



# Reinforcing Computational Thinking Throughout Chemical Engineering Curriculum with MATLAB and Simulink

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Customer Success Engineer

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Industry Marketing

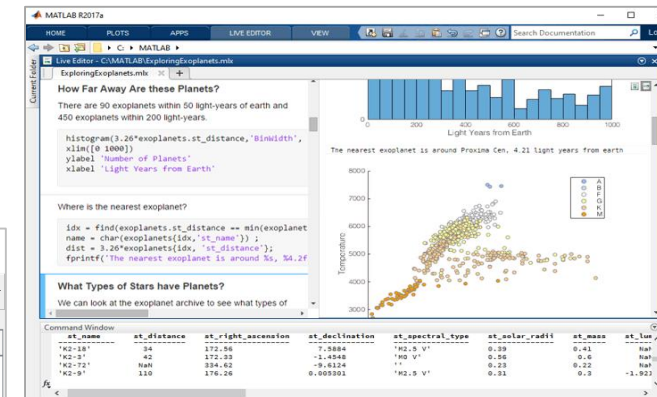
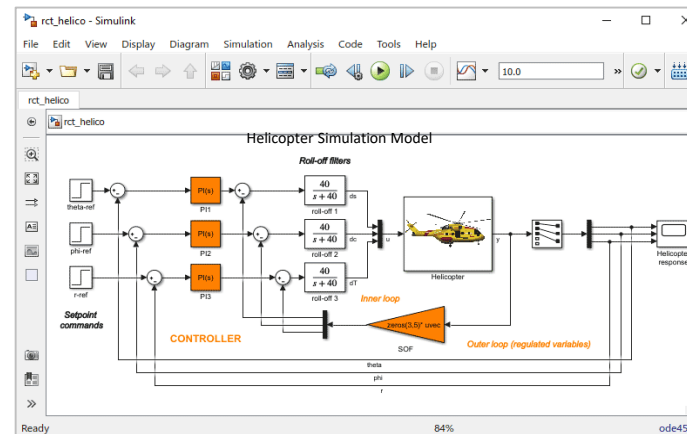
# Our Products MATLAB® & SIMULINK®



## MATLAB

- MATLAB is a programming environment for algorithm development, data analysis, visualization, and numeric computation.
- Simulink is a graphical environment for designing, simulating, and testing systems.
- 100 add-on products for specialized tasks.

## Simulink



## Chemicals and Petrochemicals

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# MATLAB and Simulink for the Chemicals and Petrochemicals Industry

<https://www.mathworks.com/solutions/chemicals-and-petrochemicals.html>

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## Tüpraş Saves Millions of Dollars Annually with Automated Control Loop Performance Monitoring

"MATLAB saved us a significant amount of time and expense by enabling us to develop our own software in-house. It also enabled us to save millions of dollars in costs that would have resulted from poor controller performance."

— Mehmet Yagci, Tüpraş



Controller health monitoring system dashboard.

### Challenge

Automate the monitoring and maintenance of almost 6000 control loops across four refineries.

### Solution

Use MATLAB to develop and test performance assessment and analysis algorithms that incorporate signal processing, spectral analysis, pattern recognition, and autoregressive models.

### Results

- Up to \$20 million saved annually
- 250 engineer-days of manual effort eliminated
- Cost-saving solution developed in-house

User Stories  User Stories - Q

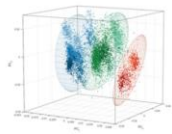
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## Auckland University of Technology and University of Auckland Researchers Analyze Dairy Processing Data with Machine Learning

"It's great to sit down with our industry partners and watch their jaws drop when they see how productive we are with MATLAB and how quickly we can analyze and plot data. Our results have enabled them to confirm hypotheses for which they lacked evidence, and have sparked new ideas for process improvement."

— David Wilson, Industrial Information and Control Centre



A 3D plot of PCA analysis of plant process variables across three powder processing plants and six years of data. The analysis shows that each plant exists in a completely separate operating space, despite producing the products with the same specifications.

### Challenge

Ensure the consistent production of high-quality milk powder in New Zealand's milk processing plants.

### Solution

Use MATLAB to preprocess and align data from multiple plants, analyze and visualize the data, and develop machine learning models capable of predicting the powder's functional properties.

### Results

- Key process flaws identified and corrected
- Multiple machine learning classifiers evaluated in hours
- Large datasets easily handled, manual processes automated

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### Wine Classification with Neural Net Pattern Recognition App

Identify the winery that particular wines came from based on **chemical** attributes of the wine.

Date: 3 Jan 2012



### Big Data and Predictive Analytics at Shell

Shell detects events and abnormalities in **chemical** plants using predictive analytics with MATLAB .

Date: 20 Oct 2014



### Big Data and Predictive Analytics at Shell - in depth

In depth: Shell detects events and abnormalities in **chemical** plants using predictive analytics with MATLAB

Date: 20 Oct 2014

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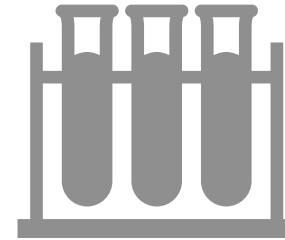
# Integrating Computational Thinking to Chemical Engineering Curriculum



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## FREE COURSES (2-3 hours)

- MATLAB Onramp
- Simulink Onramp
- Stateflow Onramp
- Machine Learning Onramp
- Deep Learning Onramp
- Image Processing Onramp
- Signal Processing Onramp
- Control Design Onramp with Simulink

