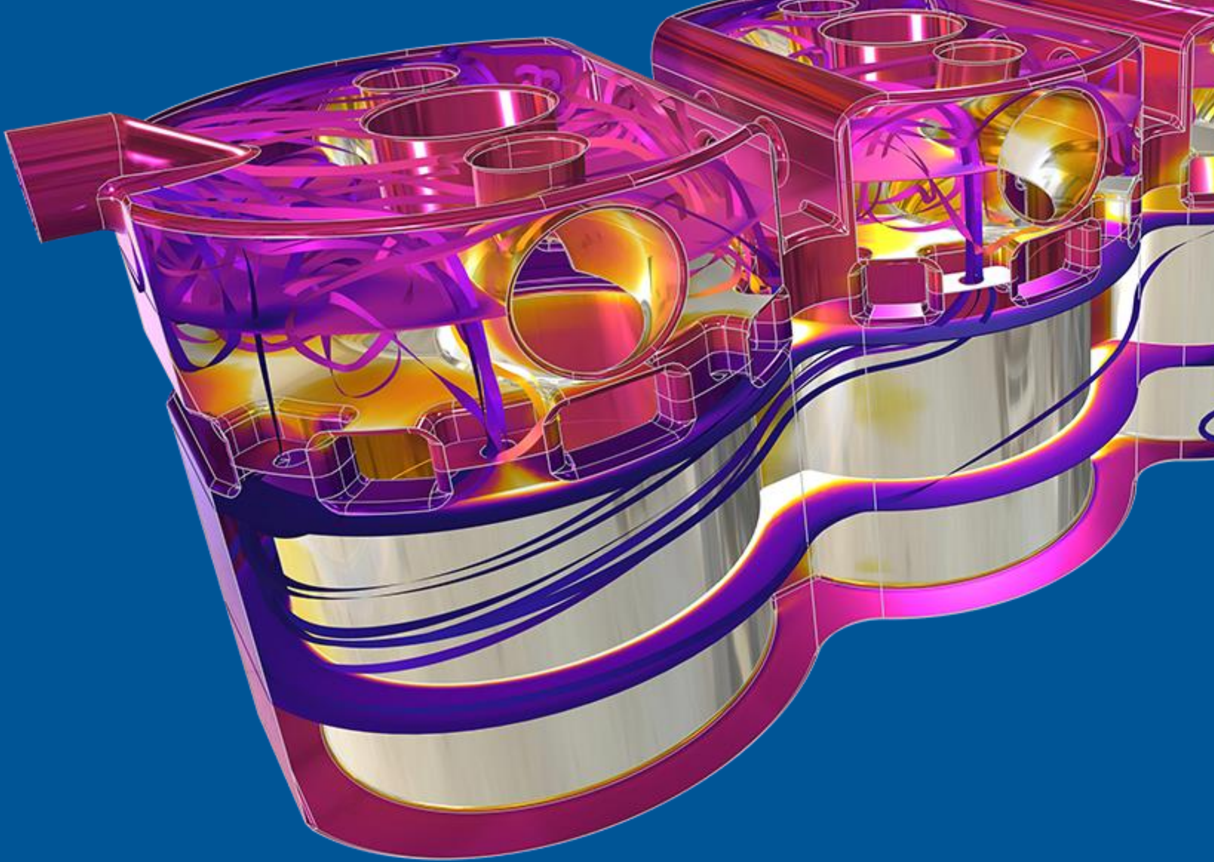
Setting up a Deep Neural Network for Structural-Thermal-Optical Model

Tomáš Vrbata
vrbata@humusoft.cz

Schedule

1. Deep Neural Networks (DNN)
2. STOP Analysis
3. Demo – Model Description
4. Demo – How to Create Surrogate model for STOP Analysis
5. Conclusions



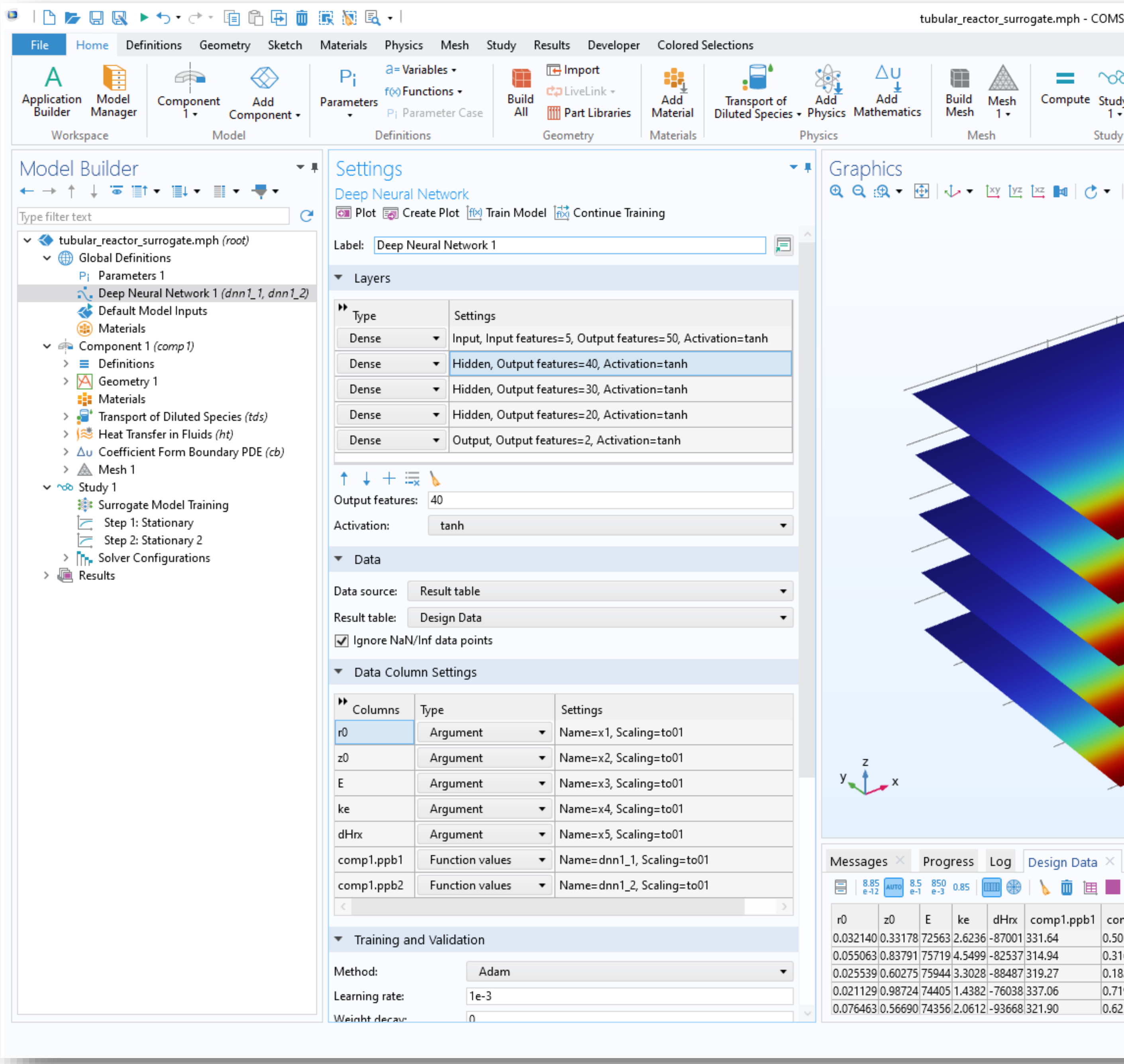
Deep Neural Networks (DNN) in COMSOL Multiphysics

Tomáš Vrbata

COMSOL

New Powerful Functionality

- DNN is a new type of function
- General multidimensional function interpolation and approximation
- Requires a training data table

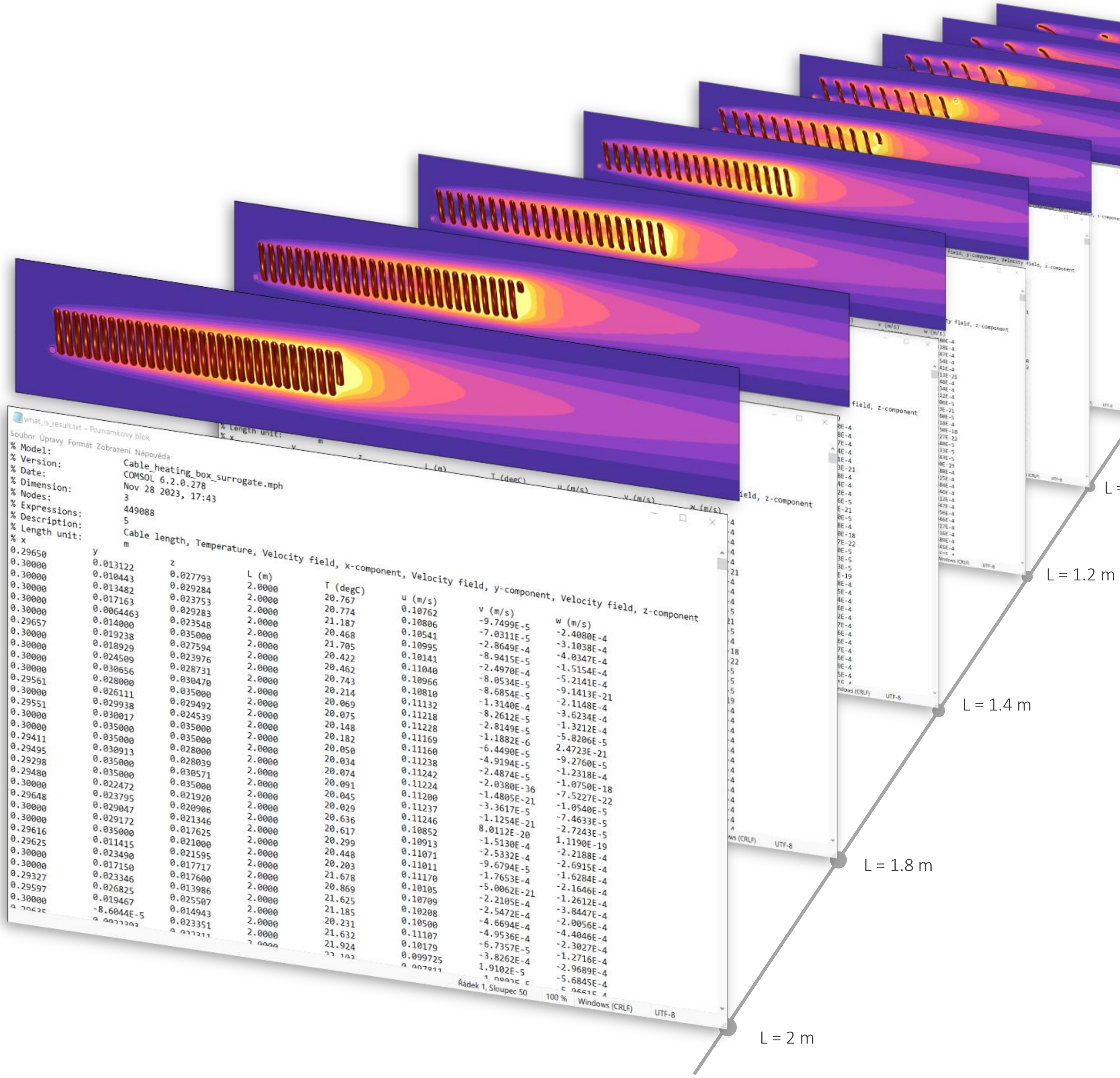


COMSOL

New Powerful Functionality

- The original parametrized 3D FEM model can be viewed as a set of large tables:

