

Introductory Slides for COT3502 – Computer Model Formulation

What is a program?

“A sequence of instructions that tells a computer to do something”



Chocolate Cake

1. *Preheat oven to 350°F and...*
2. *Microwave 4 oz chopped chocolate for...*
3. ...

Check whether **x** is prime

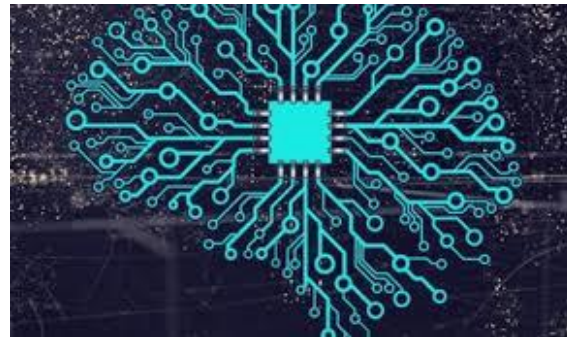
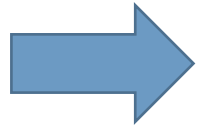
1. Check if **x** is divisible by 2
2. Check if **x** is divisible by 3
3. ...

What can programs make computers do?

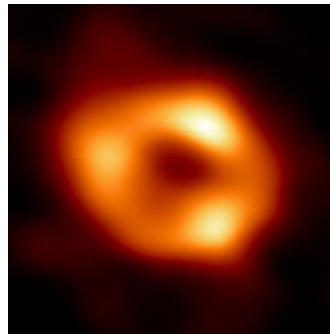
Anything! From simple calculations to the technological cutting edge!

AI / Machine Learning

Check
whether x
is prime



Astronomy Data Analysis



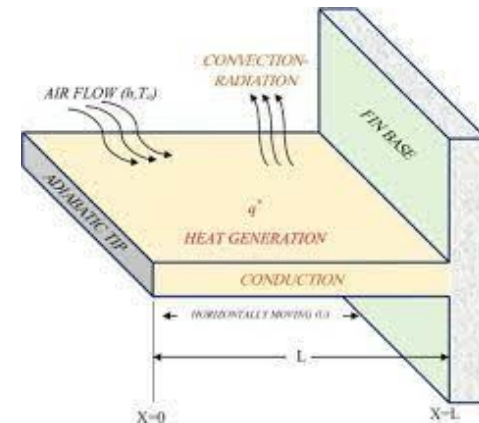
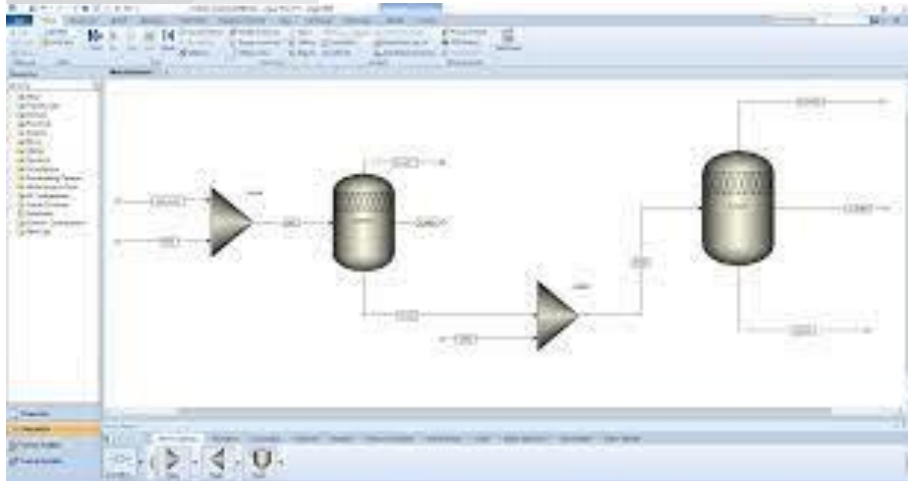
Interactive Software