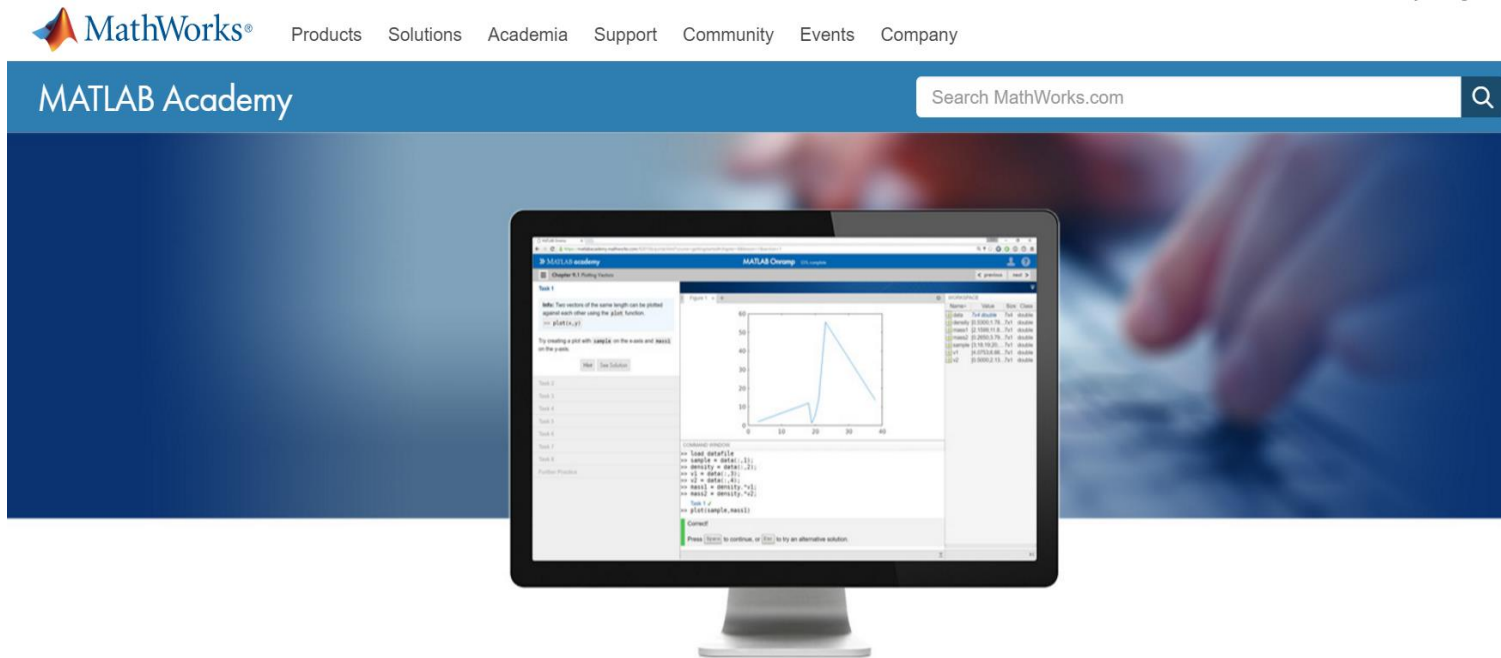
## FOCUSED COURSES

### FOUNDATIONAL COURSES (17-21 hours)

- MATLAB Fundamentals
- MATLAB Programming Techniques
- MATLAB for Financial Applications
- MATLAB for Data Processing and Visualization
- Machine Learning with MATLAB
- Deep Learning with MATLAB

### COMPUTATIONAL MATH COURSES (2-3 hours)

- Introduction to Linear Algebra
- Solving Ordinary Differential Equations
- Introduction to Statistical Methods
- Solving Non-Linear Equations
- Introduction to Symbolic Math



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# MATLAB Apps

# App Designer

**MACHINE LEARNING AND DEEP LEARNING**

- Classification Learner
- Deep Network Designer
- Neural Net Clustering
- Neural Net Fitting
- Neural Net Pattern Reco...
- Neural Net Time Series
- Regression Learner

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- Color Thresholder
- DICOM Browser
- Image Acquisition
- Image Batch Processor
- Image Browser
- Image Labeler
- Registration Estimator
- Stereo Camera Calibrator
- Video Labeler
- Video Viewer
- Volume Viewer

**MATH, STATISTICS AND OPTIMIZATION**

- Curve Fitting
- Distribution Fitter
- Optimization
- PDE Modeler

**CONTROL SYSTEM DESIGN AND ANALYSIS**

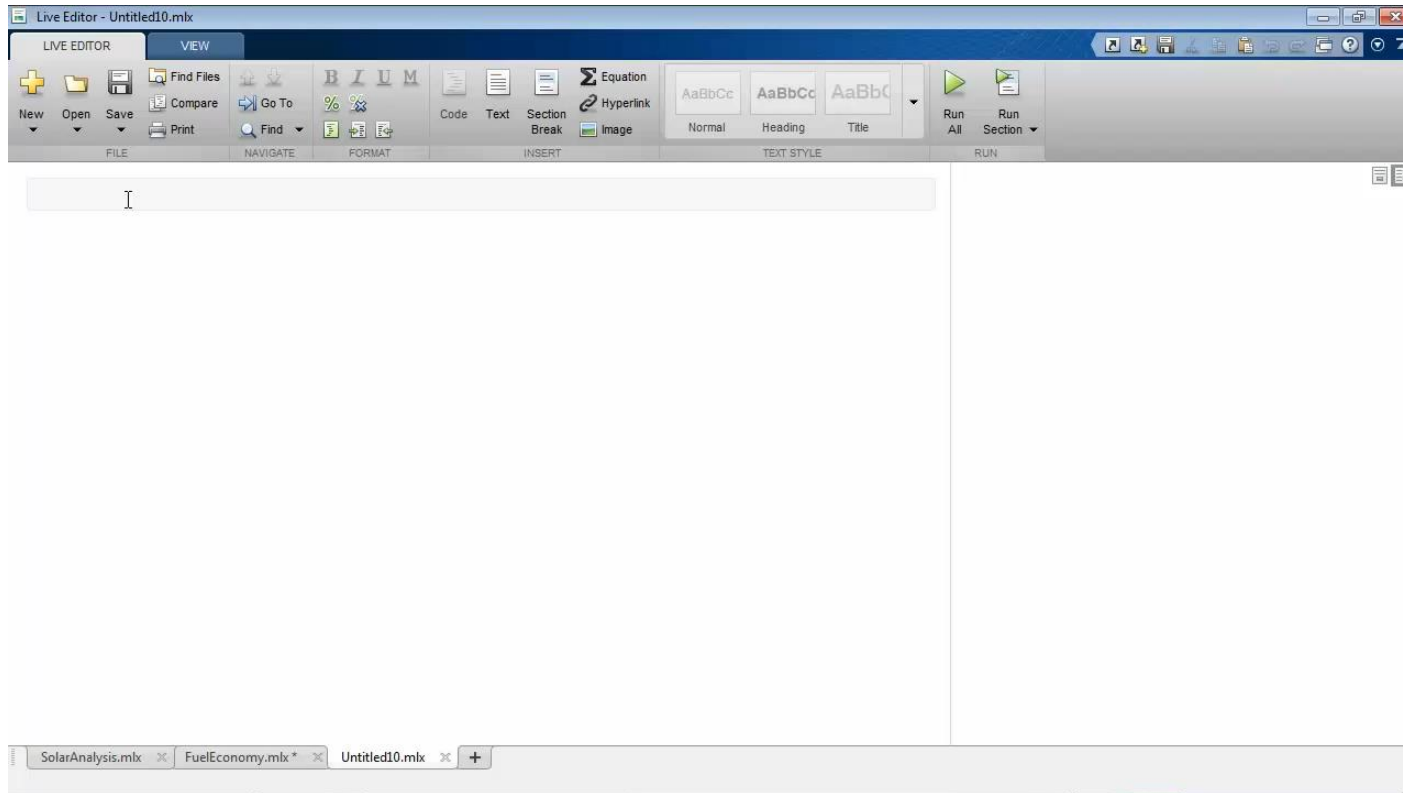
- Control System Designer
- Control System Tuner
- Diagnostic Feature Desi...
- Fuzzy Logic Designer
- Linear System Analyzer
- Model Reducer
- MPC Designer

