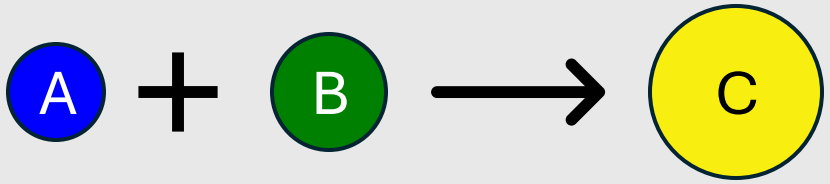
Simulating Continuous Systems

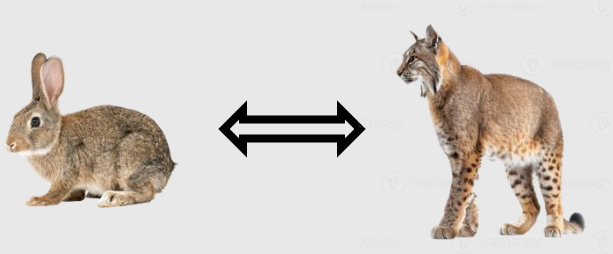
CMSC 326 Simulations

Simulating Continuous Systems

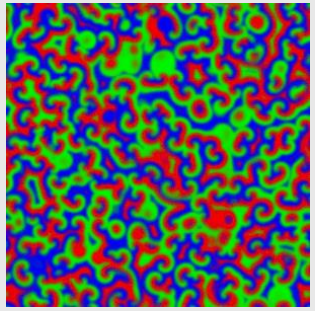
Simple chemical reaction



Rabbit–Lynx “reaction”

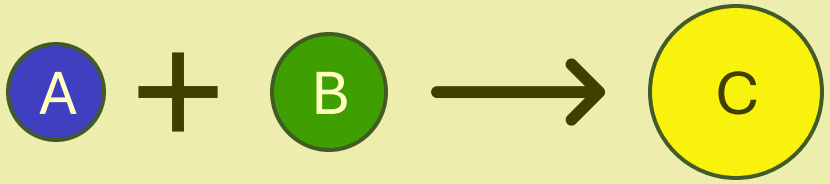


B-Z reaction

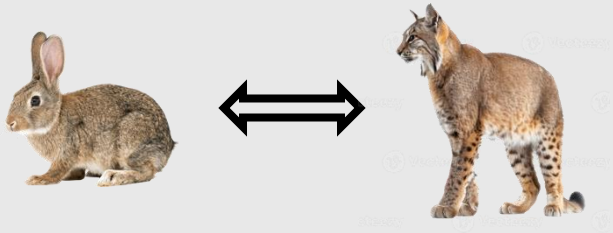


Simulating Continuous Systems

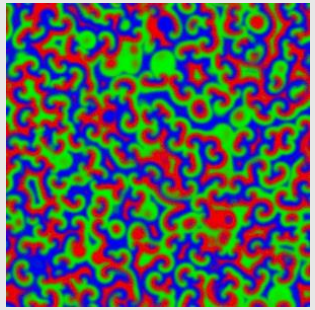
Simple chemical reaction



Rabbit–Lynx “reaction”



B-Z reaction

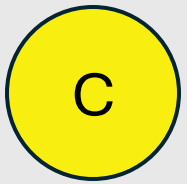


Simulation: Simple Chemical Reaction

Three molecules:

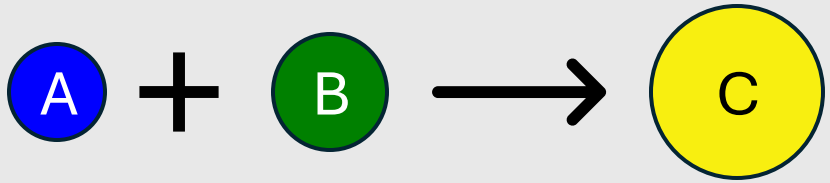
Substance 

Substance 

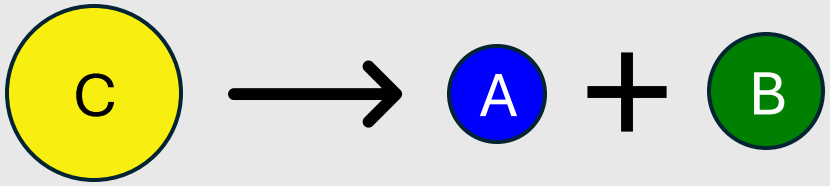
Substance 

Simulation: Simple Chemical Reaction

Reaction 1:
One molecule of **A** *reacts*
with one molecule of **B**
to produce one molecule of **C**

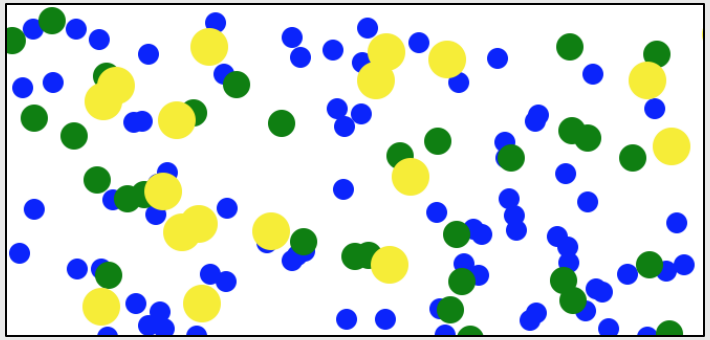


Reaction 2:
A molecule of **C** can *breakdown*
to produce one of each **A** and **B**