  x, y, z, parameters, computed quantities

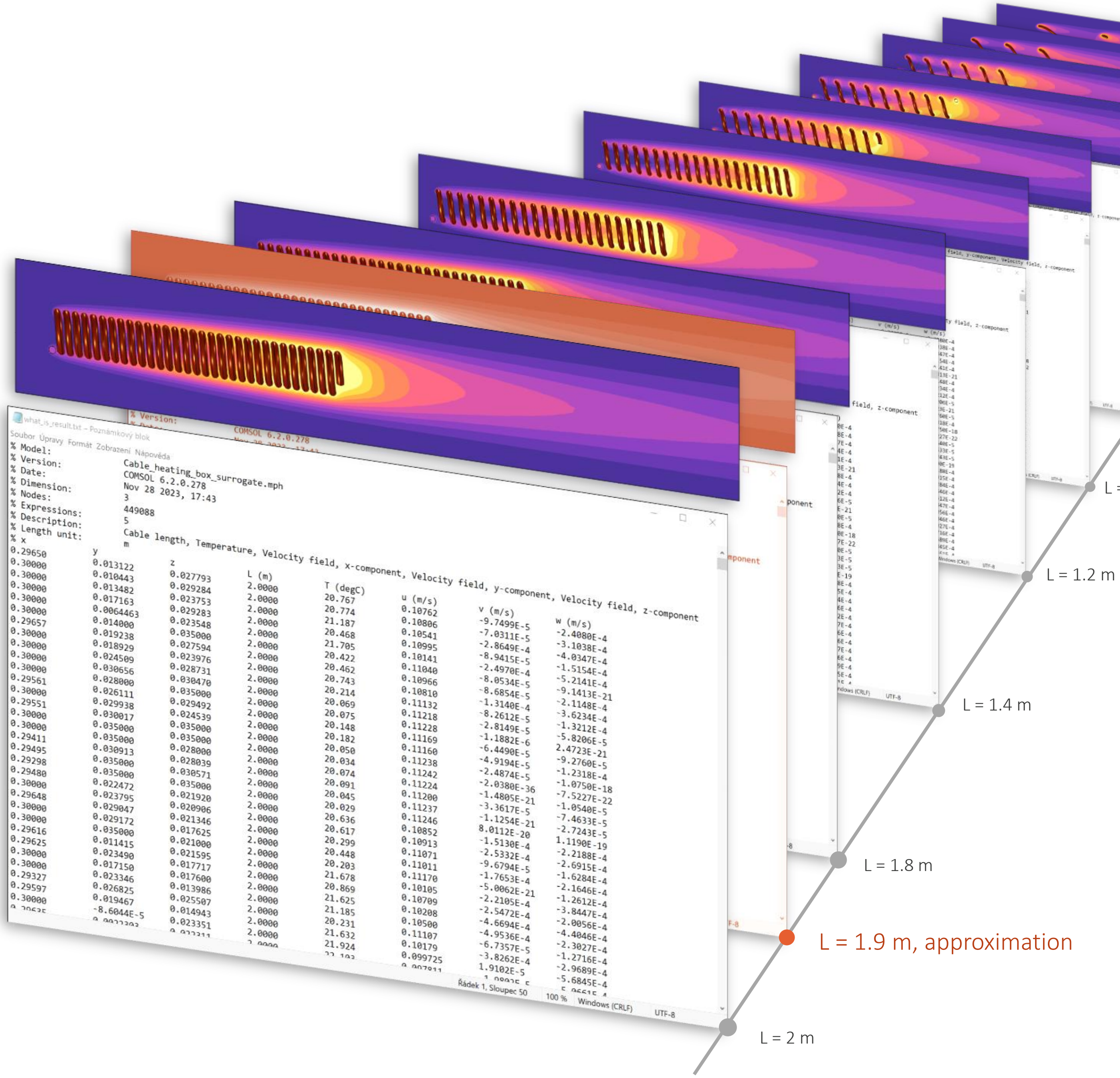


New Powerful Functionality

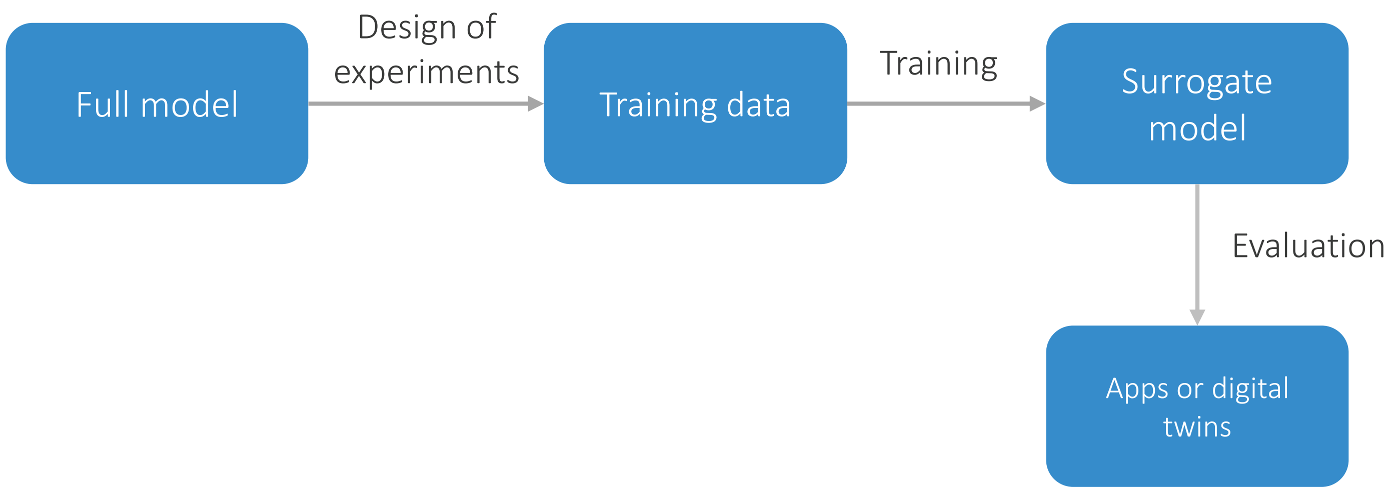
- The original parametrized 3D FEM model can be viewed as a set of large tables:

  x, y, z, parameters, computed quantities

- The surrogate model replaces the original model with new DNN function that approximate the model in the whole space of parameters

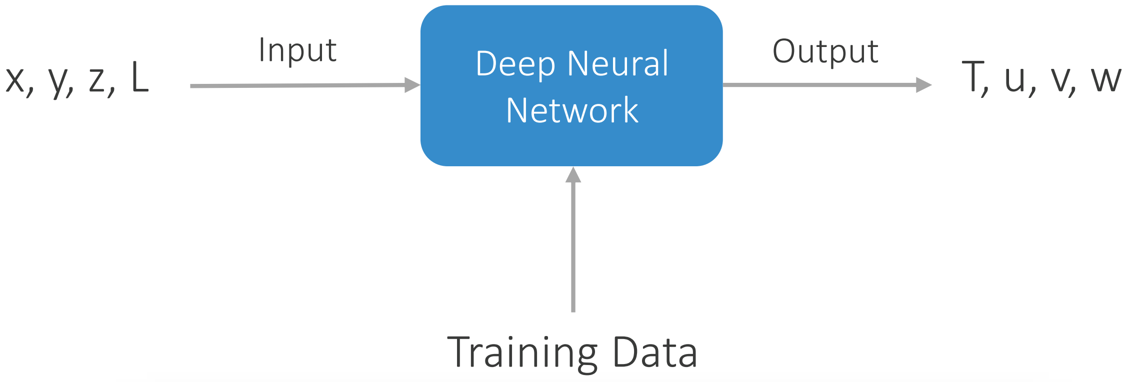


Surrogate Model Workflow



How Training Data look like?

- Inputs and Outputs together
- Data file (*.csv, *.txt, *.dat) or result table



what_is_result.txt – Poznámkový blok

Soubor Úpravy Formát Zobrazení Nápověda

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% Model:              Cable_heating_box_surrogate.mph
% Version:            COMSOL 6.2.0.278
% Date:               Nov 28 2023, 17:43
% Dimension:          3
% Nodes:              449088
% Expressions:        5
% Description:        Cable length, Temperature, Velocity field, x-component, Velocity field, y-component, Velocity field, z-component
% Length unit:        m
% x            y            z            L (m)        T (degC)     u (m/s)      v (m/s)      w (m/s)
0.29650        0.013122     0.027793     2.0000       20.767       0.10762      -9.7499E-5   -2.4080E-4
0.30000        0.010443     0.029284     2.0000       20.774       0.10806      -7.0311E-5   -3.1038E-4
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0.30000        0.014000     0.035000     2.0000       20.422       0.11040      -8.0534E-5   -9.1413E-21
0.29657        0.019238     0.027594     2.0000       20.462       0.10966      -8.6854E-5   -2.1148E-4
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0.30000        0.024509     0.028731     2.0000       20.214       0.11132      -8.2612E-5   -1.3212E-4
0.30000        0.030656     0.030470     2.0000       20.069       0.11218      -2.8149E-5   -5.8206E-5
0.30000        0.028000     0.035000     2.0000       20.075       0.11228      -1.1882E-6   2.4723E-21
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0.30000        0.029938     0.024539     2.0000       20.182       0.11160      -4.9194E-5   -1.2318E-4
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```

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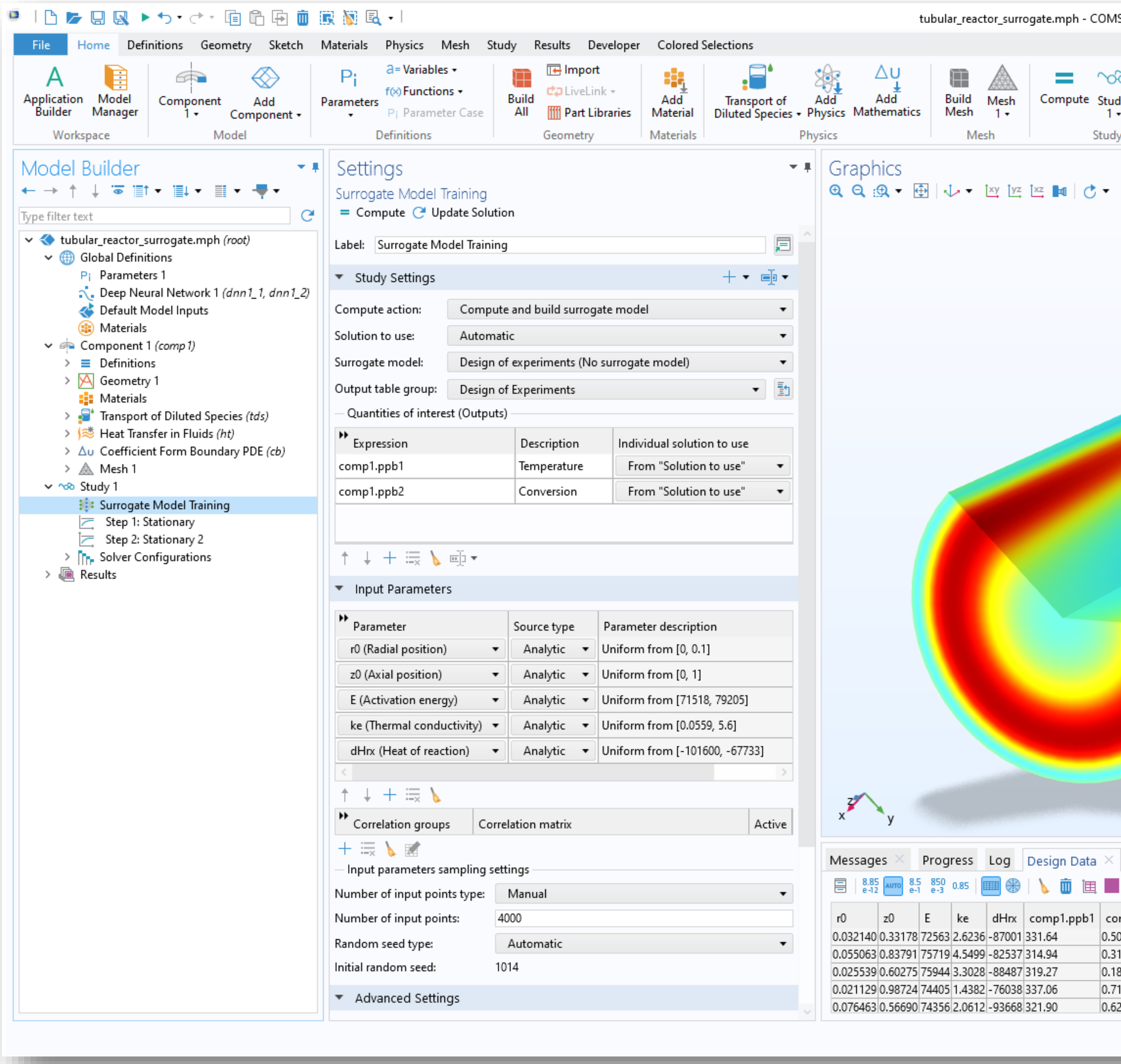
COMSOL

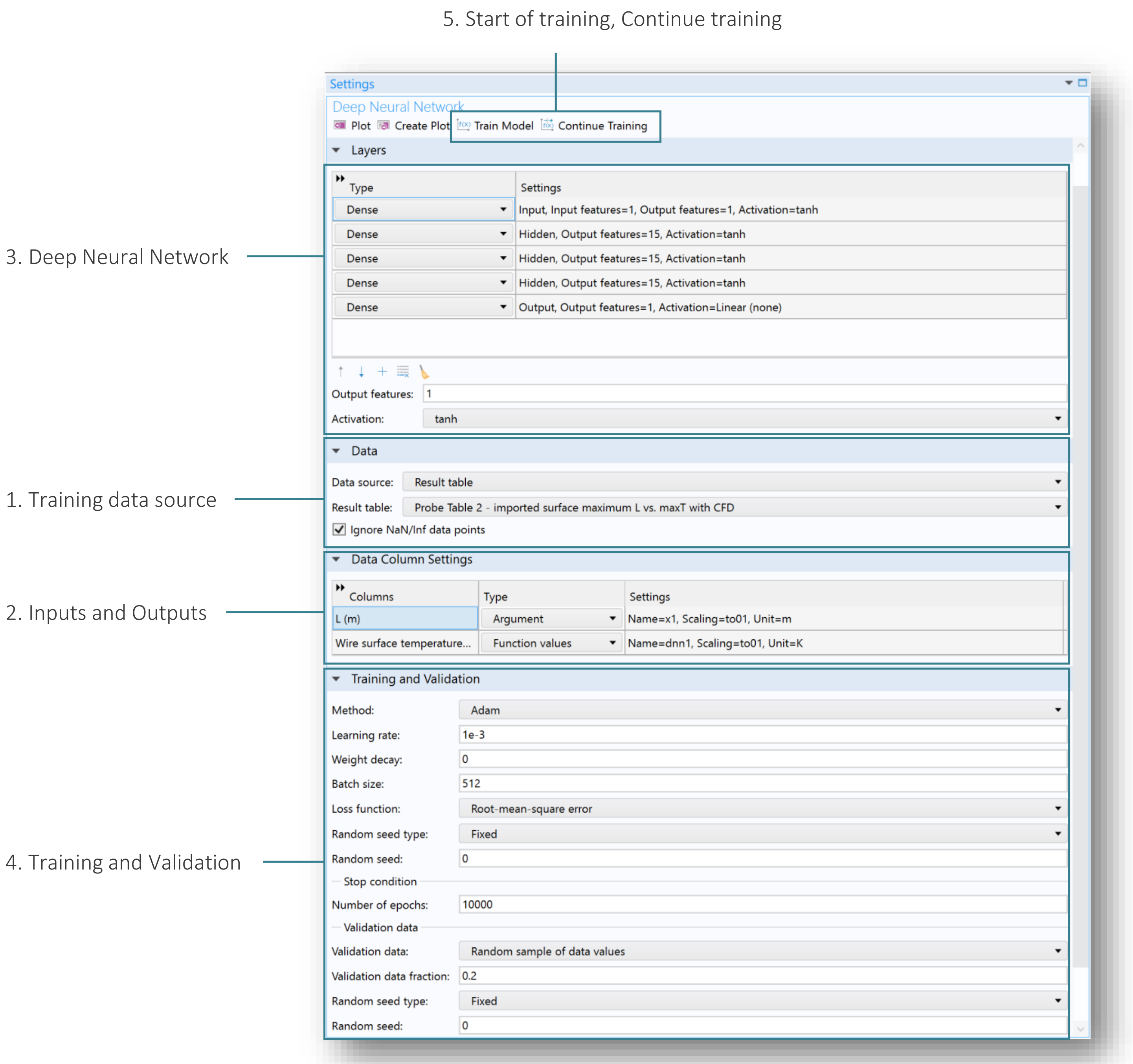
How to Generate Training Data?