The screenshot displays the MATLAB App Designer environment. The main canvas shows a mortgage app layout with the following components:

- Loan Amount:** A text input field containing the value 300000.
- Interest Rate %:** A numeric edit field containing the value 4, highlighted with a red circle 2.
- Loan Period (Years):** A text input field containing the value 30.
- Monthly Payment:** A text input field containing the value 0.00.
- Amortization Schedule:** A plot area with the title "Amortization Schedule" and a red circle 4. The y-axis is labeled "Principal and Interest" and the x-axis is labeled "Loan Period".

The interface includes a **COMPONENT LIBRARY** on the left with various UI elements like Buttons, Check Boxes, Drop Downs, Edit Fields, Labels, List Boxes, Radio Button Groups, Sliders, Spinners, State Buttons, and Text Areas. A red circle 1 highlights the "Check Box" component. On the right, the **COMPONENT BROWSER** shows the app's component tree, with "app.numInterestRate" selected and highlighted in blue. Below it, the **EDIT FIELD (NUMERIC) PROPERTIES** panel shows configuration options for the interest rate field, with a red circle 3 highlighting the "Value" property set to 4.

# Interactive programming with Live Editor



## Features

- Teach with interactive documents
- Accelerate exploratory programming
- Create an interactive narrative
- Publish consistent reports

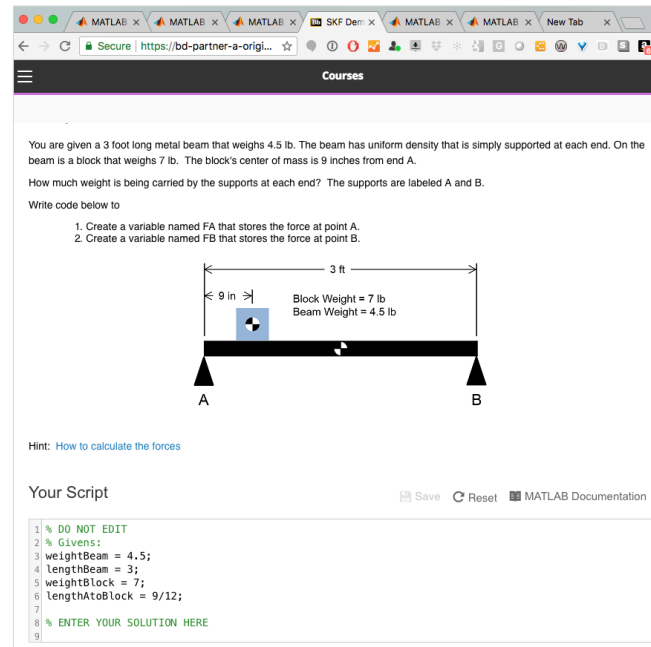
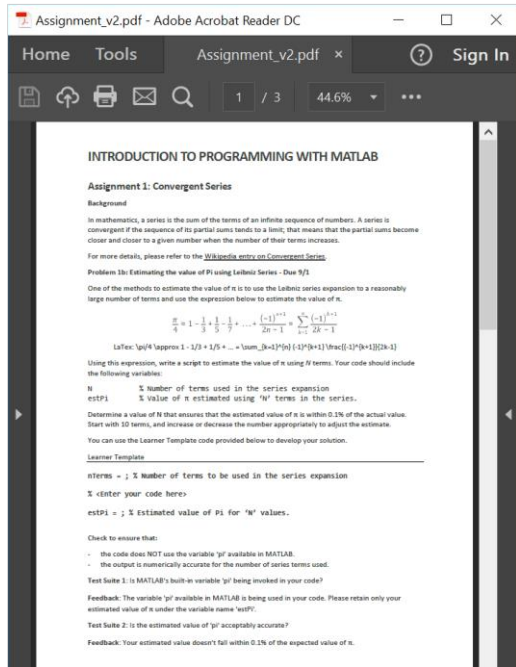
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# MATLAB Grader

Automatically grade MATLAB code in any learning environment.



“The approach enables students to **learn more quickly** from their mistakes on their own.”

– Dr. Bob Canfield, Virginia Tech

DIGITAL/PHYSICAL HANDOUTS

ONLINE AUTOGRADING ENVIRONMENT

<https://www.mathworks.com/products/matlab-grader.html>  
<http://grader.mathworks.com>

# MATLAB Grader Problem Collections

MATLAB Grader

---

Overview
System Requirements
What's New
Problem Collections

## Introduction to Programming:

Collection of 111 problems on introductory programming using MATLAB.

- Intended for use in Introduction to Programming courses and courses that require prerequisite knowledge of introductory programming concepts.
- Problems draw from a variety of applications including physics, engineering, and finance, but do not require prerequisite knowledge in these fields.
- Concepts covered: Introduction to variables and data types, Matrices & Operators, Input/Output, Flow Control and Loops, Functions, and Graphing.

### Prerequisites:

- Problems assume prerequisite mathematics knowledge up to and including pre-calculus.
- No prior computer programming experience is required.

## Numerical Methods:

Collection of 10 problems on concepts taught in courses on numerical methods.

- Intended for use in Numerical Methods and Analysis courses. The problems can also be used in courses that require corequisite knowledge of numerical methods.
- Concepts covered: modeling, computers and error analysis, equation solving, linear algebraic functions, curve fitting/approximation, numerical quadrature, numerical differentiation, and ordinary differential equations.

### Prerequisites:

- Problems assume prerequisite knowledge of calculus, linear algebra, and differential equations.
- Beginner-level programming experience is recommended, which can be achieved by taking MATLAB

## Add Problem

### Blank Problem

Create a script or function problem from scratch.