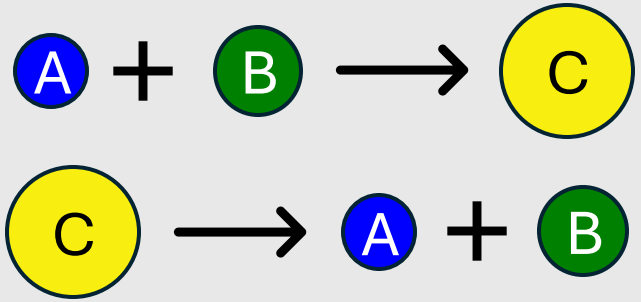


Simulate molecules in two dimensions

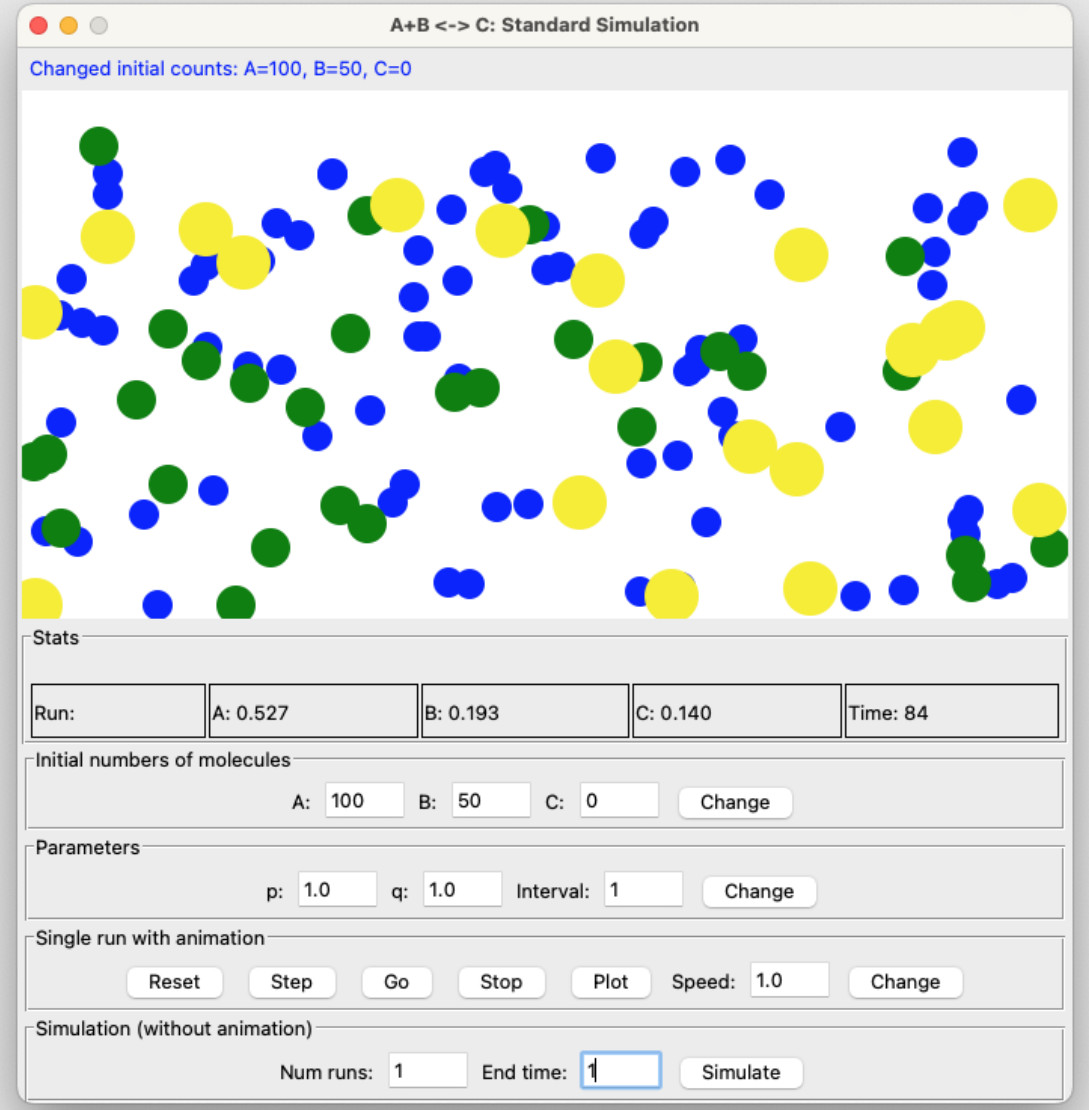
Molecules move about randomly in a solution or a gaseous state



