
1.832\text{e-}9 & 2.8\text{e-}9 & 7.5e-12 & 1.263\text{e-}9 & 1.7e-15 & e^{0} = 1
\end{array}\right]$$

$\Sigma(\chi, \chi)$

$\Sigma(\chi, X_n)$

$\Sigma(X_n, \chi)$

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

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

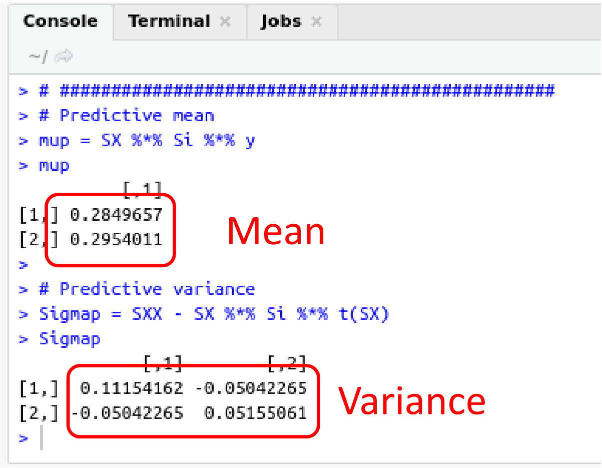
The diagonal terms are the variances at prediction points 1 and 2

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

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

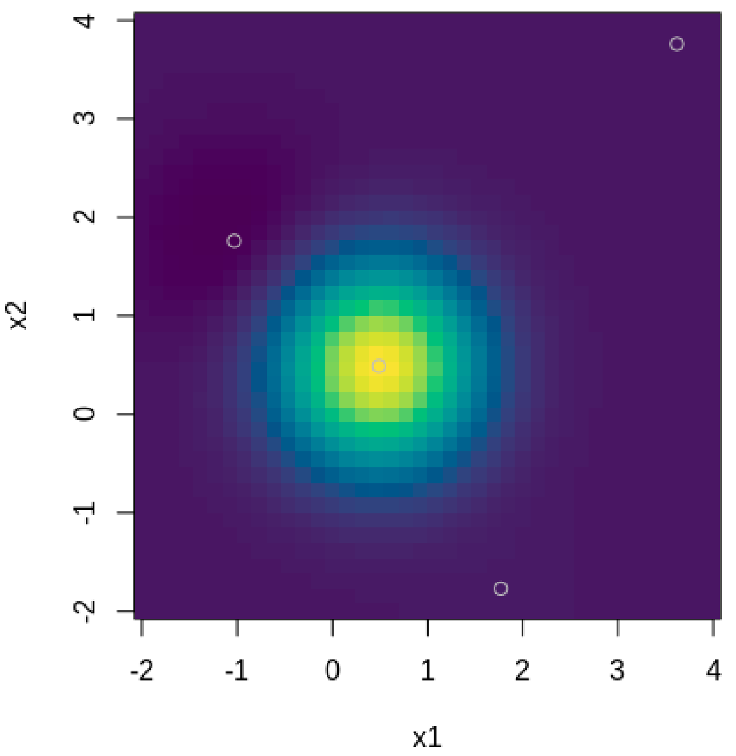


R
Code to replicate this example in R with Plots

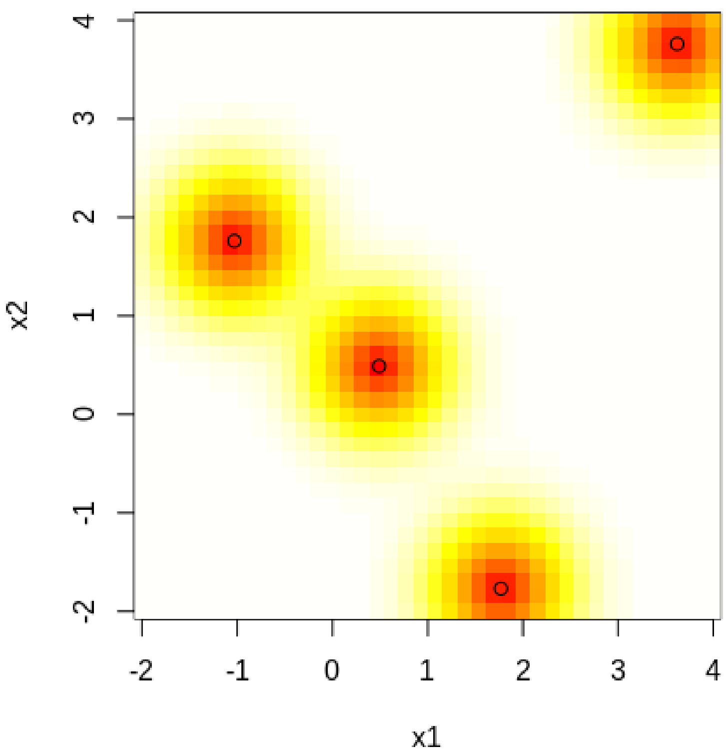
```
library(plgp)
library(lhs)

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)



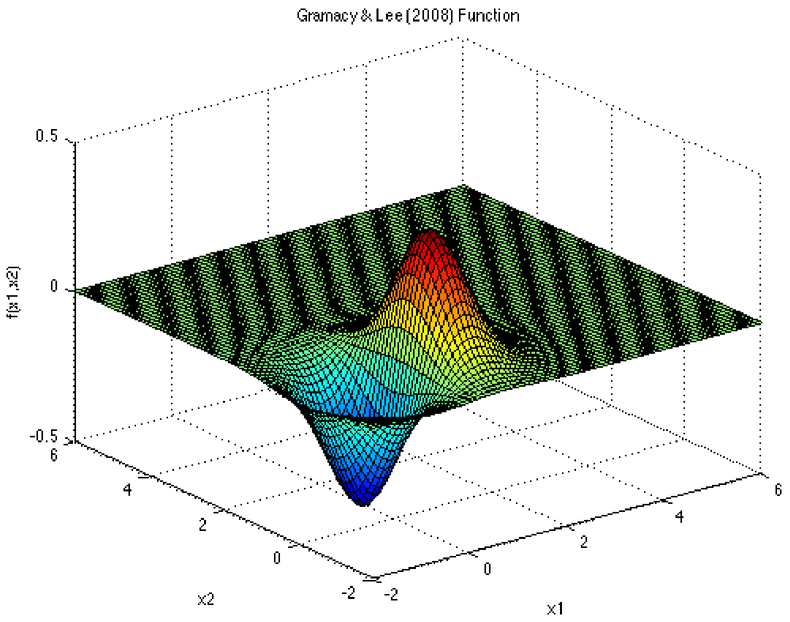
Not Good – High Standard Deviation – High Variance – High Prediction uncertainty (Prediction is not reliable)

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 ($\mu(\chi)$)