### Sample Problems From MathWorks ?

#### Getting Started with MATLAB Grader

13 problems

#### Introduction to Programming

Created By: Eric Davishahl  
111 problems

#### Digital Signal Processing

Created By: MathWorks  
10 problems

#### Numerical Methods

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10 problems

#### System Dynamics and Control

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#### Dynamics

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#### Symbolic Math Toolbox

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#### Calculus II

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#### Calculus I

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<https://www.mathworks.com/products/matlab-grader/assessment-content.html>

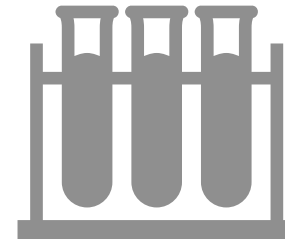
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# Reaction Kinetics

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- « Modeling
- « Build Models

Construct a Simple Model

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### Construct a Simple Model

This example shows you how to construct a simple model with two species (A and B) and a reaction. The reaction is  $A \rightarrow B$ , which follows mass action kinetics with the forward rate parameter  $k$ . Hence the rate of change is  $dA/dt = -k * A$ .

Create a SimBiology model named simpleModel.

```
m1 = sbiomodel('simpleModel');
```

Add a reaction that involves two species A and B, where A is converted to B.

```
r1 = addreaction(m1, 'A -> B');
```

SimBiology automatically add species A and B to the model.

```
m1.species
```

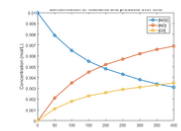
```
ans =
SimBiology Species Array

Index:  Compartment:  Name:  Value:  Units:
1       unnamed     A     0       0
2       unnamed     B     0       0
```

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Enter Cody Contest 2020. Win prizes!

Solve coding problems. Improve MATLAB skills. Have fun. See details and register.



## Chemical Kinetics with MATLAB

version 1.0.0.0 (187 KB) by Balaji **STAFF**  
This interactive MATLAB document covers concepts relating to chemical kinetics and reaction rates.

Overview Examples

This interactive MATLAB document covers concepts relating to chemical kinetics and reaction rates. This module covers concepts that are typically a part of courses on General Chemistry. Specifically, it would address the following questions:

- How are chemical reactions represented mathematically using differential equations?
- How can I use MATLAB to compute symbolic solutions to these representations?
- How can I use MATLAB to compute numerical solutions to these representations?
- How can I use MATLAB to import and evaluate experimental data to estimate reaction parameters?
- How can I use MATLAB to document and publish my solutions and conclusions?

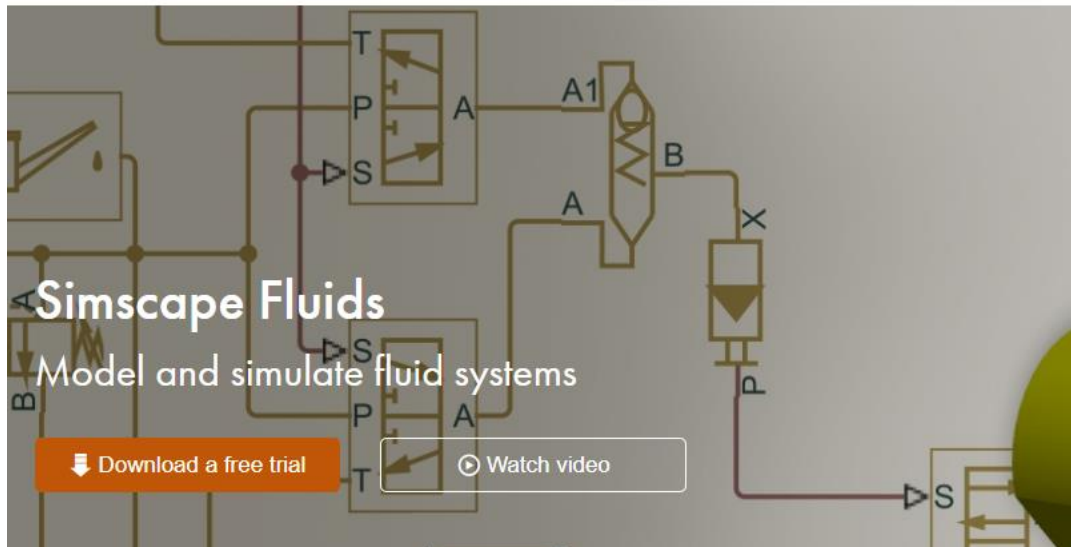
- <https://www.mathworks.com/matlabcentral/fileexchange/63104-chemical-kinetics-with-matlab>
- <https://www.mathworks.com/academia/courseware/teaching-chemistry-with-matlab.html>
- <https://www.mathworks.com/help/simbio/gs/construct-a-simple-model.html>
- <https://www.mathworks.com/products/simbiology.html>

# Fluid Dynamics

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### Hydraulic Resistive Tube

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Library

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## Hydraulic Resistive Tube

Hydraulic pipeline which accounts for friction losses only

### Library

Hydraulic Elements



### Description

The Hydraulic Resistive Tube block models hydraulic pipelines with circular and noncircular cross-sections. Fluid inertia is not considered in the model, meaning that features such as transient flow are not modeled.

The end effects are also not considered, assuming that the flow is fully developed along the total length of all the resistances is added to the pipe geometrical length.

Pressure loss due to friction is computed with the Darcy equation, in which losses are determined with the friction factor during transition from laminar to turbulent regimes is determined with the

$$p = f \frac{(L + L_{eq})}{D_H} \frac{\rho}{2A^2} q \cdot |q|$$

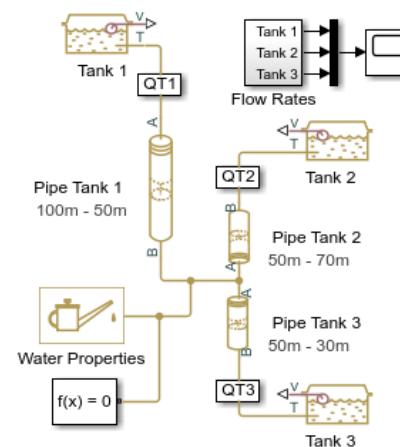
$$\begin{cases} K_s / Re & \text{for } Re \leq Re_L \\ f_L + \frac{f_T - f_L}{Re_T - Re_L} (Re - Re_L) & \text{for } Re_L < Re < Re_T \end{cases}$$

## Three Constant Head Tanks

This example shows a classical problem of fluid transportation: to determine flow rates in a common node located at 50 meters with respect to a reference point.

The pipelines are simulated with the Segmented Pipe LP block, which accounts for friction losses.