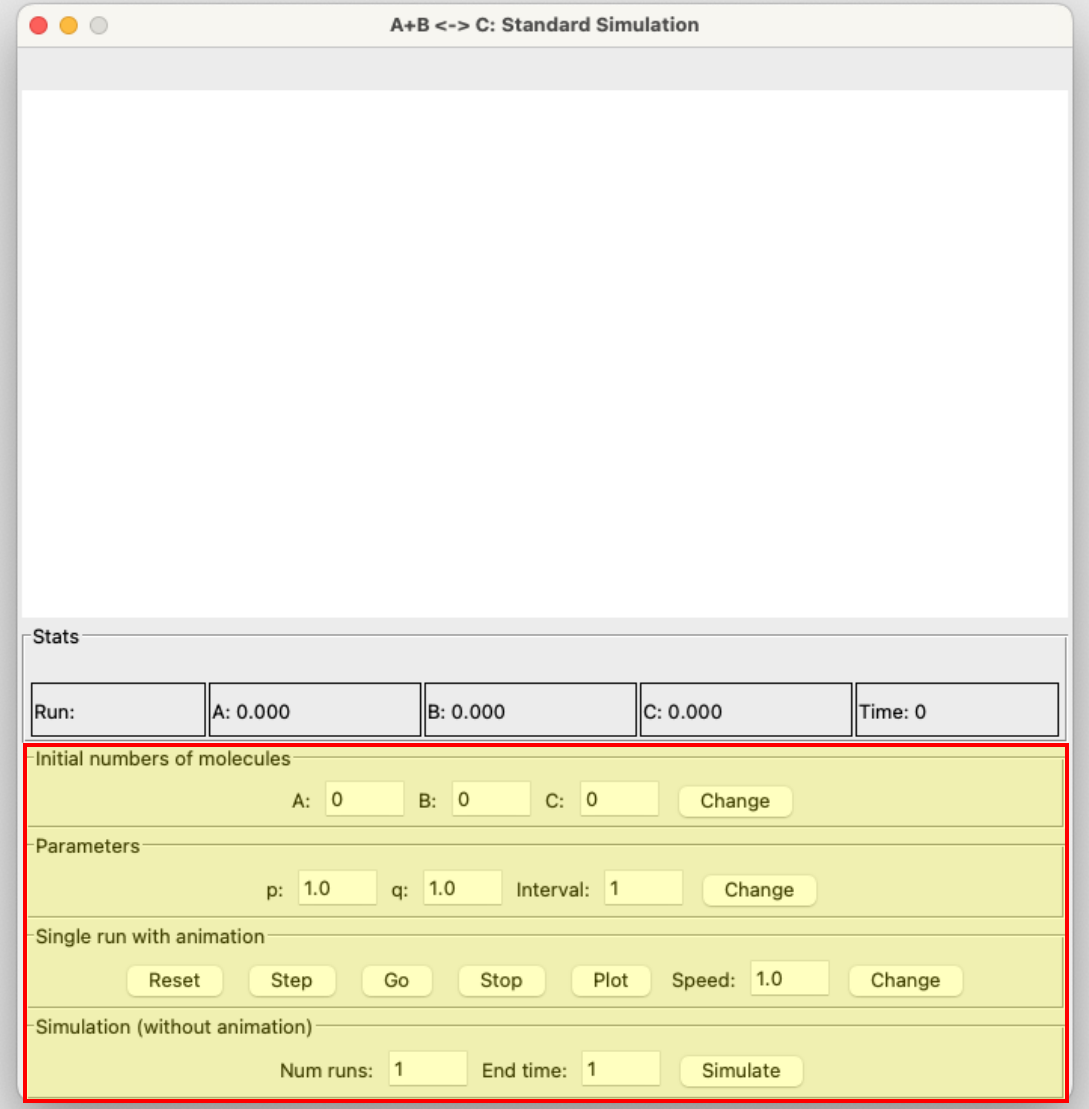
At any given instant, exactly one of the two reactions takes place



Demo: Simple Chemical Reaction



Setup the Simulation



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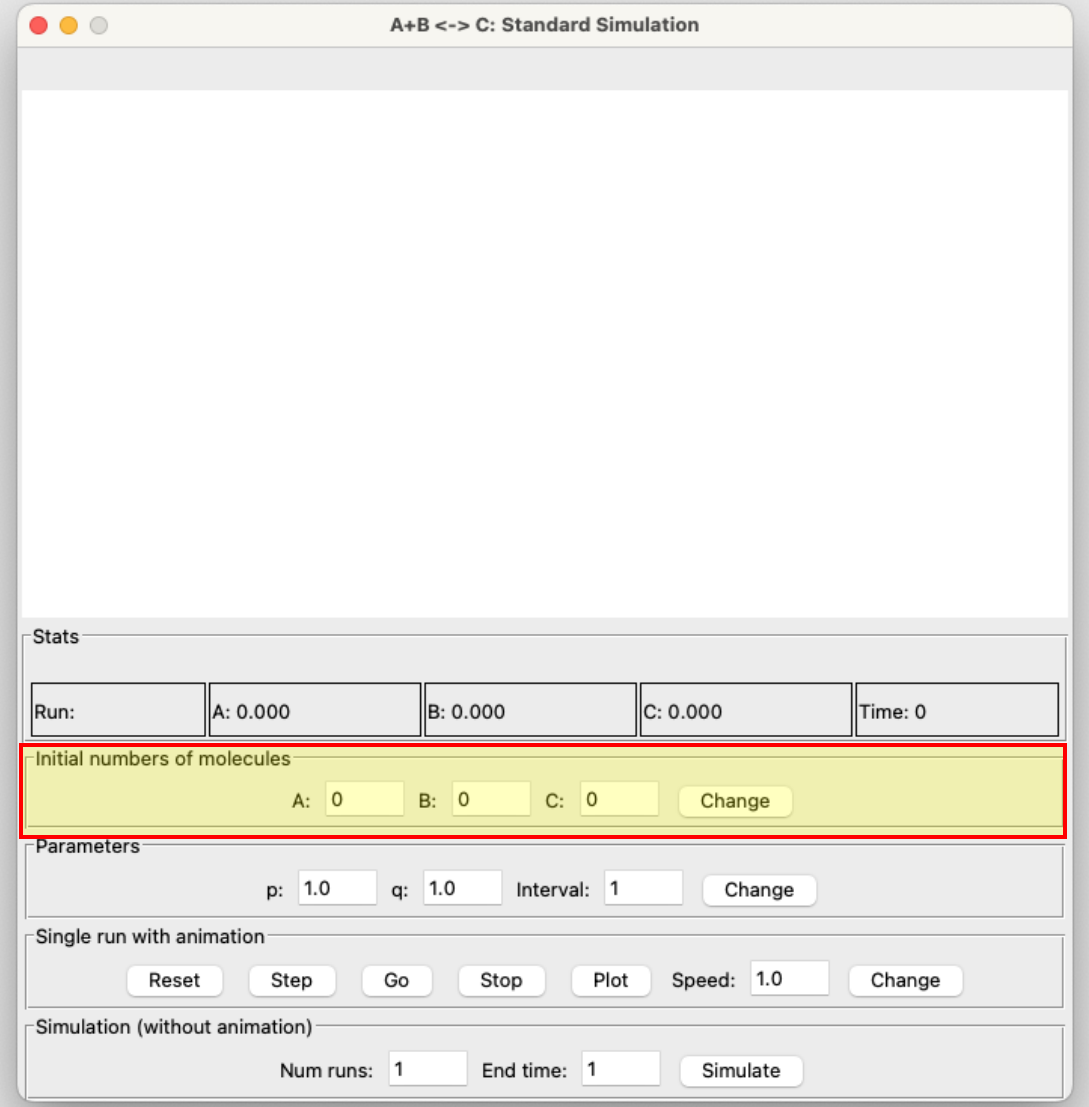