- Third-party data
  - External data file
- Parametric study results
  - Manual setting of sampling (range)
  - Time-consuming for larger number of parameters
- Surrogate Model Training study
  - Design Of Experiments method generates dataset automatically
  - Default option is Latin Hypercube Sampling (LHS)
  - More strategic approach for larger number of parameters



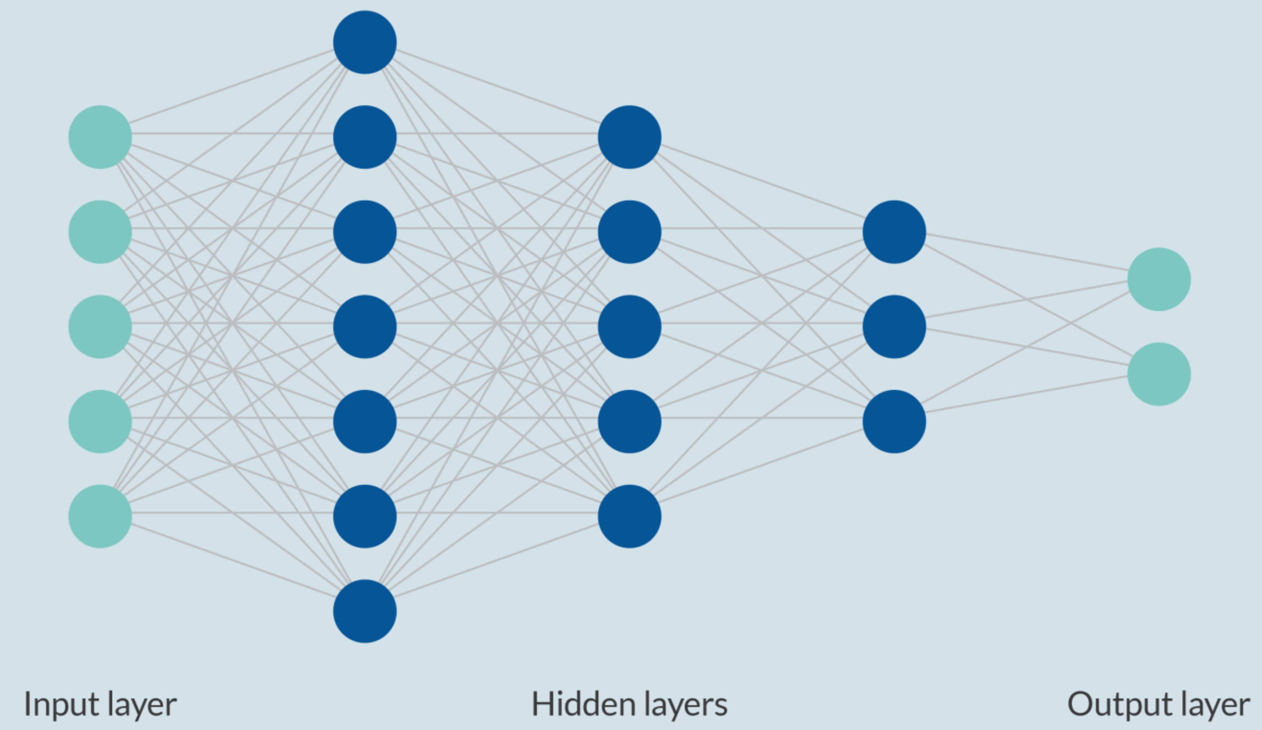
Deep Neural Network Settings

1. Training data source
2. Data source column settings
   - Inputs: arguments
   - Outputs: function value
3. Deep Neural Network settings
   - Number of layers
   - Output features (neurons) per layer
   - Activation function
4. Training and Validation settings
5. Training / Continue training



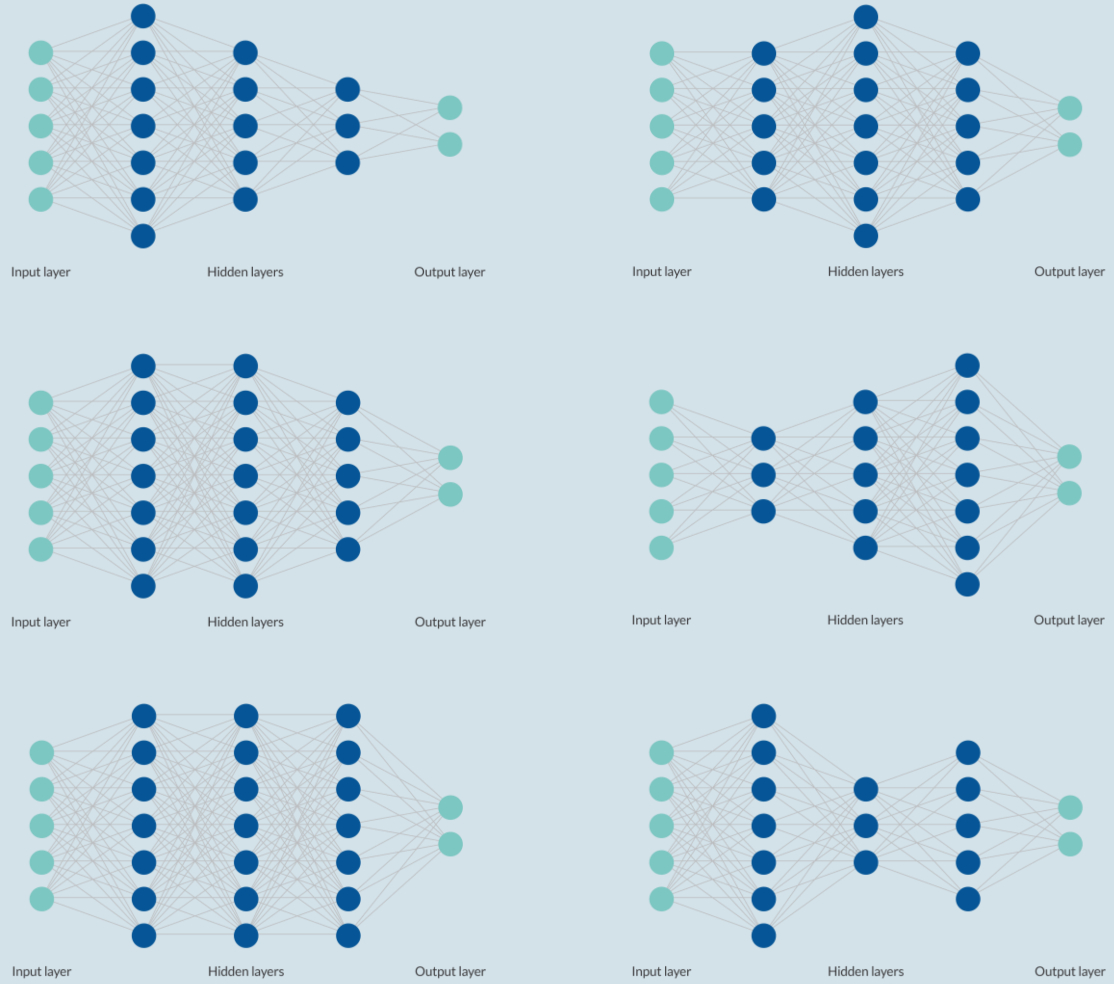
Deep Neural Network

- A DNN model consists of an input layer, a series of hidden layers, and an output layer.
- Each layer consists of a number of nodes, or neurons, or output features. The figure shows a graph for a network with three hidden layers, 5 input nodes, and 2 output nodes.
- You can define any number of layers and nodes for a DNN surrogate model.



Optimizing Neural Network Architecture

- Selection of layers and nodes is iterative and based on:
  - Problem-specific knowledge
  - Empirical testing



Optimizing Neural Network Architecture

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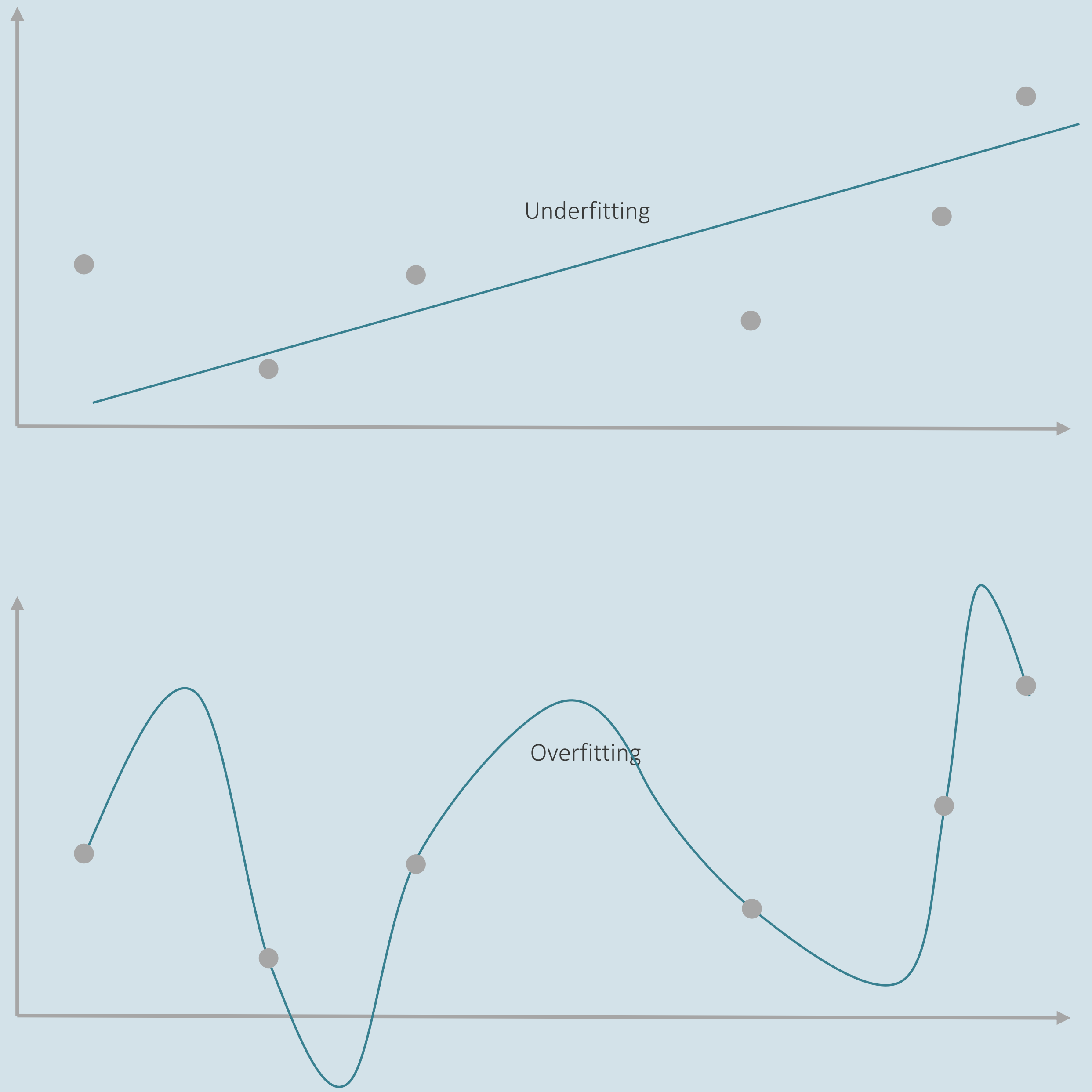
- Balance is key:
  - Too few layers/nodes may lead to underfitting and be inadequate for complex surrogate modeling.
  - Excess layers/nodes can cause overfitting, yielding high accuracy on training data but poor generalization.



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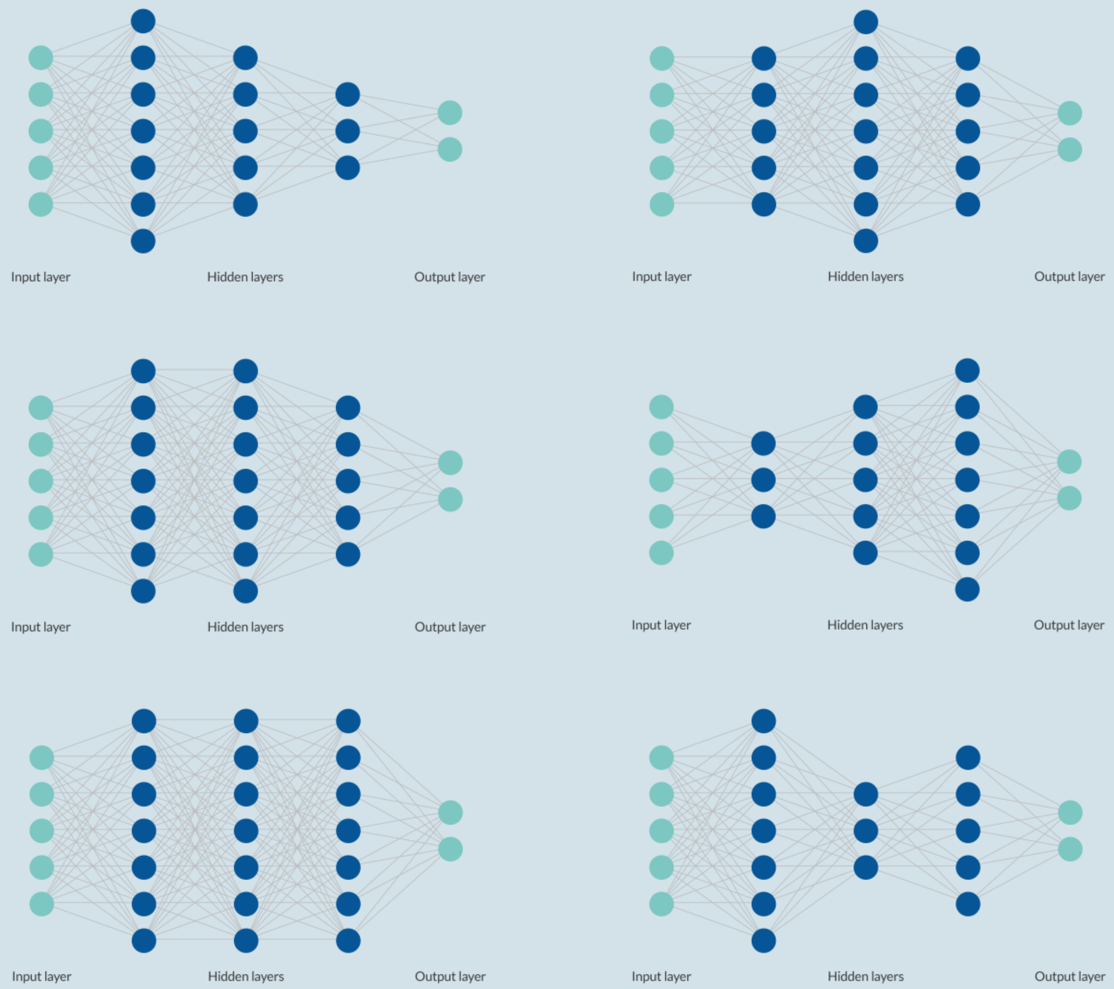
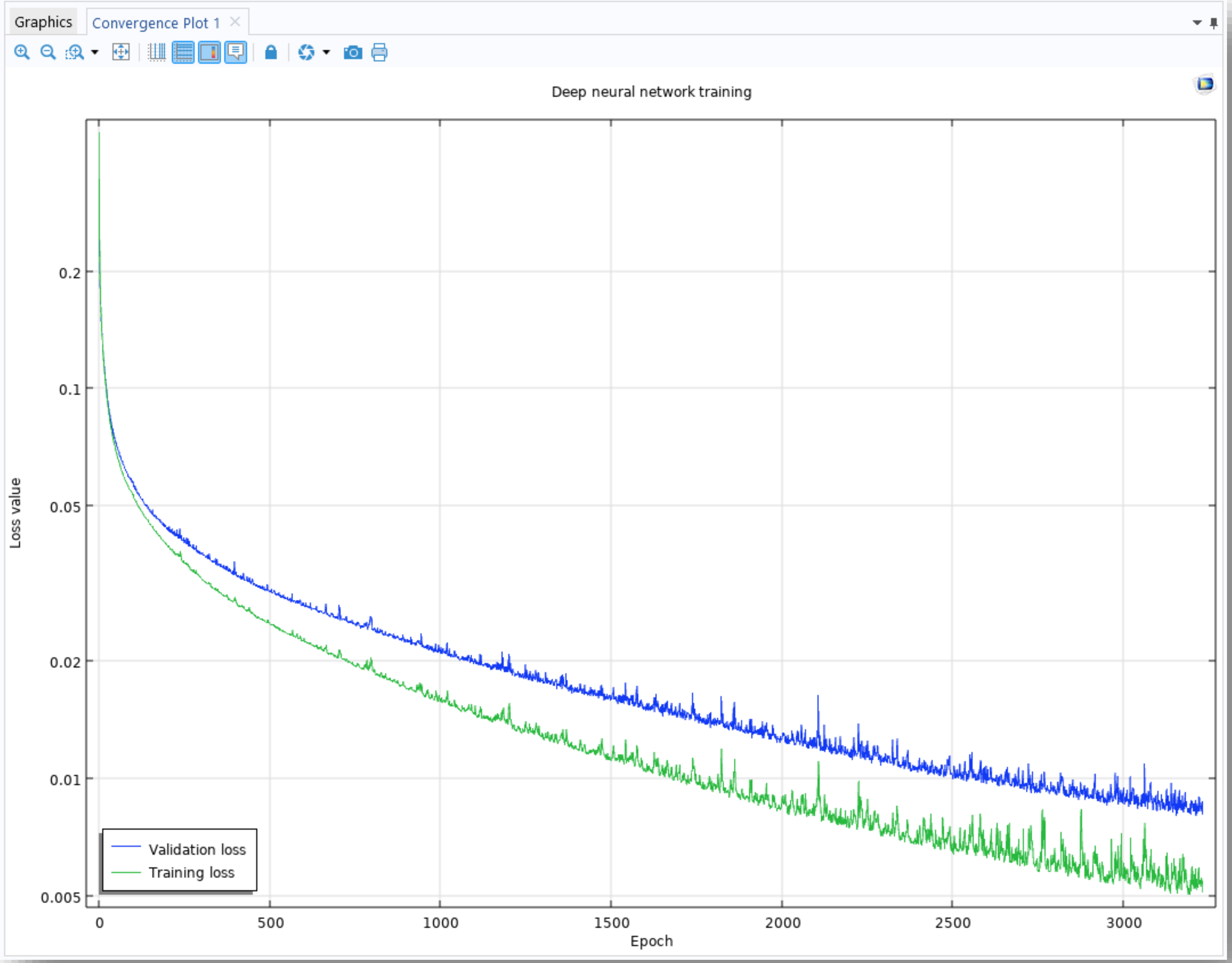
- Consider computational costs:
  - More layers/nodes increase model evaluation time.
  - Rule-of-thumb starting point: 3 hidden layers with 64, 32, and 16 nodes