### Model



### Three Constant Head Tanks

1. Plot flow rate and volume in tanks (see code)
2. Explore simulation results using sscxplorer
3. Learn more about this example

# Heat Transfer



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## Partial Differential Equation Toolbox

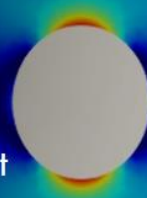
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### Partial Differential Equation Toolbox

Solve partial differential equations using finite element analysis

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### Category

- Get Started with Partial Differential Equation Toolbox
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- Structural Mechanics
- Heat Transfer**
- Electromagnetics
- General PDEs

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### Heat Transfer

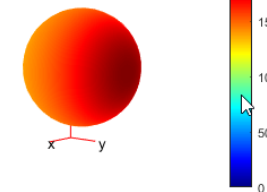
Solve conduction-dominant heat transfer problems with convection and radiation occurring at boundaries

Address challenges with thermal management by analyzing the temperature distributions of components based on material properties, external heat sources, and boundary conditions.

A typical programmatic workflow for solving a heat transfer problem includes the following steps:

- Create a special thermal model container for a steady-state or transient thermal model.
- Define 2-D or 3-D geometry and mesh it.
- Assign thermal properties of the material, such as thermal conductivity  $k$ , specific heat  $c$ , and mass density  $\rho$ .
- Specify internal heat sources  $Q$  within the geometry.
- Specify temperatures on the boundaries or heat fluxes through the boundaries. For convective heat flux through the boundary  $h(T - T_\infty)$ , the ambient temperature  $T_\infty$ , emissivity  $\epsilon$ , and Stefan-Boltzmann constant  $\sigma$ .
- Set an initial temperature or initial guess.
- Solve and plot results, such as the resulting temperatures, temperature gradients, heat fluxes, and heat rates.

Temperature at Time 50



<https://www.mathworks.com/help/pde/heat-transfer-and-diffusion-equations.html>  
<https://www.mathworks.com/products/pde.html>

- « Documentation Home
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- « Control System Design and Tuning
- « Classical Control Design

**Design Internal Model Controller for Chemical Reactor Plant**

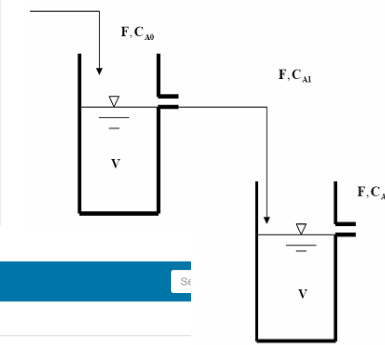
- ON THIS PAGE
- Plant Model
  - Linear Plant Models
  - Define IMC Structure in Control System Designer
  - Tune Compensator
  - Control Performance with Model Mismatch
  - See Also
  - Related Topics

**Design Internal Model Controller for Chemical Reactor Plant**

This example shows how to design a compensator in an IMC structure for series chemical reactors, using Control System Designer. Model-based process control applications.

**Plant Model**

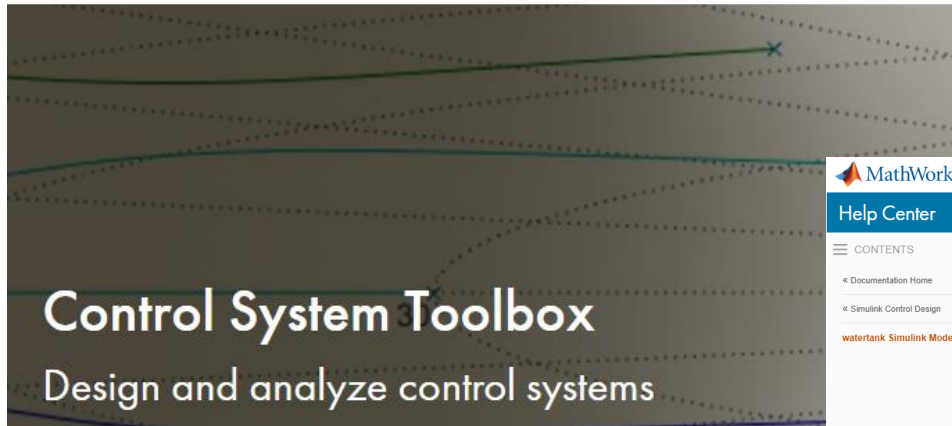
The plant for this example is a chemical reactor system, comprised of two well-mixed tanks.



# Process Control



## Control System Toolbox



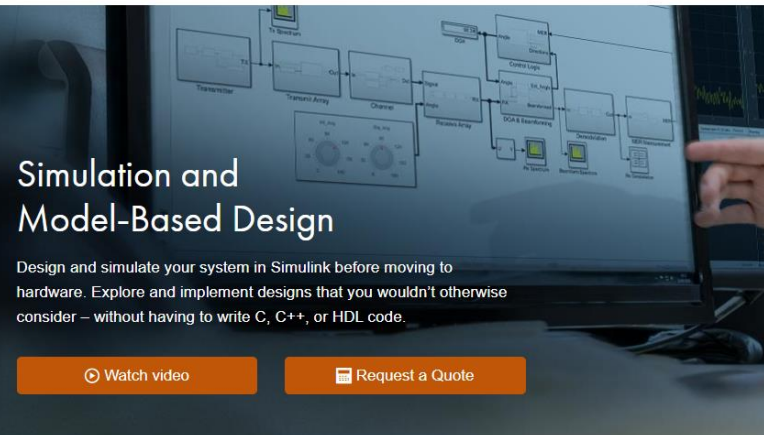
## Control System Toolbox

Design and analyze control systems



## Simulink

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## Simulation and Model-Based Design

Design and simulate your system in Simulink before moving to hardware. Explore and implement designs that you wouldn't otherwise consider – without having to write C, C++, or HDL code.

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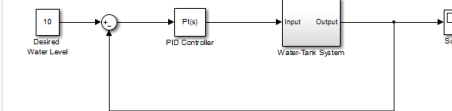


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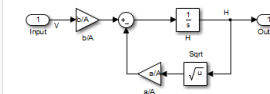
**watertank Simulink Model**

**watertank Simulink Model**

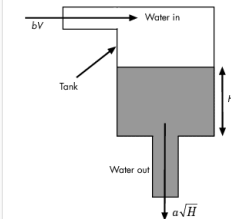
The Simulink® model watertank includes the nonlinear Water-Tank System plant and a PI controller in a single-loop feedback system.



The Water-Tank System is shown in the following figure.



Water enters the tank from the top at a rate proportional to the voltage,  $V$ , applied to the pump. The water leaves through an opening in the tank base. flow rate results in a nonlinear plant.