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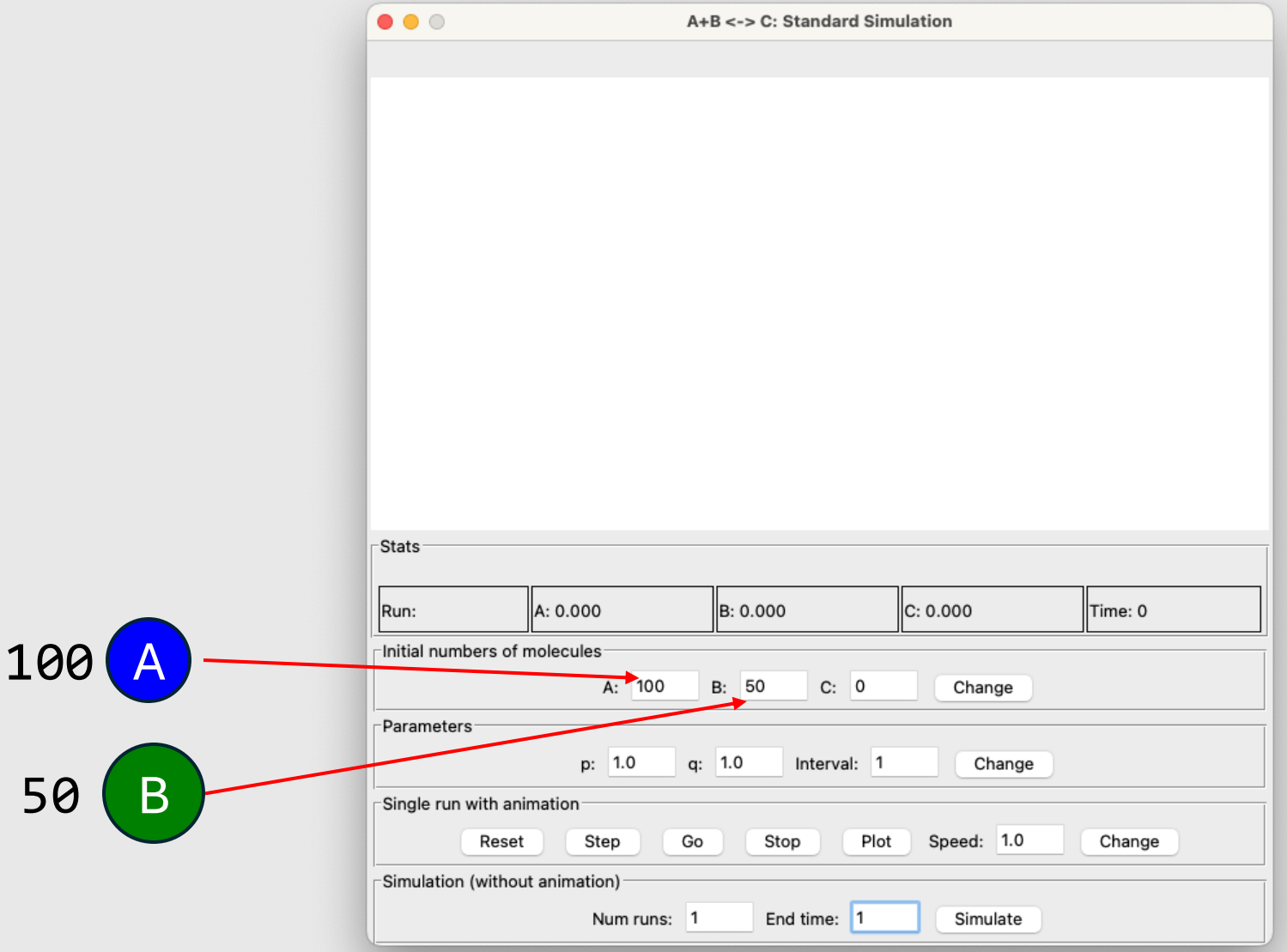