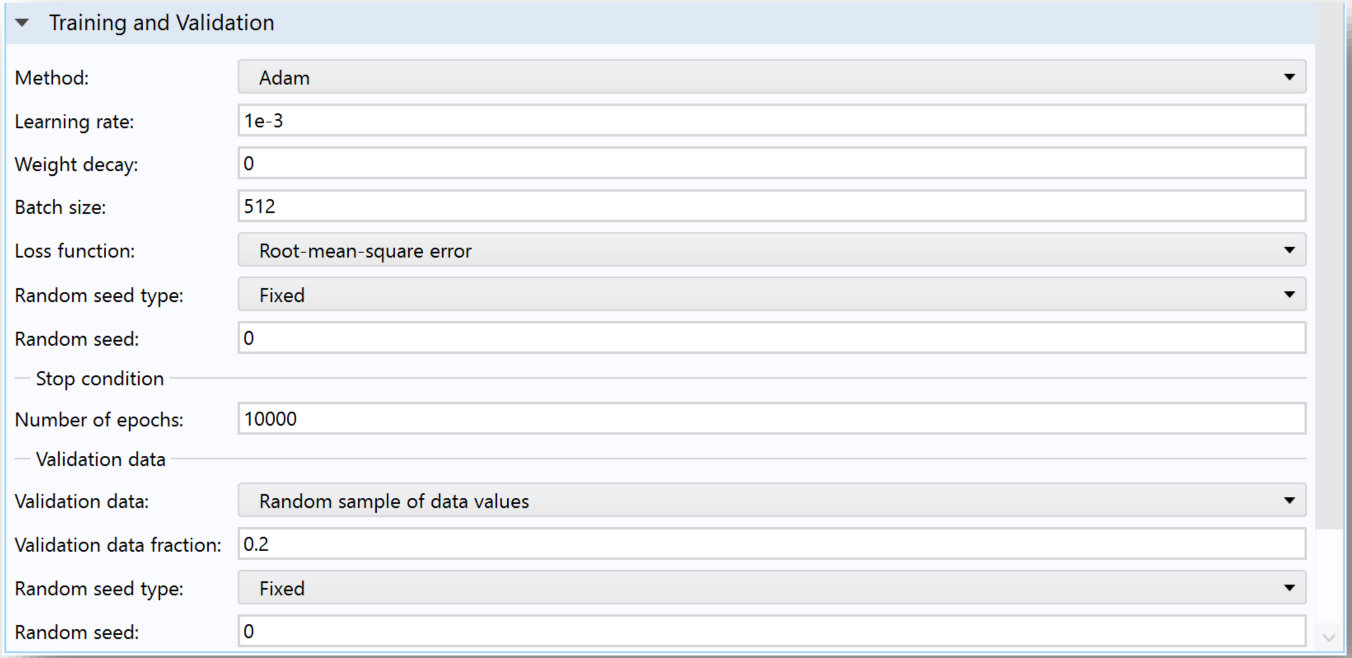
Training a DNN

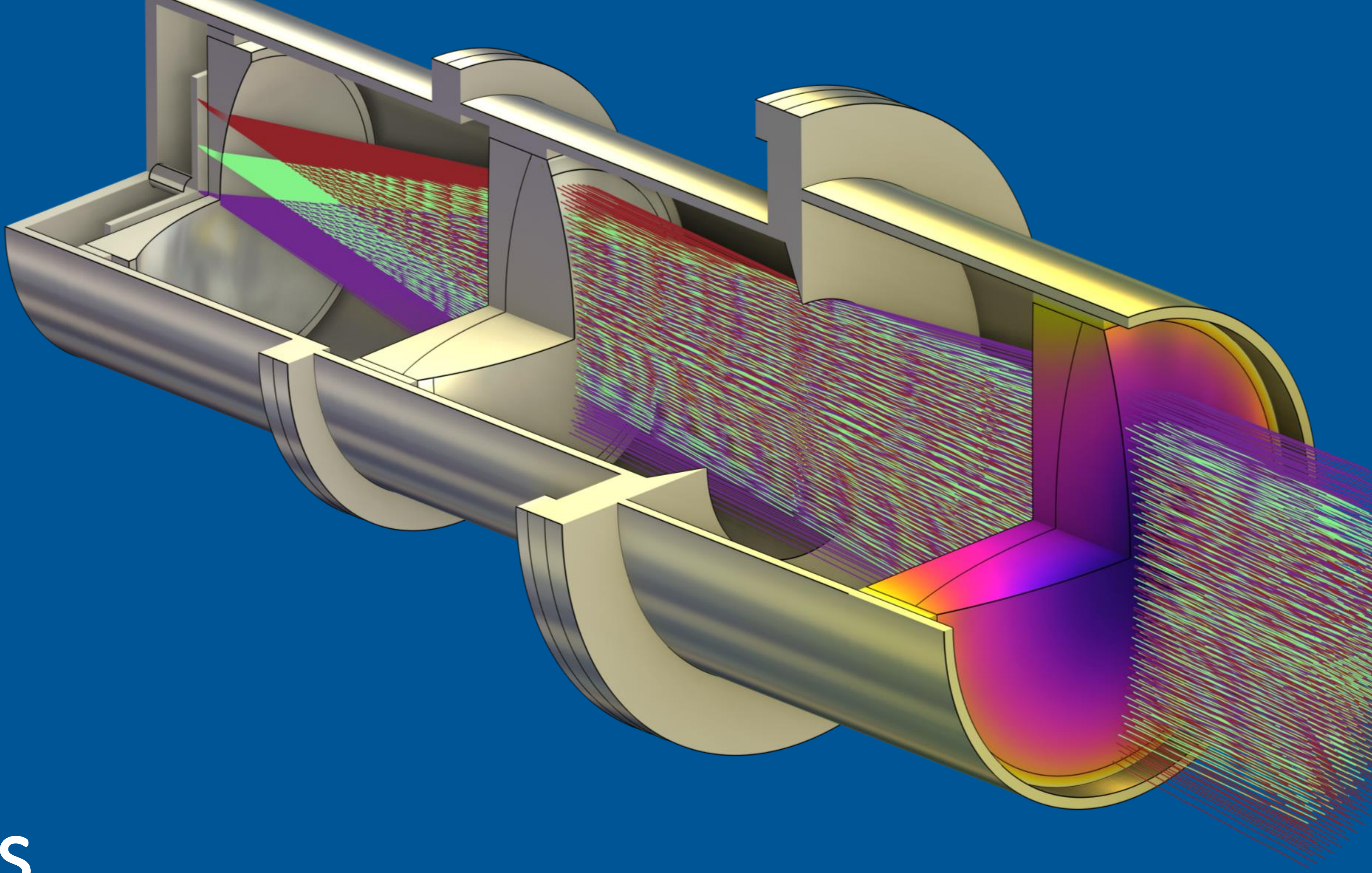
- The internal parameters of the neural network are called weights and biases
- Training involves optimizing weights and biases to minimize error
- Objective of training: Align surrogate model closely with the finite element model
- Error measurement is done via the loss function
- Default loss function is root mean squared error (RMSE)



Training and Validation Settings

- The DNN is trained using a specialized optimization solver.
- The solver settings are called *hyperparameters*. Some of the most important are:
  - *Learning rate*:
    - Controls optimization step size
    - Analogous to numerical damping in nonlinear solvers
  - *Batch size*:
    - Determines subdivision of training data into subsets
  - *Number of epochs*:
    - Indicates total passes through the full dataset





STOP Analysis

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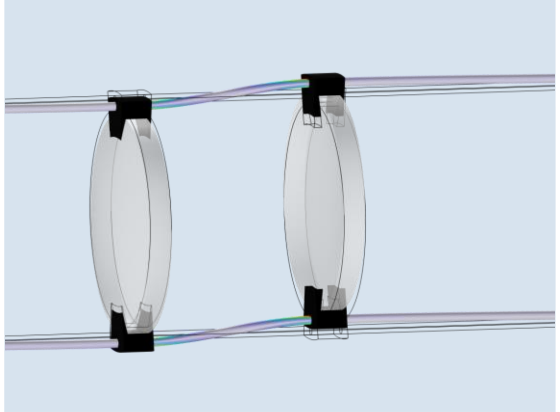
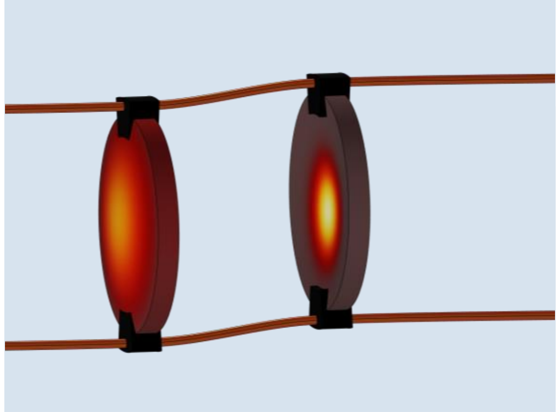
STOP Analysis in COMSOL®



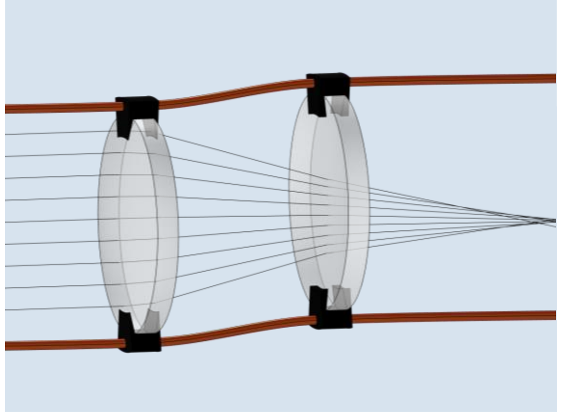
Structural

Model the structural displacements in an optical system.



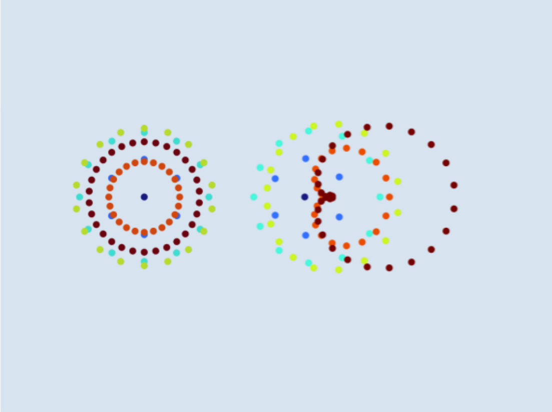
Thermal

Apply a fixed operating temperature or simulate the temperature distribution. Heat sources may include absorption from the beam itself.



Optical

With the local temperature and displacement considered, model how light will propagate through the system.