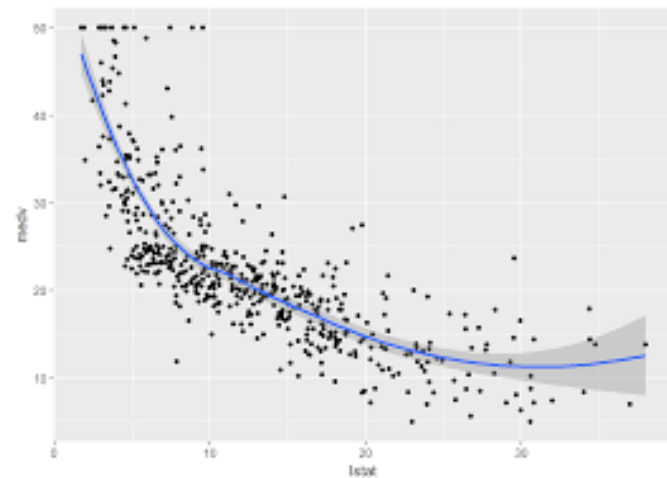
What do chemical engineers write programs to do?

Mass & Energy Transfer Modeling

Process Control / Automation



Regression & Optimization



What will you do in COT3502?

Do math you couldn't do by hand...

$$\int_0^5 x^2 \exp(-x) dx$$

$$\frac{dP}{dt} = -Pm + bHP$$

$$\frac{dH}{dt} = Hr - aHP$$

$$\begin{cases} P = P(t) & \text{Number of Predators} \\ H = H(t) & \text{Number of Prey} \end{cases}$$

$$\text{Xylene: } 0.07D_1 + 0.18B_1 + 0.15D_2 + 0.24B_2 = 0.15F$$

$$\text{Styrene: } 0.04D_1 + 0.24B_1 + 0.10D_2 + 0.65B_2 = 0.25F$$

$$\text{Toluene: } 0.54D_1 + 0.42B_1 + 0.54D_2 + 0.10B_2 = 0.40F$$

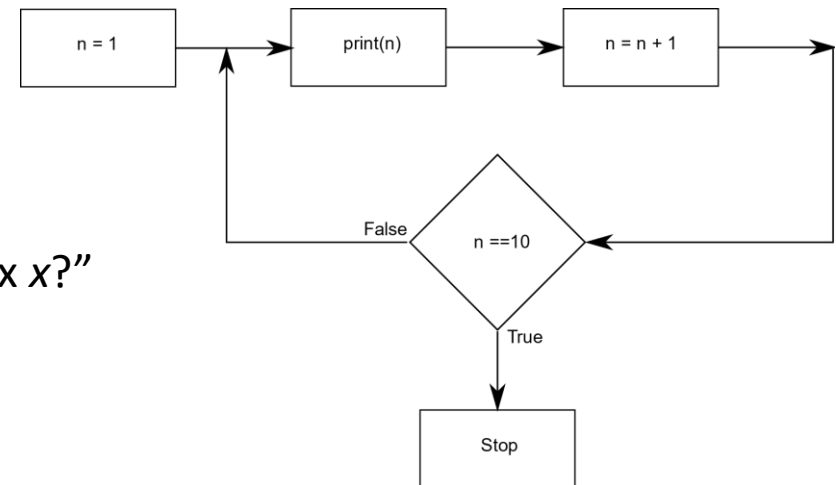
$$\text{Benzene: } 0.35D_1 + 0.16B_1 + 0.21D_2 + 0.01B_2 = 0.20F$$

Learn new ways to approach problems...

“How do I put a , b , and c together to do x ?”

“How do I modify a to do b instead?”

“If x isn't working, how do I devise a plan to fix x ?”



...and anything else you explore along the way

```
In [15]: import antigravity
```

```
In [15]: import this.py|
```

We will be using Python in COT3502 – Why Python?

Easy to learn!

Print in Python:

```
print("Hello World")
```

Print in C++:

```
std::cout << "Hello World" << std::endl;
```

Free!



**(You can download this on
any computer at any time)**

We will be using Python in COT3502 – Why Python?

Versatile!

Math, arrays
and matrices



Data /
spreadsheet
operations

Advanced
functions and
solvers



Plotting tools

...all in one language

Popular!

Over 50% of
chemical
engineers on
Github use
Python