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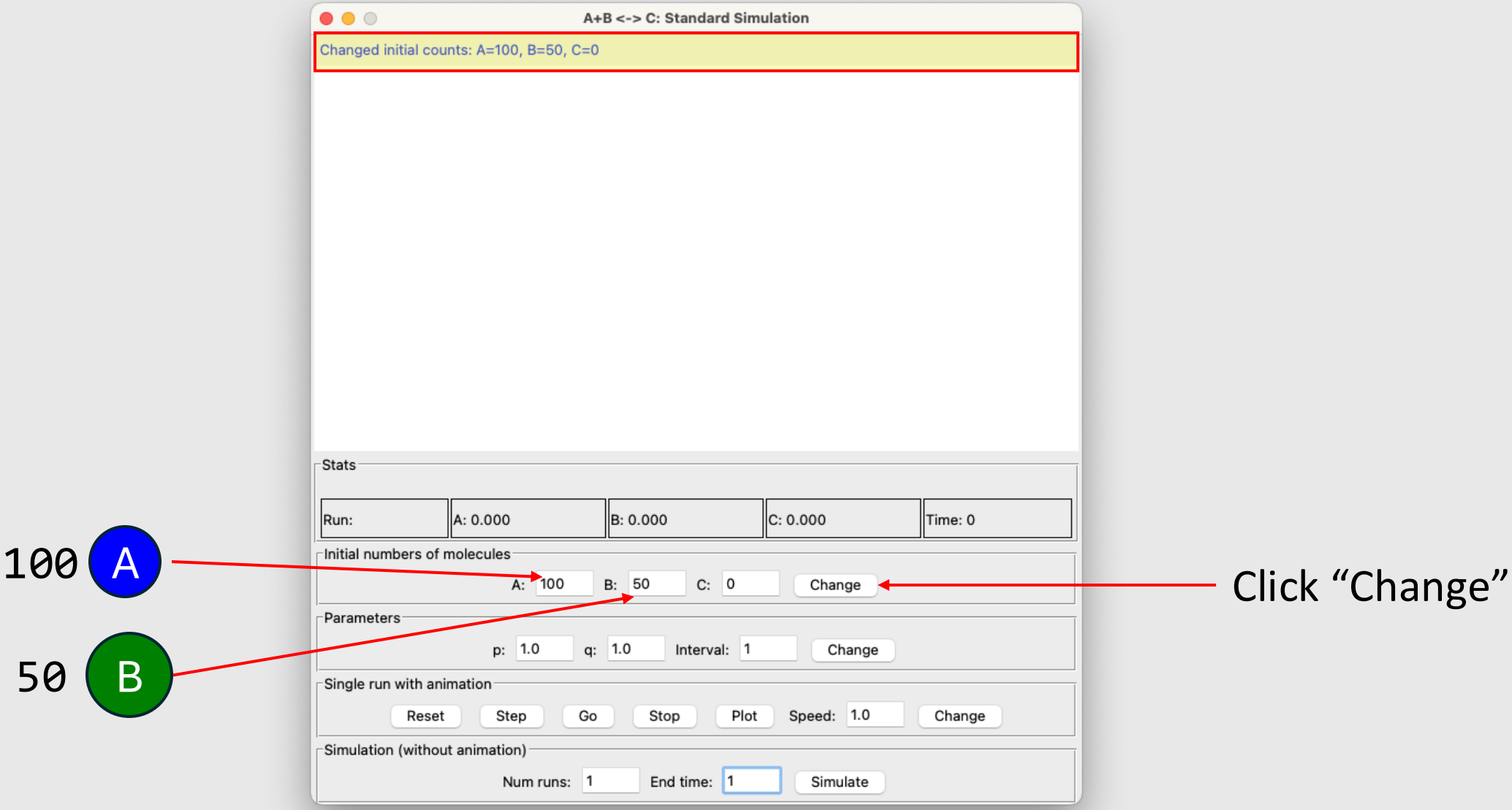

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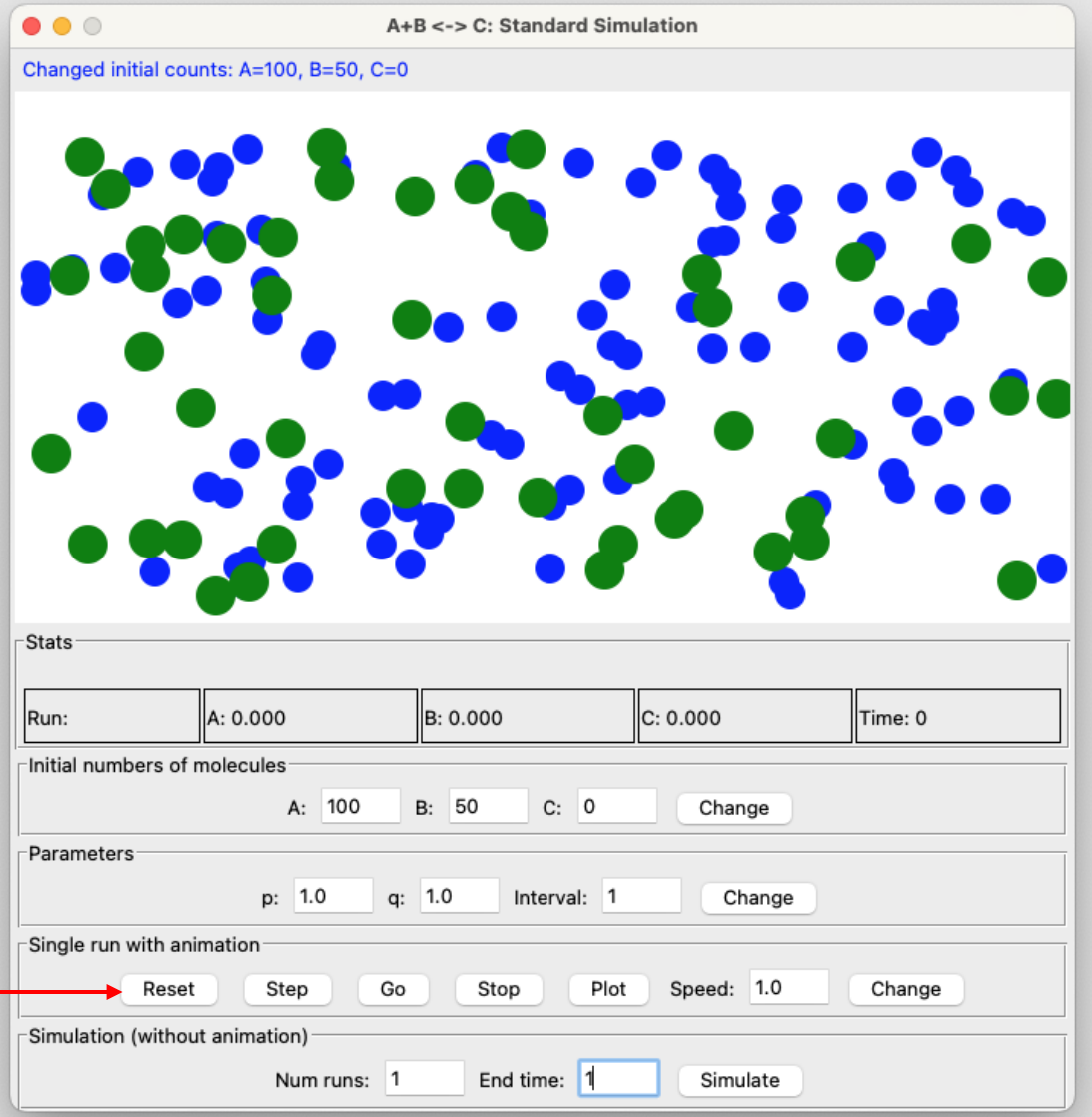
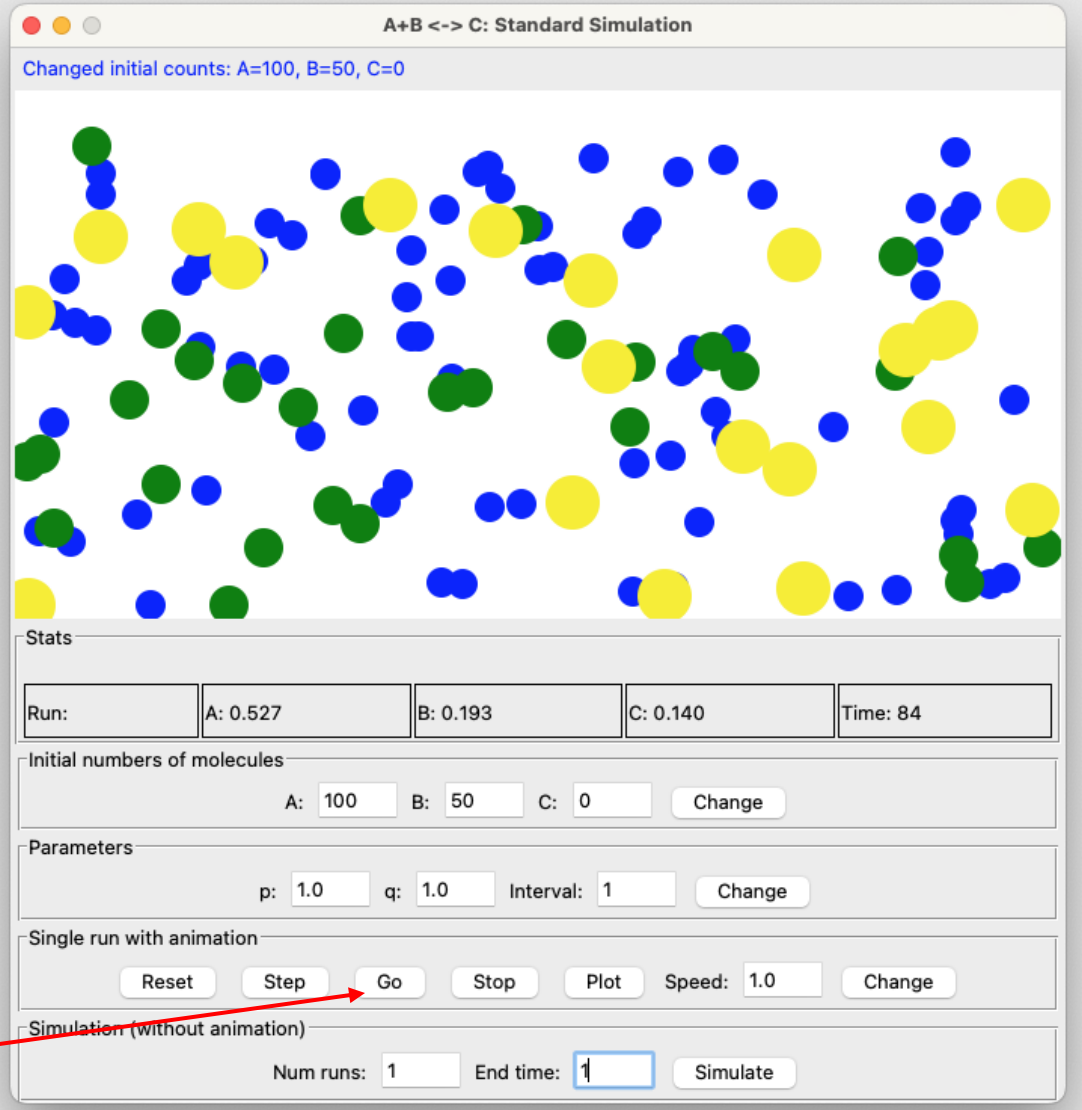