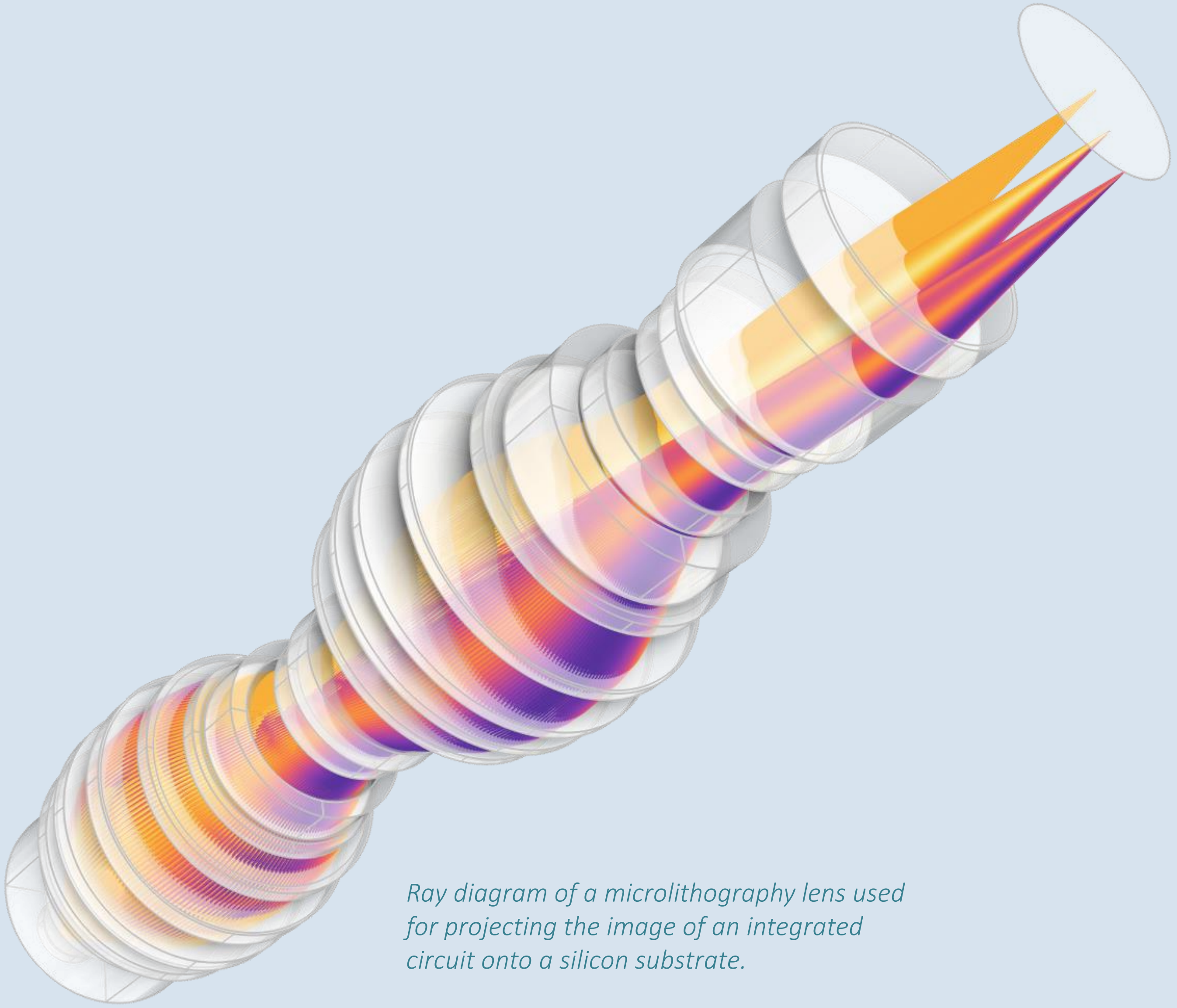
Performance

Evaluate the optical performance under the influence of thermal and structural loads.

OVERVIEW

Geometrical Optics

- Ray tracing in homogeneous and graded media
- Detailed analysis of ray intensity and polarization
- Variety of features for releasing rays and controlling interaction with boundaries
- Functionality for multiscale electromagnetics modeling
- Multiphysics couplings for STOP analysis



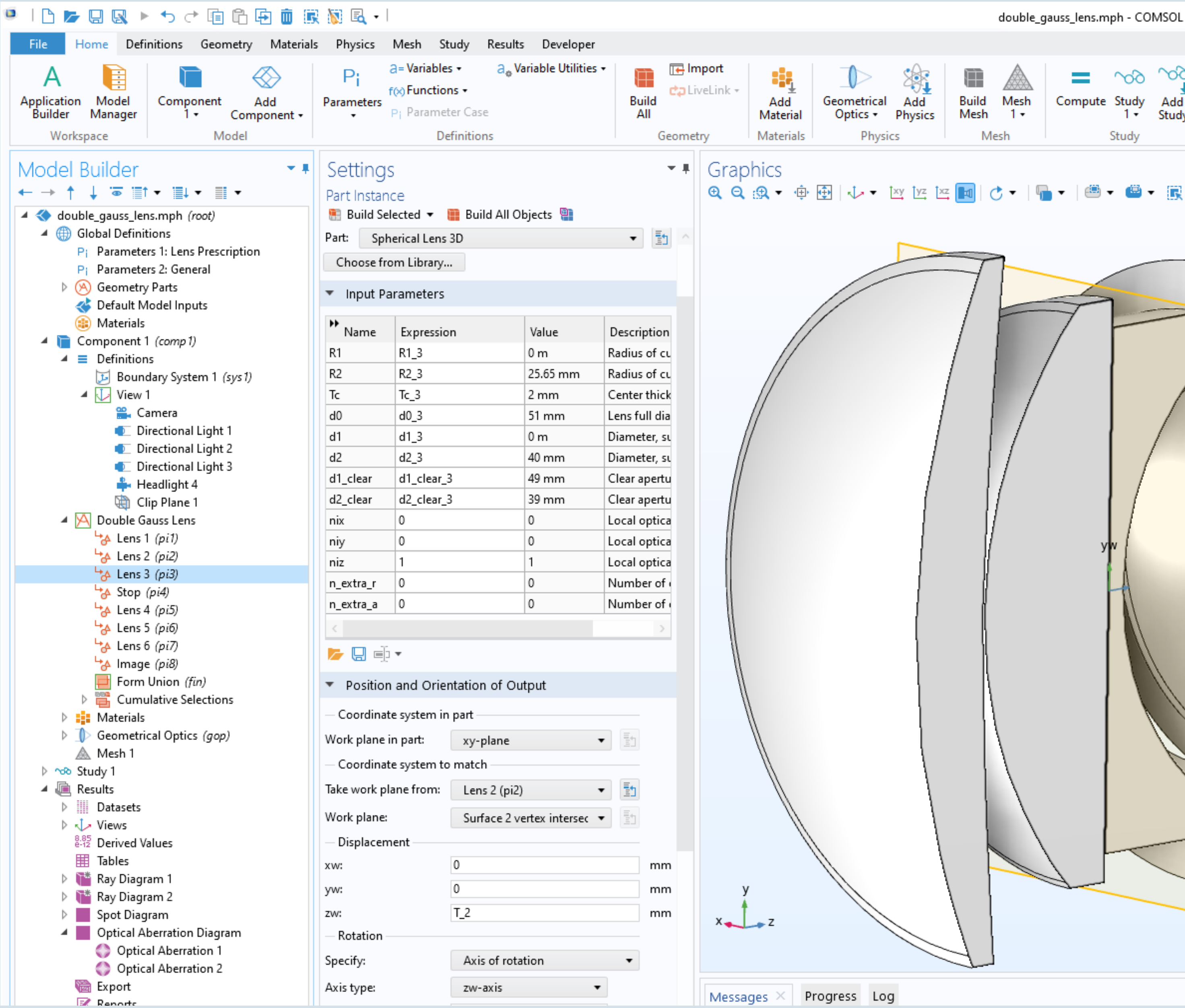
Ray diagram of a microlithography lens used for projecting the image of an integrated circuit onto a silicon substrate.

Ray Optics Module Part Library

The Ray Optics Module Part Library contains parameterized geometry parts for optical systems:

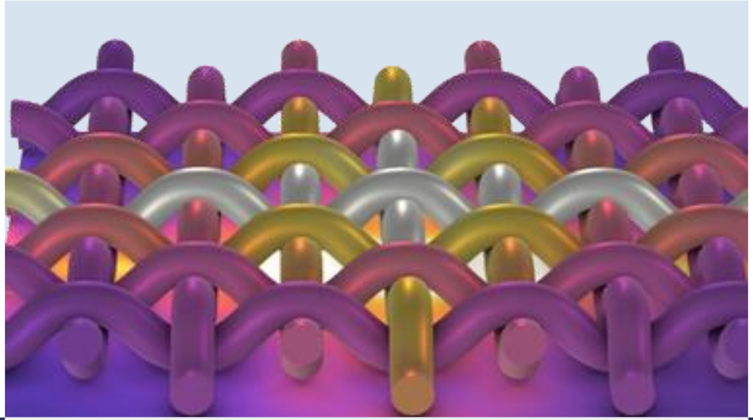
- Apertures and obstructions
- Aspheric, cylindrical, doublet, triplet, and spherical lenses
- Beam splitters and prisms
- Mirrors and reflectors

The parts include predefined selections for convenient set up of boundary conditions



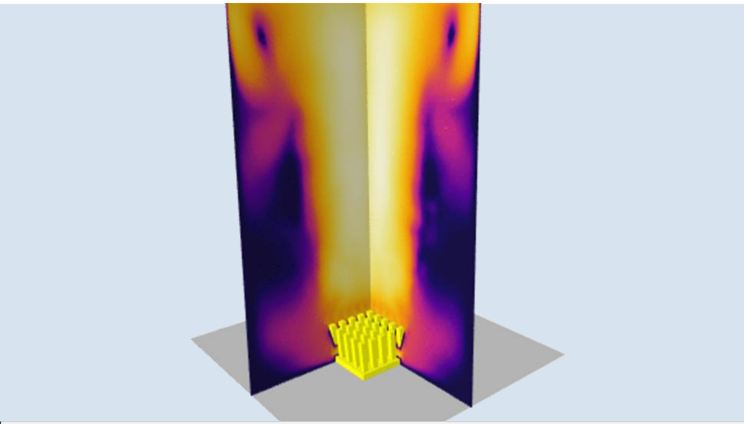
OVERVIEW

Heat Transfer Functionality



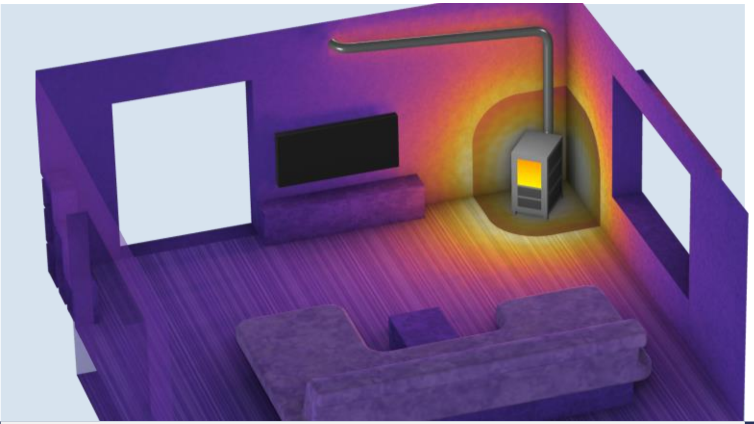
Conduction

- Isotropic, anisotropic, linear, and nonlinear thermal conductivity
- Thermal contact
- Thin layers



Convection

- Free and forced convection
- Laminar and turbulent flow
- Effective material properties

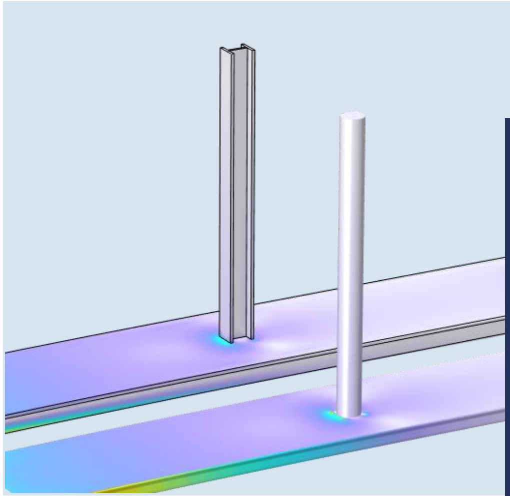


Radiation

- Surface-to-ambient and surface-to-surface radiation
- External radiation sources
- Radiation in participating media

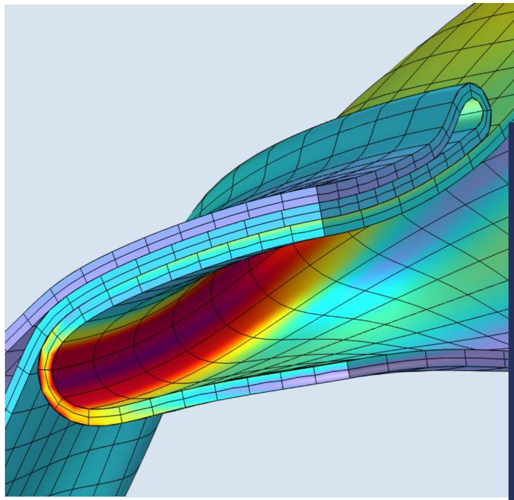
OVERVIEW

Structural Mechanics Functionality



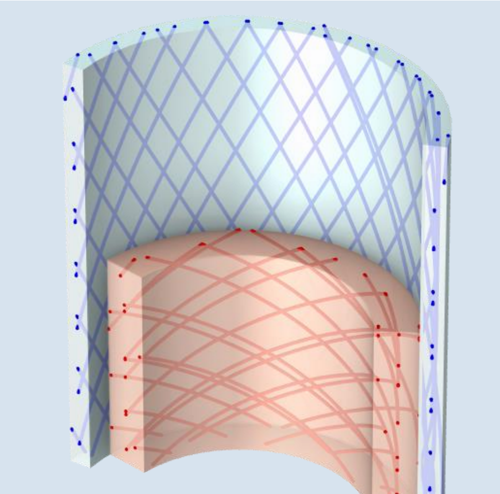
Formulations

Combine solids, single and layered shells, plates, membranes, beams, pipes, trusses, and wires.



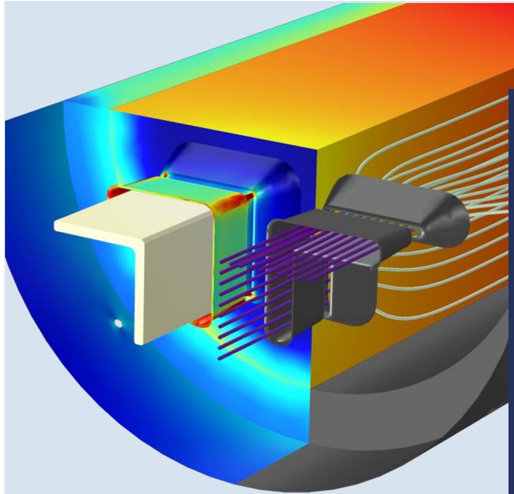
Analysis Types

Run stationary, transient, and frequency response analyses, as well as specialized analyses such as mechanical contact, buckling, and fatigue.