<https://www.mathworks.com/products/simulink.html>

<https://www.mathworks.com/products/control.html>

<https://www.mathworks.com/help/slcontrol/gs/watertank-simulink-model.html>

<https://www.mathworks.com/help/control/ug/internal-model-control-design-for-a-chemical-reactor-plant.html>

# Process Design

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  - Linearize Plant Using Aspen Plus Control Design Interface
  - Create Scaled and Reduced LTI State-Space Model
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  - Design Model Predictive Controller
  - Cosimulate MPC Controller and Nonlinear Plant
  - See Also

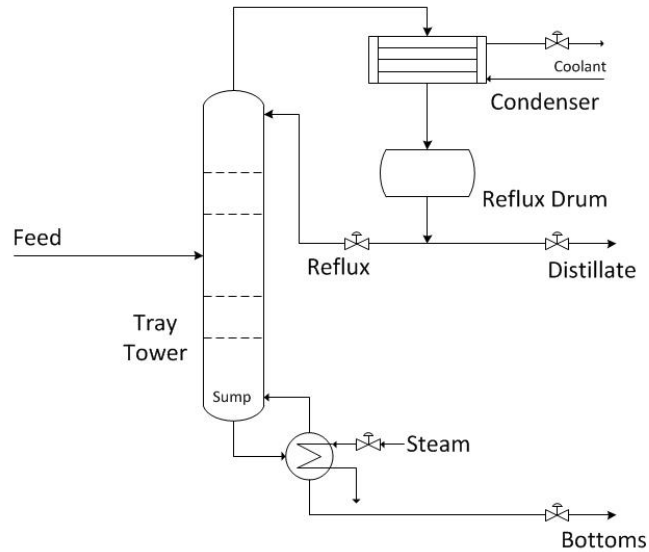
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### Design and Cosimulate Control of High-Fidelity Distillation Tower with Aspen Plus Dynamics

This example shows how to design a model predictive controller in MATLAB for a high-fidelity distillation tower model built in Aspen Plus Dynamics®. The controller performance is then verified through cosimulation and Aspen Plus Dynamics.

#### Distillation Tower

The distillation tower uses 29 ideal stages to separate a mixture of benzene, toluene, and xylenes (represented by p-xylene). The distillation process is continuous. The equipment includes a reboiler and a total condenser below:



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### Linking MATLAB to Process Simulators

Researchers and engineers have connected MATLAB® with process simulators for a variety of purposes—optimization, machine learning, controls, and several others. You can find a list of papers on the topic [here](#). Explore three ways MATLAB can connect to process simulators like Aspen Plus.

#### Option 1: Native Integration

- **Aspen Dynamics:** The Control Design Interface tool, included in Aspen Dynamics, enables you to extract a linear state space model from Aspen Dynamics. You can load this into MATLAB and use it with Control System Toolbox™ when designing a process control system.
- **UniSim:** Honeywell's UniSim Design Suite lets you design processes and perform process simulations. UniSim Design links to MATLAB, making it easier to leverage the strengths of both applications.

<https://www.mathworks.com/solutions/chemicals-and-petrochemicals/interconnectivity.html>

<https://www.mathworks.com/help/mpc/ug/design-and-cosimulate-control-of-high-fidelity-distillation-tower-with-aspen-plus-dynamics.html>



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Data preparation, design, simulation, and deployment for deep neural networks

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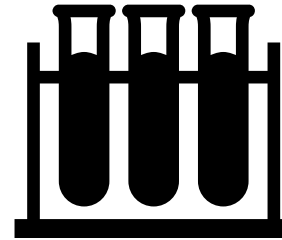
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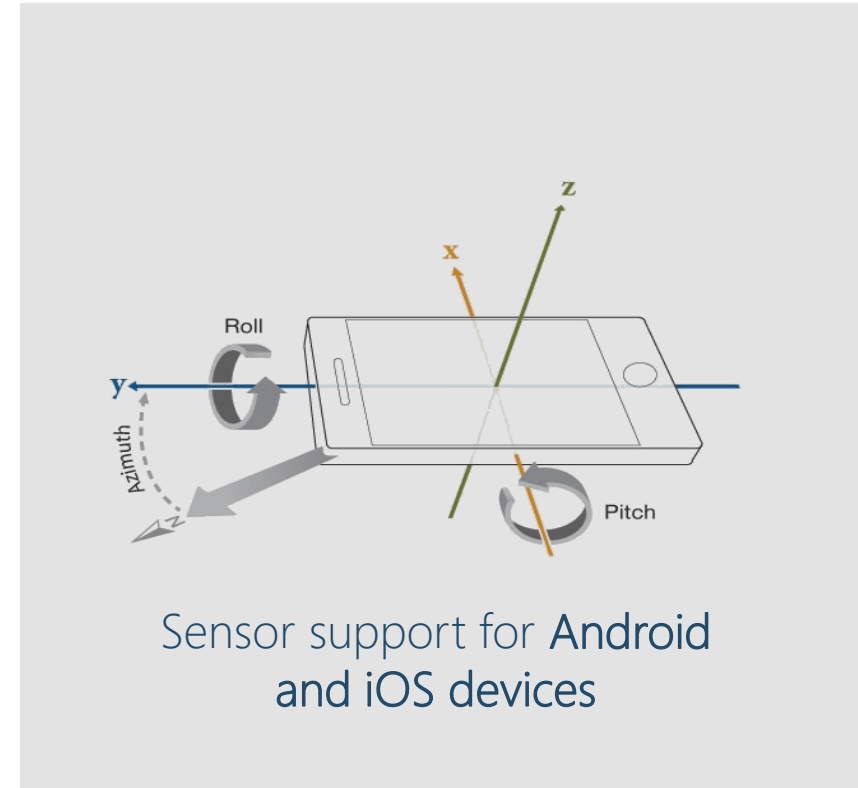
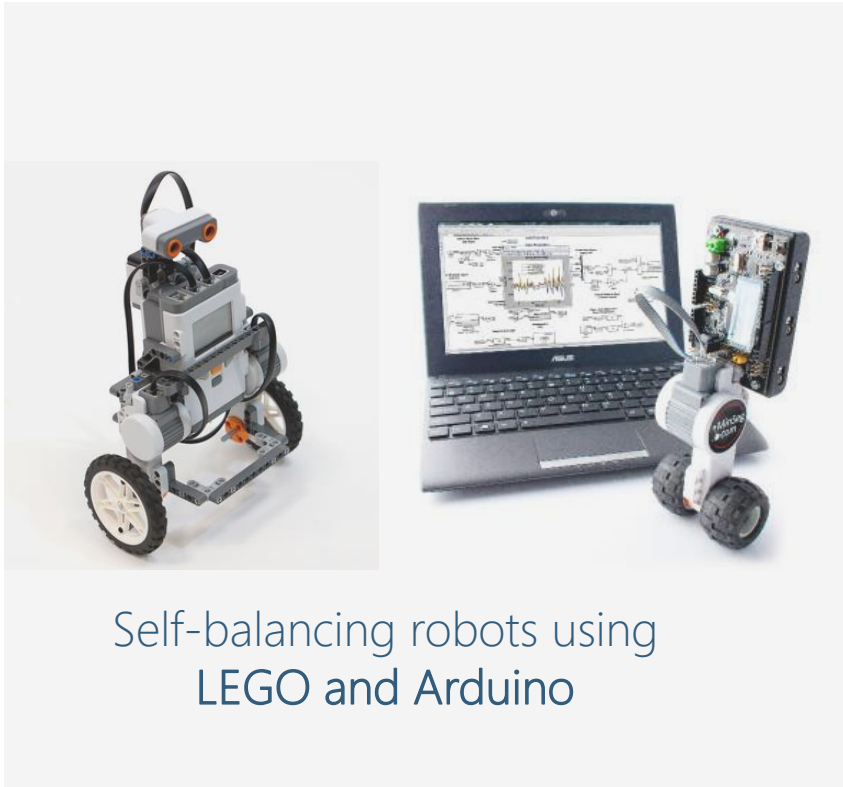