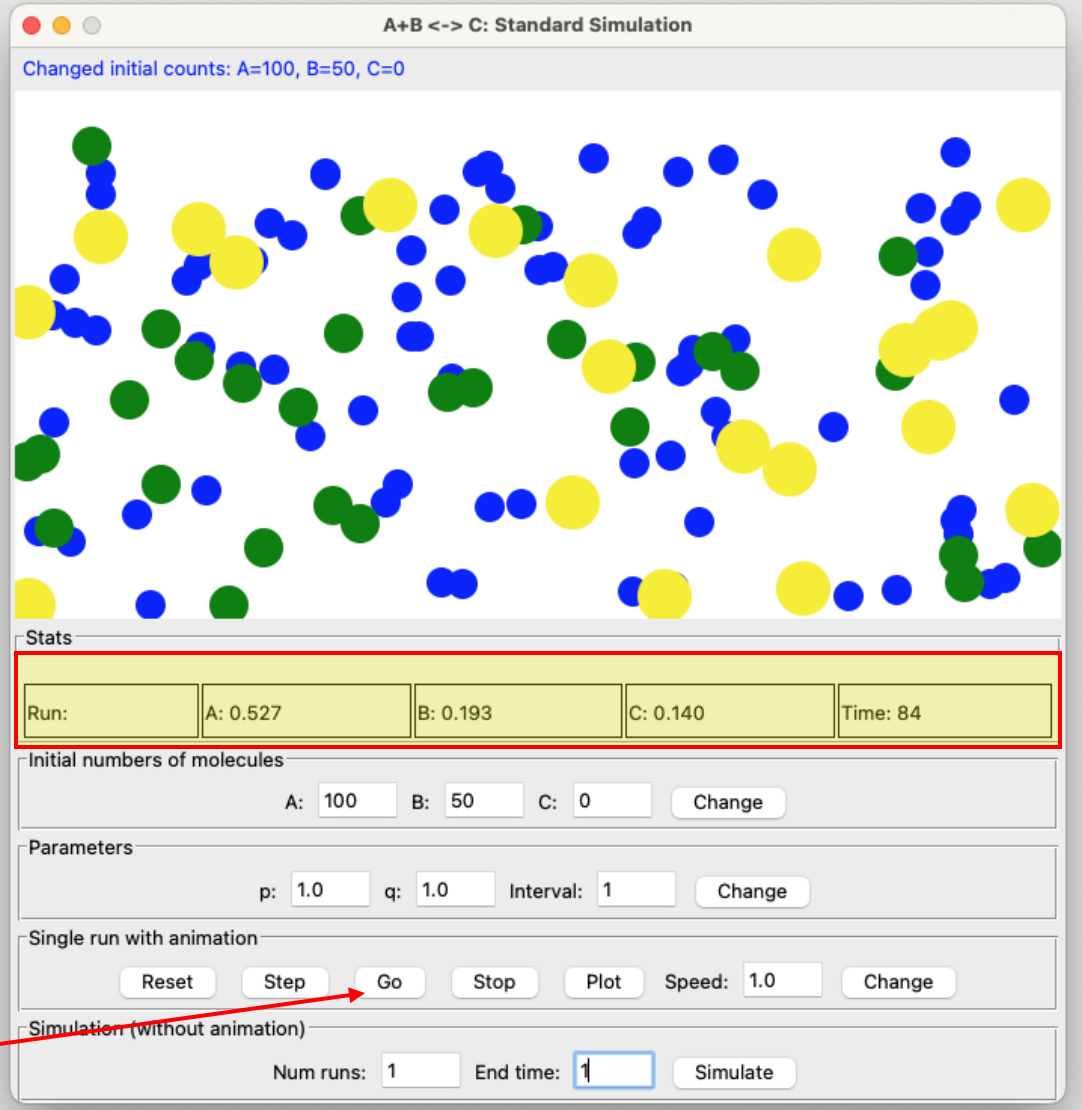
Click “Reset”