Material Models

Choose from a wide variety of elastic, viscoelastic, hyperelastic, elastoplastic, and composite material models. Materials can be spatially varying, anisotropic, and dependent on other variables.



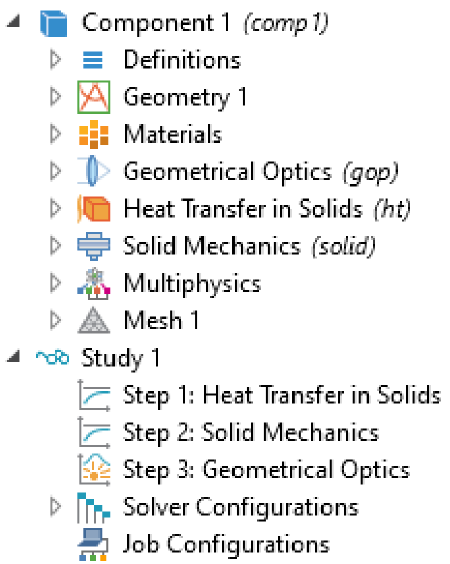
Multiphysics

Multiphysics couplings with heat transfer, CFD, acoustics, electromagnetics, optics, and more are available.

Study Setup

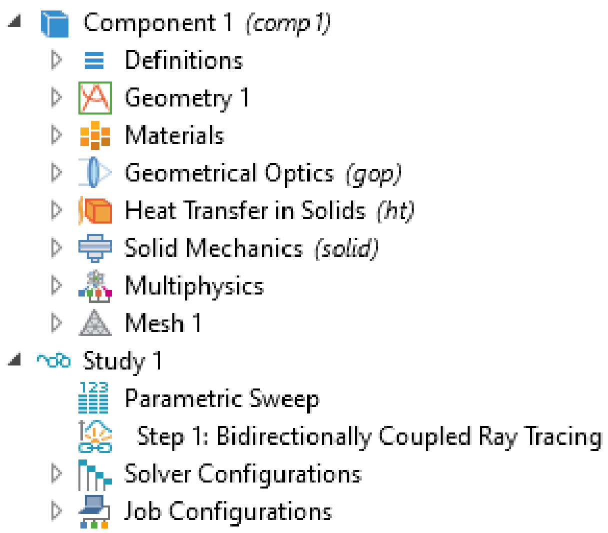
One-Way Coupled STOP Analysis

- With the temperatures affecting the deformations, and both temperatures and deformations influencing the ray paths, you can solve for the different physics interfaces one at a time.



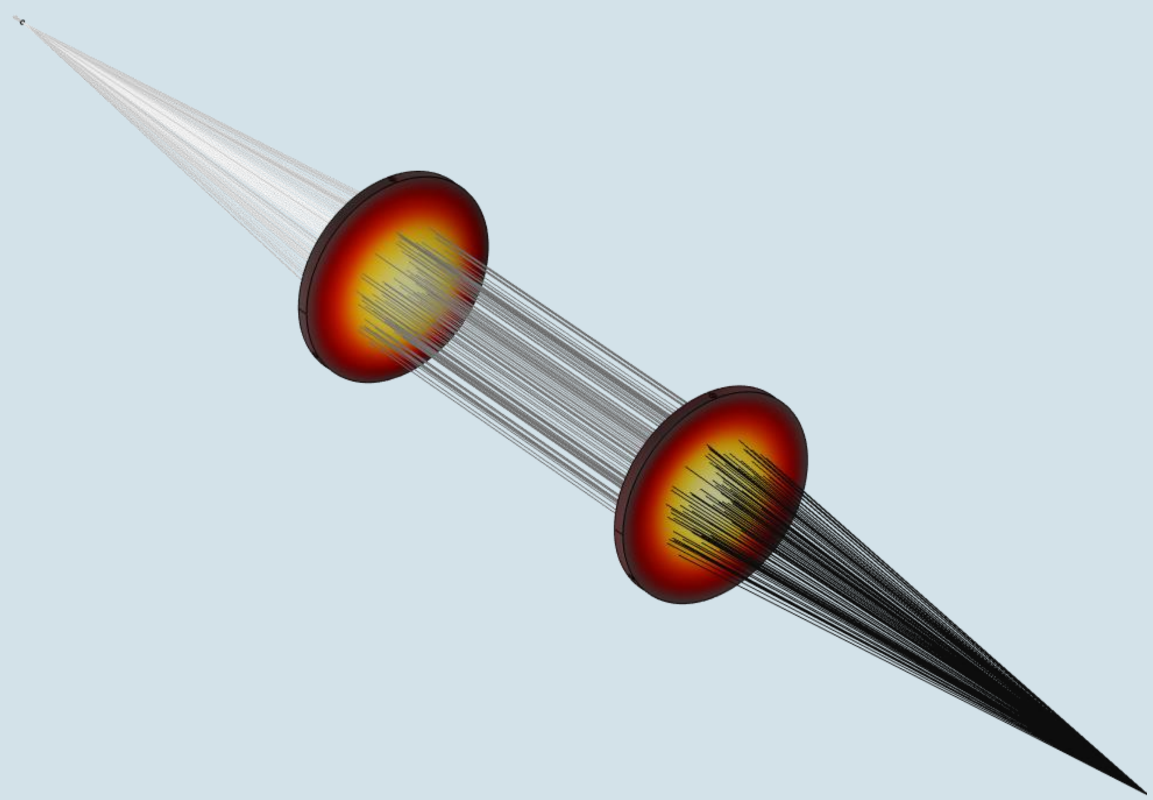
STOP Analysis with Ray Heating

- The dedicated *Bidirectionally Coupled Ray Tracing* study type, along with the *Ray Heat Source* feature, will automatically follow the iteration scheme in the previous slide.



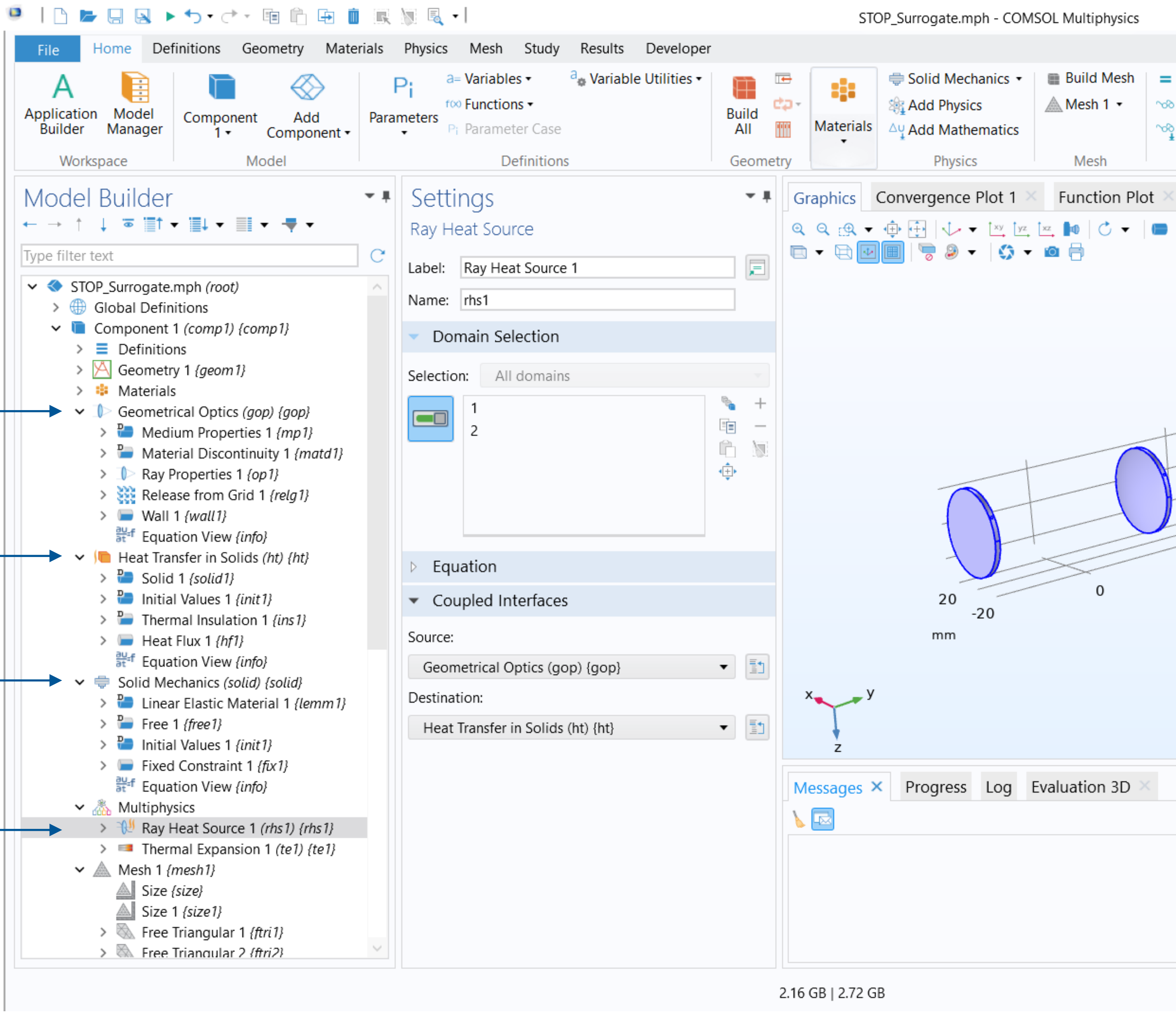
DEMO:
Surrogate model for STOP Analysis

- Creation of a digital twin of Laser Focusing System to obtain instantaneous values of temperature, stress and lens deformation.



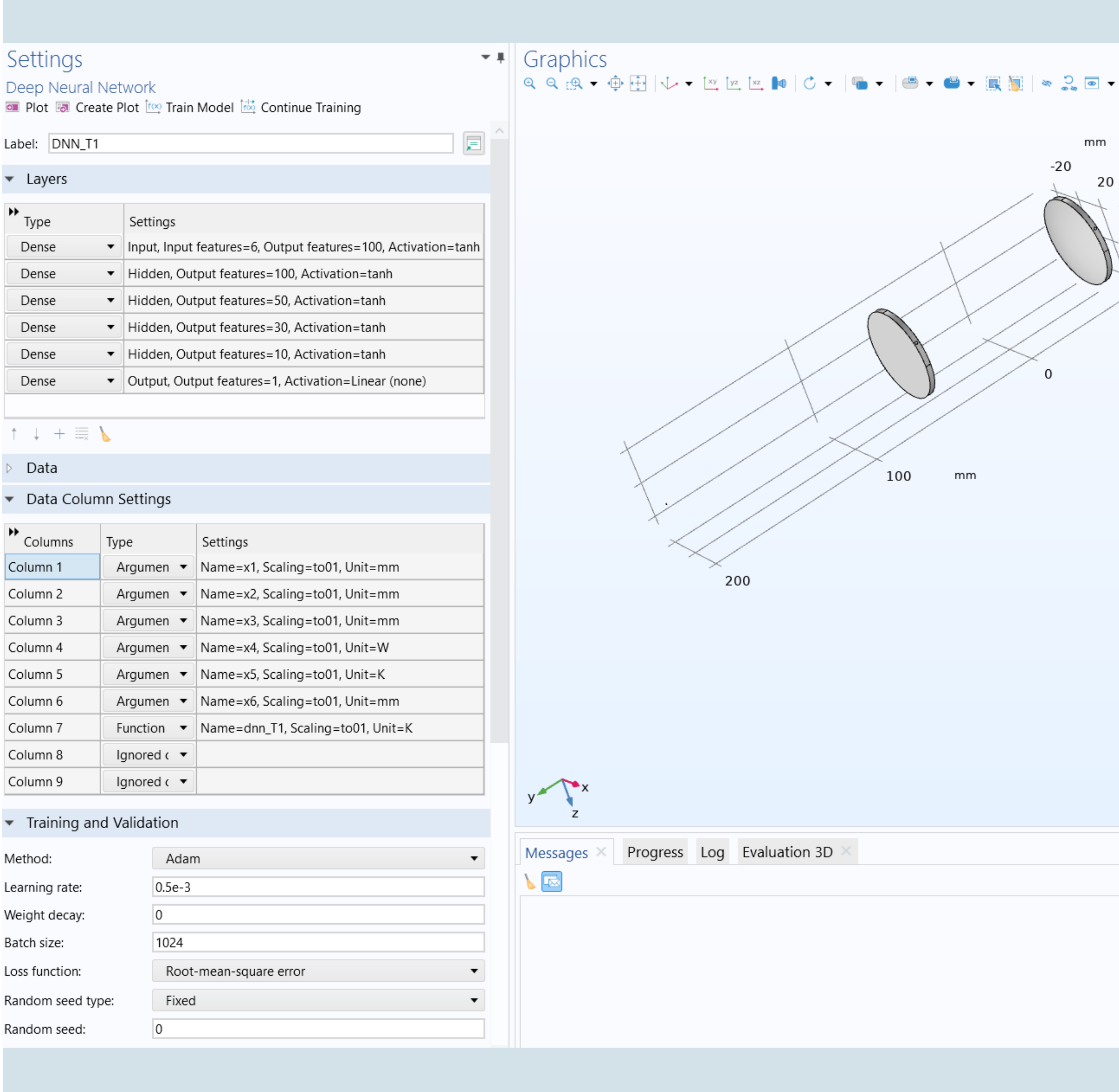
COMSOL Multiphysics

- Geometrical Optics
- Heat Transfer
- Solid Mechanics
- Ray Heat Source
  Thermal Expansion

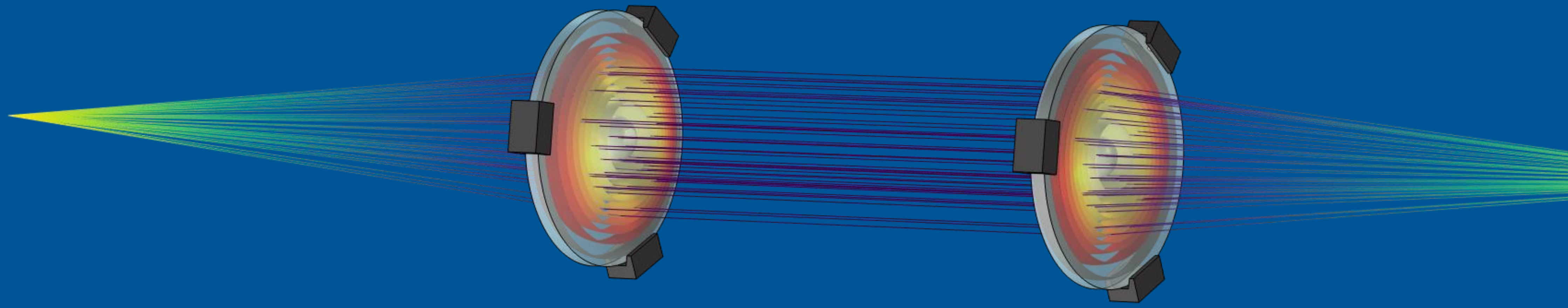


Our Neural Networks for STOP Model

- 6 DNNs in total (3 for each lens)
- 6 input parameters: x, y, z, lrms, T0, lam*
- Output parameters: temperature, stress, displacement
- Training data for 300 parameter combinations (lrms, T0, lam)
- 4 hidden layers, number of neurons: 100, 50, 30, 10
- Activations:
  - Output layers activation: linear
  - Other layers activation: tanh