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# Project-based learning with low-cost hardware



<http://hardware.mathworks.com>  
<https://www.mathworks.com/products/matlab-mobile.html>

# ThingSpeak

IoT analytics platform



Send sensor data privately to the cloud.



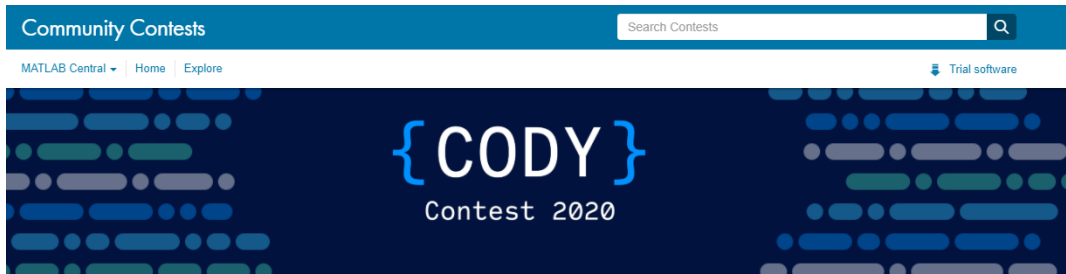
Analyze and visualize your data with MATLAB.



Trigger a reaction.

<https://thingspeak.com/>

# Student Competitions and Community Contests



Community Contests

Search Contests

MATLAB Central Home Explore

Trial software

## { CODY }

Contest 2020

### Solve and Rate Cody Problems. Win Prizes!

Solve MATLAB coding problems and rate their difficulty to win cool prizes. The more you complete, the greater your chances of winning. The contest runs from October 1 to December 31.

#### Two ways to win

- **Be a top scorer** - The top three Cody scorers during the contest win prizes.
- **Rate problem difficulty** - Each rating gets you an entry in our weekly prize raffle.

#### Contest Is Underway!

Play until December 31, 2020

59 06 11 26  
Days Hours Minutes Seconds

Register

Simply click Register and you're in!



<https://www.mathworks.com/academia/student-competitions.html>

<https://www.mathworks.com/matlabcentral/contests/cody-2020.html?q=&page=1>

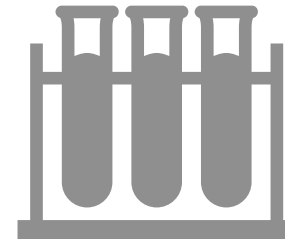
# Integrating Computational Thinking to Chemical Engineering Curriculum



Introduce



Reinforce



Apply



Getting Help

# Resources for Educators

Products Solutions Academia Support **Community** Events

Distance Learning Community

Search Distance Learning Community

MATLAB Central Home Explore Contribute My Activity

## Keep Teaching through Distance Learning

Posted by Loren Shure, March 23, 2020

As many universities are moving quickly to distance learning, it is vital for educators to think carefully about how to adapt their approach to still deliver key learning outcomes for students in an online setting.

» Read more...

## Discussions

Start a discussion

### Welcome to the Distance Learning Community

Latest activity by jiro on 30 Mar 2020 at 13:17

Tags: distance\_learning

### Tell us your story

Latest activity by jiro on 30 Mar 2020 at 13:05

Tags: distance\_learning



Welcome to the Distance Learning Community

Moderator:  
Jiro Deke

This is a world-wide community for educators who are teaching remotely or online using MathWorks tools. It houses resources, such as articles, code examples, and videos, as well as an area where community members can ask questions or hold discussions



Products Solutions Academia Support Community Events

## Academia

For Students For Educators For Researchers

## Teaching with MATLAB

Engage your students and scale your instruction with online learning tools from MathWorks

Launch the course

## Teach and Learn with MATLAB and Simulink

The tools used at more than 6500 universities worldwide.

## Help Center

chemical engineering

Get MATLAB

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AI, Data Science, and Statistics	2
Control Systems	7

### Resource

Documentation	19
Functions	3
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Examples	9
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### Source

MathWorks	9
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Documentation 19 Examples 9 Functions 3 Blocks 1 Apps 0 Videos 23 Answers 74 Bug Reports 0 File Exchange 89

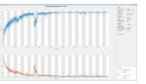
FILTERED BY Examples x Remove All

Results 1 - 9 of 9

### Chemical Process Fault Detection Using Deep Learning

This example shows how to use simulation data to train a neural network that can detect faults in a chemical process.

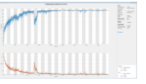
Documentation / Deep Learning Toolbox / Deep Learning with Time Series, Sequences, and Text



### Chemical Process Fault Detection Using Deep Learning

Use simulation data to train a neural network that can detect faults in a chemical process.

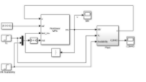
Documentation / Predictive Maintenance Toolbox / Detect and Predict Faults / Detect and Diagnose Faults



### Economic MPC Control of Ethylene Oxide Production

... "Economic model predictive control designs for input rate-of-change constraint handling and guaranteed economic performance." Computers and Chemical Engineering, Vol. 92, 2016, pp 18-36. Related Topics.

Documentation / Model Predictive Control Toolbox / Nonlinear MPC Design



### Gaussian Models

... science and engineering. For example, Gaussian peaks can describe line emission spectra and chemical concentration assays. Fit Gaussian Models Interactively Open the Curve Fitting app by entering cftool.

## Educators

Teach with MATLAB and Simulink Curriculum Resources Online Teaching Campus-Wide License

## Virtual Labs and Projects with MATLAB and Simulink

You can bring interactive labs to your online courses to enable student participation and active learning. Use MATLAB and Simulink to build engaging virtual labs by incorporating modeling and simulation.