Run the Simulation



Click “Go”

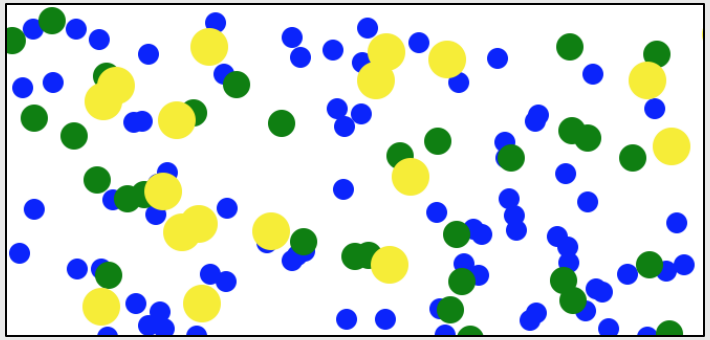
Run the Simulation



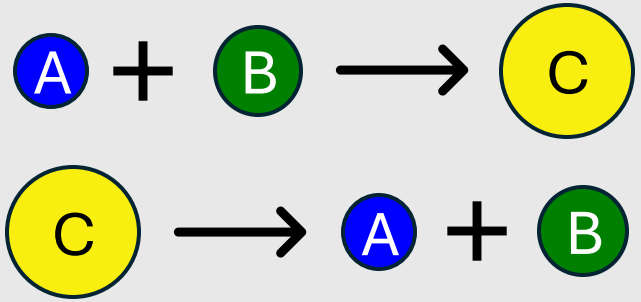
Click “Go”

Simulate molecules in two dimensions

Molecules move about randomly in a solution or a gaseous state



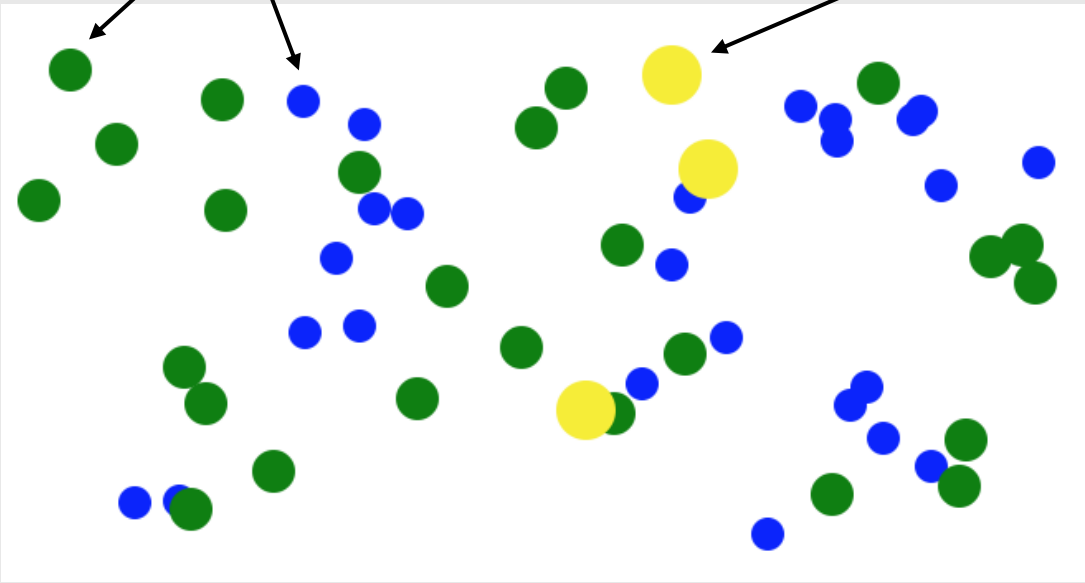
At any given instant, exactly one of the two reactions takes place



How do we decide which reaction?