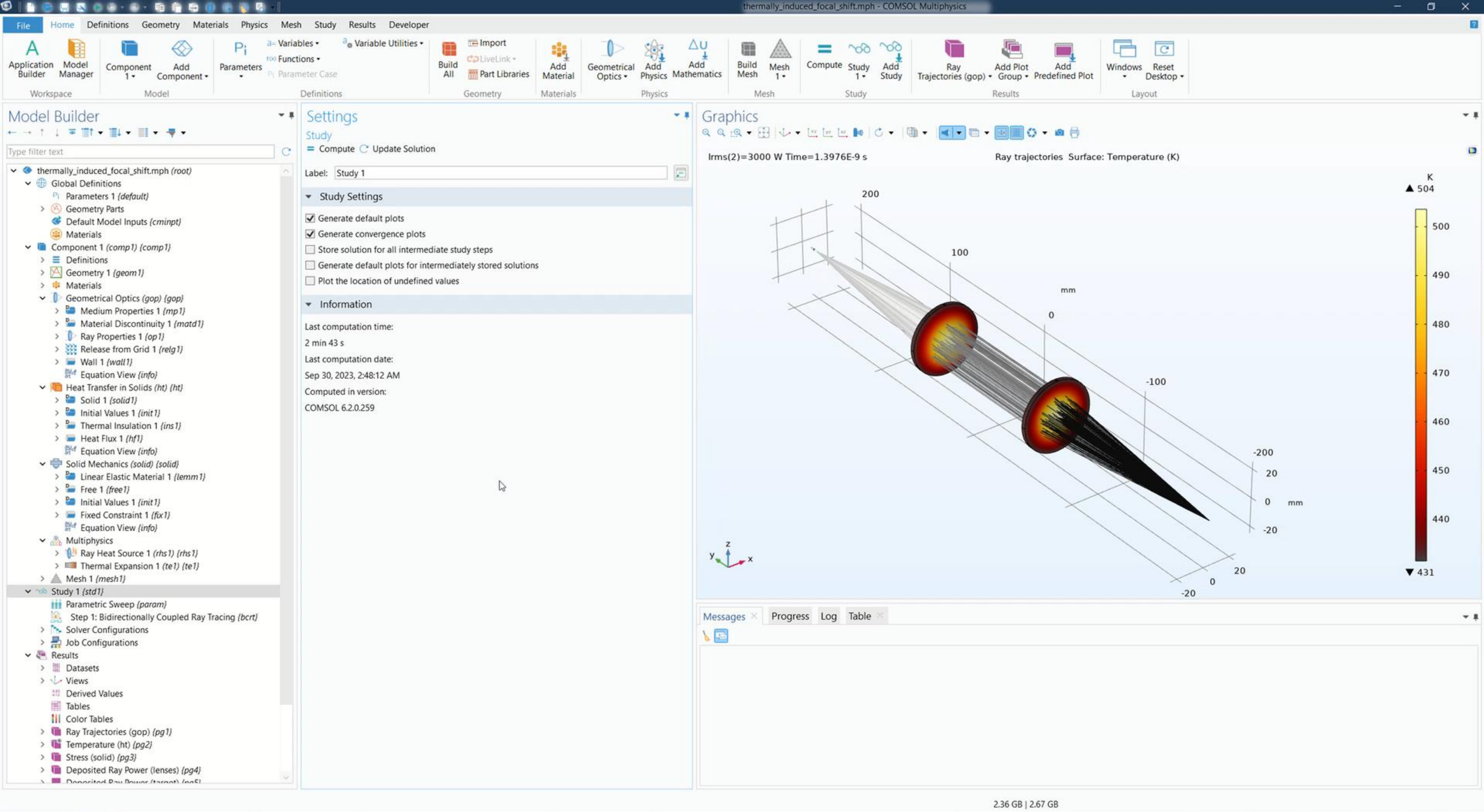
* Lrms = laser power, T0 = room temperature, lam = laser wavelength



How to Create Surrogate Model from STOP Simulation

Tomáš Vrbata

Setting up Surrogate Model Training


thermally_induced_focal_shift.mph - COMSOL Multiphysics
File
Home
Definitions
Geometry
Materials
Physics
Mesh
Study
Results
Developer
Application Builder
Model Manager
Workspace
Component 1
Add Component
Model
Parameters
Variables
Functions
Parameter Case
Variable Utilities
Definitions
Build All
Import
LiveLink
Part Libraries
Geometry
Add Material
Materials
Geometrical Optics
Add Physics
Add Mathematics
Physics
Build Mesh
Mesh 1
Mesh
Compute
Study 1
Add Study
Study
Ray Trajectories (gop)
Add Plot Group
Add Predefined Plot
Results
Windows
Reset Desktop
Layout
Model Builder
Type filter text
thermally_induced_focal_shift.mph (root)
Global Definitions
Parameters 1 (default)
Geometry Parts
Default Model Inputs (cminpt)
Materials
Component 1 (comp1) (comp1)
Definitions
Geometry 1 (geom1)
Materials
Geometrical Optics (gop) (gop)
Medium Properties 1 (mp1)
Material Discontinuity 1 (matd1)
Ray Properties 1 (op1)
Release from Grid 1 (relg1)
Wall 1 (wall1)
Equation View (info)
Heat Transfer in Solids (ht) (ht)
Solid 1 (solid1)
Initial Values 1 (init1)
Thermal Insulation 1 (ins1)
Heat Flux 1 (hf1)
Equation View (info)
Solid Mechanics (solid) (solid)
Linear Elastic Material 1 (lemm1)
Free 1 (free1)
Initial Values 1 (init1)
Fixed Constraint 1 (fix1)
Equation View (info)
Multiphysics
Ray Heat Source 1 (rhs1) (rhs1)
Thermal Expansion 1 (te1) (te1)
Mesh 1 (mesh1)
Study 1 (std1)
Parametric Sweep (param)
Step 1: Bidirectionally Coupled Ray Tracing (bcrt)
Solver Configurations
Job Configurations
Results
Datasets
Views
Derived Values
Tables
Color Tables
Ray Trajectories (gop) (pg1)
Temperature (ht) (pg2)
Stress (solid) (pg3)
Deposited Ray Power (lenses) (pg4)
Settings
Study
Compute
Update Solution
Label:
Study 1
Study Settings
Generate default plots
Generate convergence plots
Store solution for all intermediate study steps
Generate default plots for intermediately stored solutions
Plot the location of undefined values
Information
Last computation time:
2 min 43 s
Last computation date:
Sep 30, 2023, 2:48:12 AM
Computed in version:
COMSOL 6.2.0.259
Graphics
Irms(2)=3000 W Time=1.3976E-9 s
Ray trajectories Surface: Temperature (K)
K
▲ 504
500
490
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470
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200
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mm
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z
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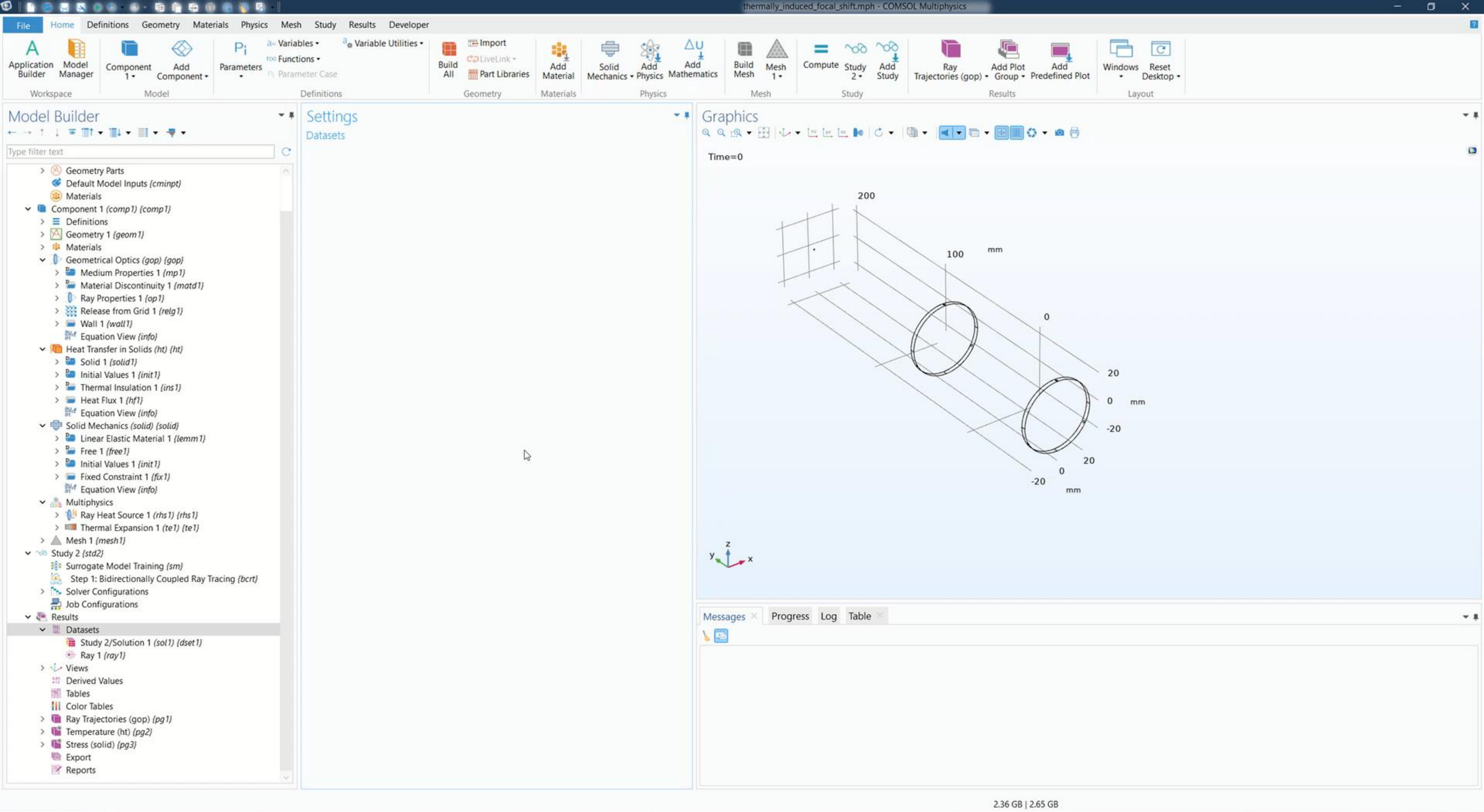
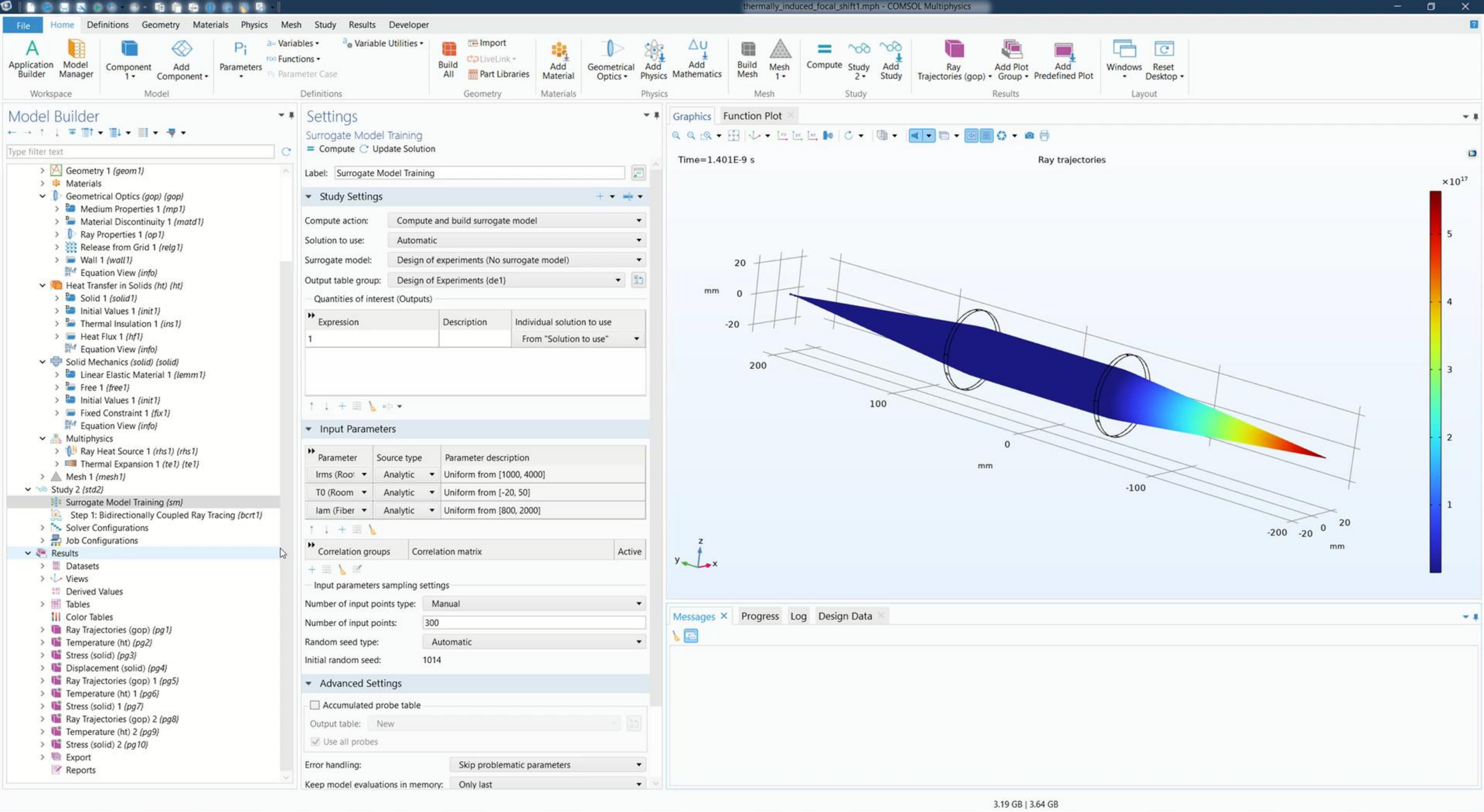
Messages
Progress
Log
Table
2.36 GB | 2.67 GB