See how *Mondragon University* used MATLAB and Simulink to model a laboratory turbine and other system components.

"Simulation with Simulink is a valuable stepping stone between theory and implementation that saves considerable time and money, particularly when a project involves a turbine or other costly system hardware."

- Carlos Garcia, *Mondragon University*

## Online Laboratories

Use MATLAB and Simulink to teach virtual or remote labs, or teach with hardware kits. As the format of lab activities varies between topics, MATLAB and Simulink contain tools to support your instruction by deploying apps, streaming data from your hardware, and utilizing mobile devices.

### Virtual

Simulates a process, test, apparatus, or other activity.

Examples:

- PID Tuner app
- Using simulation in dynamic systems labs at the University of Pittsburgh

### Remote

Campus-based hardware is accessed, viewed, or operated.

Examples:

- Analyzing vehicle traffic with ThingSpeak
- Robotarium remote-access robotics lab

### Hardware at Home

Students use kits or mobile devices, or collect data.

Examples:

- Arduino Engineering Kit
- Classifying images using deep learning with MATLAB Mobile

[www.mathworks.com/academia/educators.html](http://www.mathworks.com/academia/educators.html)  
[www.mathworks.com/matlabcentral/topics/distance-learning.html](http://www.mathworks.com/matlabcentral/topics/distance-learning.html)  
<https://www.mathworks.com/learn/teaching-with-matlab.html>

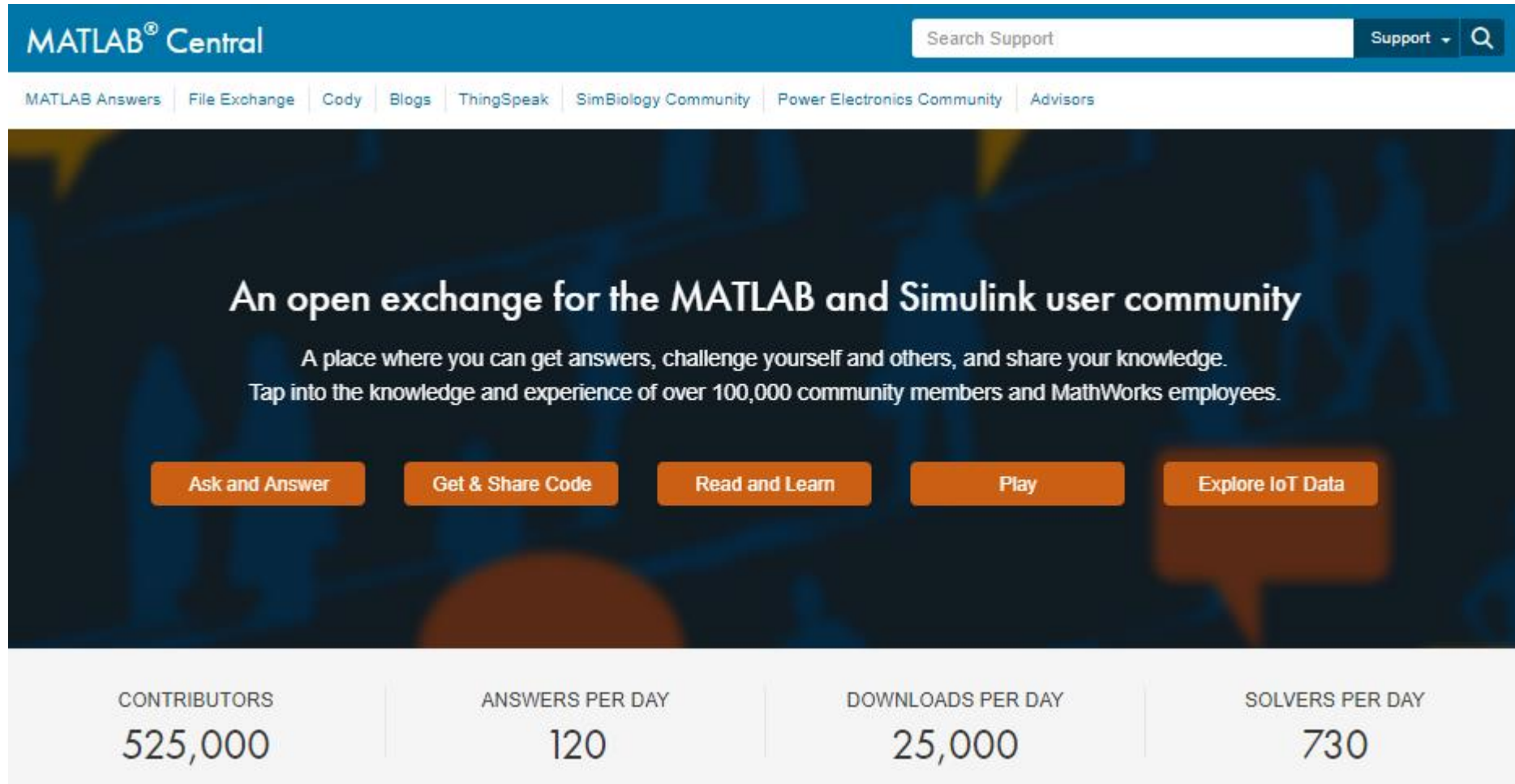
Access to MATLAB through your web browser

MATLAB integrated file sharing

Hands-on exercises with automated assessments and feedback

Ready-to-use resources to enhance your instruction

# MATLAB Central



The screenshot shows the MATLAB Central homepage. At the top, there is a blue header with the 'MATLAB® Central' logo on the left, a search bar labeled 'Search Support' in the center, and a 'Support' dropdown menu with a search icon on the right. Below the header is a navigation bar with links for 'MATLAB Answers', 'File Exchange', 'Cody', 'Blogs', 'ThingSpeak', 'SimBiology Community', 'Power Electronics Community', and 'Advisors'. The main content area features a dark blue background with a grid of people silhouettes. The central text reads: 'An open exchange for the MATLAB and Simulink user community'. Below this, it says: 'A place where you can get answers, challenge yourself and others, and share your knowledge. Tap into the knowledge and experience of over 100,000 community members and MathWorks employees.' There are five orange buttons: 'Ask and Answer', 'Get & Share Code', 'Read and Learn', 'Play', and 'Explore IoT Data'. At the bottom, a white bar displays four statistics: 'CONTRIBUTORS 525,000', 'ANSWERS PER DAY 120', 'DOWNLOADS PER DAY 25,000', and 'SOLVERS PER DAY 730'.



# MathWorks Customer Success Engineers

consult with faculty and researchers to support them with their STEM initiatives, including integrating computational or systems thinking into their curriculum.