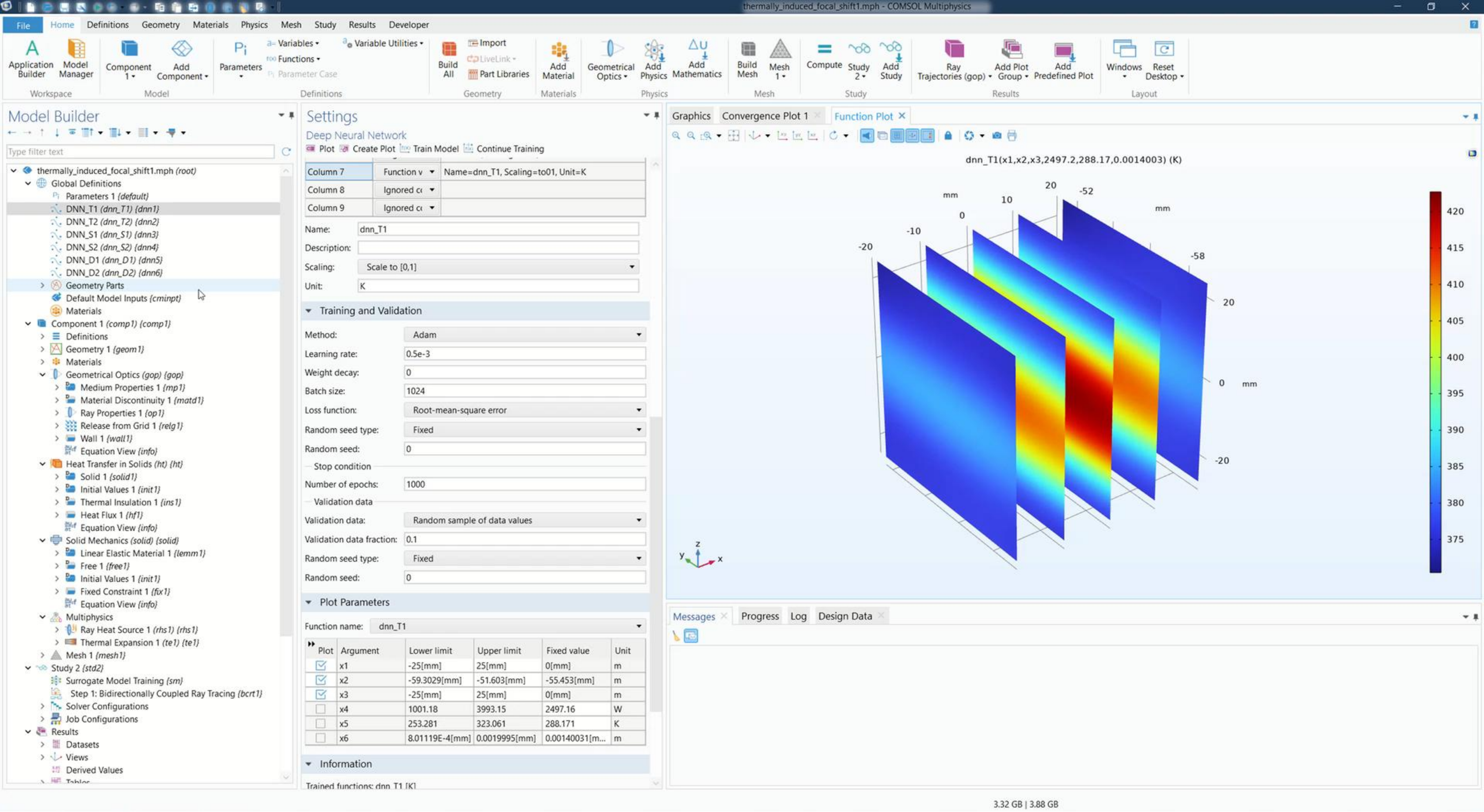
Generation of training data


thermally_induced_focal_shift.mph - COMSOL Multiphysics
File
Home
Definitions
Geometry
Materials
Physics
Mesh
Study
Results
Developer
Application Builder
Model Manager
Workspace
Component 1
Add Component
Model
Parameters
Variables
Functions
Parameter Case
Variable Utilities
Definitions
Build All
Import
LiveLink
Part Libraries
Geometry
Add Material
Materials
Solid Mechanics
Add Physics
Add Mathematics
Physics
Build Mesh
Mesh 1
Mesh
Compute
Study 2
Add Study
Study
Ray Trajectories (gop)
Add Plot Group
Add Predefined Plot
Results
Windows
Reset Desktop
Layout
Model Builder
Type filter text
Geometry Parts
Default Model Inputs {cminpt}
Materials
Component 1 (comp1) {comp1}
Definitions
Geometry 1 {geom1}
Materials
Geometrical Optics (gop) {gop}
Medium Properties 1 {mp1}
Material Discontinuity 1 {matd1}
Ray Properties 1 {op1}
Release from Grid 1 {relg1}
Wall 1 {wall1}
Equation View {info}
Heat Transfer in Solids (ht) {ht}
Solid 1 {solid1}
Initial Values 1 {init1}
Thermal Insulation 1 {ins1}
Heat Flux 1 {hf1}
Equation View {info}
Solid Mechanics (solid) {solid}
Linear Elastic Material 1 {lemm1}
Free 1 {free1}
Initial Values 1 {init1}
Fixed Constraint 1 {fix1}
Equation View {info}
Multiphysics
Ray Heat Source 1 (rhs1) {rhs1}
Thermal Expansion 1 (te1) {te1}
Mesh 1 {mesh1}
Study 2 {std2}
Surrogate Model Training {sm}
Step 1: Bidirectionally Coupled Ray Tracing {bcrt}
Solver Configurations
Job Configurations
Results
Datasets
Study 2/Solution 1 (sol1) {dset1}
Ray 1 {ray1}
Views
Derived Values
Tables
Color Tables
Ray Trajectories (gop) {pg1}
Temperature (ht) {pg2}
Stress (solid) {pg3}
Export
Reports
Settings
Datasets
Graphics
Time=0
200
100
mm
0
20
0
mm
-20
20
0
-20
mm
z
y
x
Messages
Progress
Log
Table
2.36 GB | 2.65 GB

Setting up a Deep Neural Network


thermally_induced_focal_shift1.mph - COMSOL Multiphysics
File
Home
Definitions
Geometry
Materials
Physics
Mesh
Study
Results
Developer
Model Builder
Geometry 1 {geom1}
Materials
Geometrical Optics (gop) {gop}
Medium Properties 1 {mp1}
Material Discontinuity 1 {matd1}
Ray Properties 1 {op1}
Release from Grid 1 {relg1}
Wall 1 {wall1}
Equation View {info}
Heat Transfer in Solids (ht) {ht}
Solid 1 {solid1}
Initial Values 1 {init1}
Thermal Insulation 1 {ins1}
Heat Flux 1 {hf1}
Equation View {info}
Solid Mechanics (solid) {solid}
Linear Elastic Material 1 {lemm1}
Free 1 {free1}
Initial Values 1 {init1}
Fixed Constraint 1 {fix1}
Equation View {info}
Multiphysics
Ray Heat Source 1 (rhs1) {rhs1}
Thermal Expansion 1 (te1) {te1}
Mesh 1 {mesh1}
Study 2 {std2}
Surrogate Model Training {sm}
Step 1: Bidirectionally Coupled Ray Tracing {bcrt1}
Solver Configurations
Job Configurations
Results
Datasets
Views
Derived Values
Tables
Color Tables
Ray Trajectories (gop) {pg1}
Temperature (ht) {pg2}
Stress (solid) {pg3}
Displacement (solid) {pg4}
Ray Trajectories (gop) 1 {pg5}
Temperature (ht) 1 {pg6}
Stress (solid) 1 {pg7}
Ray Trajectories (gop) 2 {pg8}
Temperature (ht) 2 {pg9}
Stress (solid) 2 {pg10}
Export
Reports
Settings
Surrogate Model Training
Compute
Update Solution
Label: Surrogate Model Training
Study Settings
Compute action: Compute and build surrogate model
Solution to use: Automatic
Surrogate model: Design of experiments (No surrogate model)
Output table group: Design of Experiments (de1)
Quantities of interest (Outputs)
Expression | Description | Individual solution to use
1 | | From "Solution to use"
Input Parameters
Parameter | Source type | Parameter description
Irms (Roo | Analytic | Uniform from [1000, 4000]
T0 (Room | Analytic | Uniform from [-20, 50]
lam (Fiber | Analytic | Uniform from [800, 2000]
Correlation groups | Correlation matrix | Active
Input parameters sampling settings
Number of input points type: Manual
Number of input points: 300
Random seed type: Automatic
Initial random seed: 1014
Advanced Settings
Accumulated probe table
Output table: New
Use all probes
Error handling: Skip problematic parameters
Keep model evaluations in memory: Only last
Graphics
Function Plot
Time=1.401E-9 s
Ray trajectories
×10^17
Messages
Progress
Log
Design Data
3.19 GB | 3.64 GB

DNN visualization and postprocessing


thermally_induced_focal_shift1.mph - COMSOL Multiphysics
File
Home
Definitions
Geometry
Materials
Physics
Mesh
Study
Results
Developer
Application Builder
Model Manager
Workspace
Component 1
Add Component
Model
Parameters
Variables
Functions
Parameter Case
Variable Utilities
Definitions
Build All
Import
LiveLink
Part Libraries
Geometry
Add Material
Materials
Geometrical Optics
Add Physics
Add Mathematics
Physics
Build Mesh
Mesh 1
Mesh
Compute
Study 2
Add Study
Study
Ray Trajectories (gop)
Add Plot Group
Add Predefined Plot
Results
Windows
Reset Desktop
Layout
Model Builder
Type filter text
thermally_induced_focal_shift1.mph (root)
Global Definitions
Parameters 1 (default)
DNN_T1 (dnn_T1) (dnn1)
DNN_T2 (dnn_T2) (dnn2)
DNN_S1 (dnn_S1) (dnn3)
DNN_S2 (dnn_S2) (dnn4)
DNN_D1 (dnn_D1) (dnn5)
DNN_D2 (dnn_D2) (dnn6)
Geometry Parts
Default Model Inputs (cminpt)
Materials
Component 1 (comp1) (comp1)
Definitions
Geometry 1 (geom1)
Materials
Geometrical Optics (gop) (gop)
Medium Properties 1 (mp1)
Material Discontinuity 1 (matd1)
Ray Properties 1 (op1)
Release from Grid 1 (relg1)
Wall 1 (wall1)
Equation View (info)
Heat Transfer in Solids (ht) (ht)
Solid 1 (solid1)
Initial Values 1 (init1)
Thermal Insulation 1 (ins1)
Heat Flux 1 (hf1)
Equation View (info)
Solid Mechanics (solid) (solid)
Linear Elastic Material 1 (lemm1)
Free 1 (free1)
Initial Values 1 (init1)
Fixed Constraint 1 (fix1)
Equation View (info)
Multiphysics
Ray Heat Source 1 (rhs1) (rhs1)
Thermal Expansion 1 (te1) (te1)
Mesh 1 (mesh1)
Study 2 (std2)
Surrogate Model Training (sm)
Step 1: Bidirectionally Coupled Ray Tracing (bcrt1)
Solver Configurations
Job Configurations
Results
Datasets
Views
Derived Values
Tables
Settings
Deep Neural Network
Plot
Create Plot
Train Model
Continue Training
Column 7
Function v
Name=dnn_T1, Scaling=to01, Unit=K
Column 8
Ignored c
Column 9
Ignored c
Name: dnn_T1
Description:
Scaling: Scale to [0,1]
Unit: K
Training and Validation
Method: Adam
Learning rate: 0.5e-3
Weight decay: 0
Batch size: 1024
Loss function: Root-mean-square error
Random seed type: Fixed
Random seed: 0
Stop condition
Number of epochs: 1000
Validation data
Validation data: Random sample of data values
Validation data fraction: 0.1
Random seed type: Fixed
Random seed: 0
Plot Parameters
Function name: dnn_T1
Plot | Argument | Lower limit | Upper limit | Fixed value | Unit
x1 | -25[mm] | 25[mm] | 0[mm] | m
x2 | -59.3029[mm] | -51.603[mm] | -55.453[mm] | m
x3 | -25[mm] | 25[mm] | 0[mm] | m
x4 | 1001.18 | 3993.15 | 2497.16 | W
x5 | 253.281 | 323.061 | 288.171 | K
x6 | 8.01119E-4[mm] | 0.0019995[mm] | 0.00140031[m... | m
Information
Trained functions: dnn_T1 [K]
Graphics
Convergence Plot 1
Function Plot
dnn_T1(x1,x2,x3,2497.2,288.17,0.0014003) (K)
mm
20
10
0
-10
-20
-52
-58
mm
20
0
-20
mm
420
415
410
405
400
395
390
385
380
375
z
y
x
Messages
Progress
Log
Design Data
3.32 GB | 3.88 GB

Application running

Making an application skipped

Application Library | COMSOL S

vulpecula.humusoft.cz:2036/app-lib

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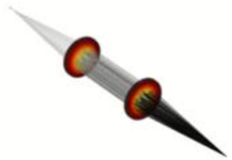
STOP Analysis - Surrogate Model



Date uploaded: 2024-05-20 15:39:22

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Air-Cooled BESS

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Thermal Actuator Surrogate Model Application

Date uploaded: 2023-11-15 08:33:52

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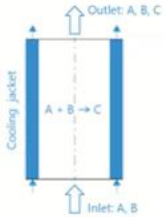
Tubular Reactor Surrogate Model Application



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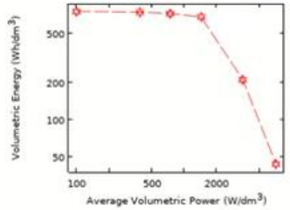
Surrogate Model Training of a Battery Rate Capability Model



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Installation Verification

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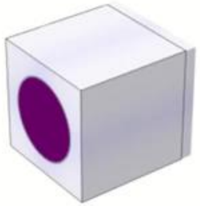
Homogenized Material Properties of Periodic Microstructures



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Lungs Ohmic Heating

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Brownian Motion

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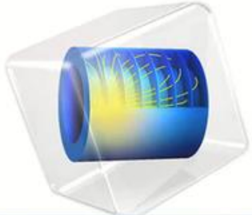
MHD 3D



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