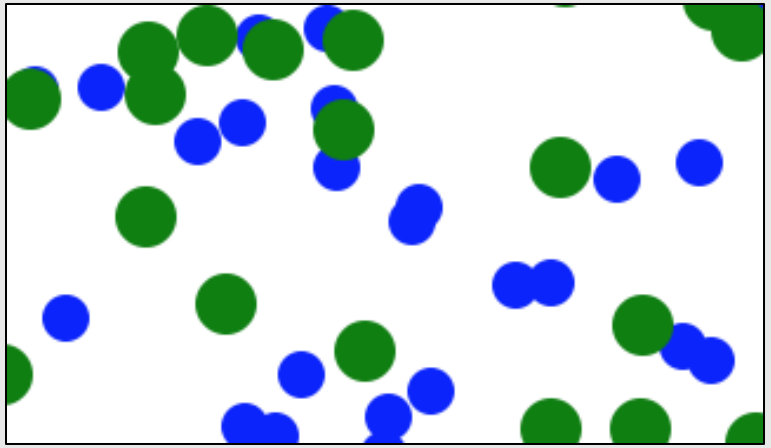
Many more **A** (green) and **B** (blue) molecules
A + B → C more likely

Fewer **C** (yellow) molecules
C → A + B less likely

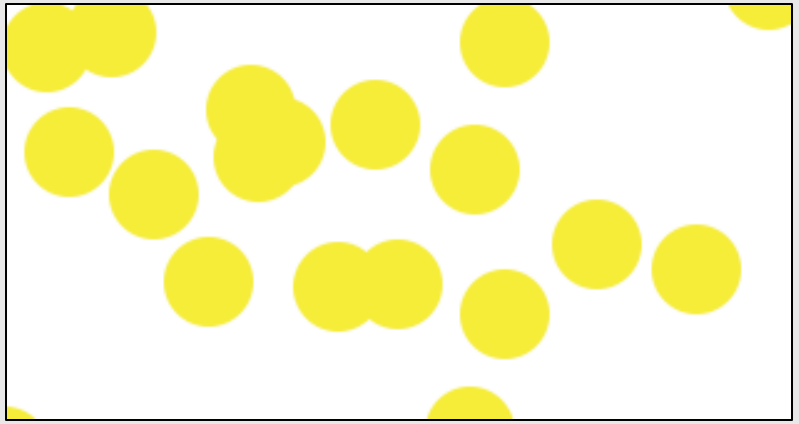


How do we decide which reaction?

The *likelihood* of the first reaction is **proportional** to the number of **A** molecules and the number of **B** molecules



The more of **C**, the *more likely* we'll have the second reaction



Reaction Model

N_A = number of A molecules

N_B = number of B molecules

N_C = number of C molecules

Reaction Model

E_A = concentration of A

E_B = concentration of B

E_C = concentration of C

Reaction Model

To get the concentration (mass per unit volume), we'll approximate the actual physical volume as:

$$V_{total} = N_A + N_B + 2N_C$$

Reaction Model

$$E_A = \frac{N_A}{V_{total}}$$

$$E_B = \frac{N_B}{V_{total}}$$

$$E_C = \frac{N_C}{V_{total}}$$

Reaction Model

Concentration of A

$$E_A = \frac{N_A}{V_{total}}$$

Concentration of B

$$E_B = \frac{N_B}{V_{total}}$$

Concentration of C

$$E_C = \frac{N_C}{V_{total}}$$

Reaction Model

R_1 = Probability that first reaction takes place

R_2 = Probability that second reaction takes place

Reaction Model

The chances of the first reaction taking place are *proportional* to both the number of **A** molecules (N_A)
and the number of **B** molecules (N_B)

Thus,

$$R_1 \propto N_A N_B$$

$$R_2 \propto N_C$$

Reaction Model

Because the numbers of molecules N_A, N_B, N_C are proportional to concentrations E_A, E_B, E_C, we can write:

$$R_1 \propto E_A E_B$$

$$R_2 \propto E_C$$

Reaction Model

The constant of proportionality may be different

To model this, we'll use constants $\mathbf{p}$ and $\mathbf{q}$

$$R_1 = pE_A E_B$$

$$R_2 = qE_C$$

Reaction Model

What happens at each step of the simulation is this:

1. Randomly choose between doing the first or second reaction, based on the relative proportion of $\mathbf{R_1}$ and $\mathbf{R_2}$

2. If it's the first, then remove one each of an **A** and a **B** molecule and create a new **C** molecule

3. If it's the second, we remove one **C** molecule and create a new **A** and a new **B** molecule

Reaction Model

```
for step in number_of_steps:

    # Compute concentrations
    V = NA + NB + (2 * NC)
    EA = NA / V
    EB = NB / V
    EC = NC / V

    # Calculate reaction probabilities
    R1 = p * EA * EB
    R2 = q * EC

    # Randomly choose one reaction
    if random.uniform(0, 1) < R1 / (R1 + R2):
        # A + B → C
        # Remove one A and one B, make one C
        ...
    else:
        # C → A + B
        # Remove one C, make one A and one B
        ...
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    else:
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        ...
```

$$N_A = 60$$
$$N_B = 30$$
$$N_C = 10$$

$$V_{total} = N_A + N_B + 2N_C$$
$$V_{total} = 60 + 30 + (2 \times 10) = 110$$

$$E_A = \frac{N_A}{V_{total}} = \frac{60}{110} = 0.5454 \ldots$$

$$E_B = \frac{N_B}{V_{total}} = \frac{30}{110} = 0.2727 \ldots$$

$$E_C = \frac{N_C}{V_{total}} = \frac{10}{110} = 0.0909 \ldots$$

Reaction Model

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for step in number_of_steps:

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    V = NA + NB + (2 * NC)
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    else:
        # C → A + B
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        ...
```

$$E_A = 0.54$$
$$E_B = 0.27$$
$$E_C = 0.09$$

$$p = 1.0$$
$$q = 1.0$$

$$R_1 = pE_AE_B = 1.0 \times 0.54 \times 0.27 = 0.1458$$

$$R_2 = qE_C = 1.0 \times 0.09 = 0.09$$

Reaction Model

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for step in number_of_steps:

    # Compute concentrations
    V = NA + NB + (2 * NC)
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Reaction Model

```python
for step in number_of_steps:

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        ...
```
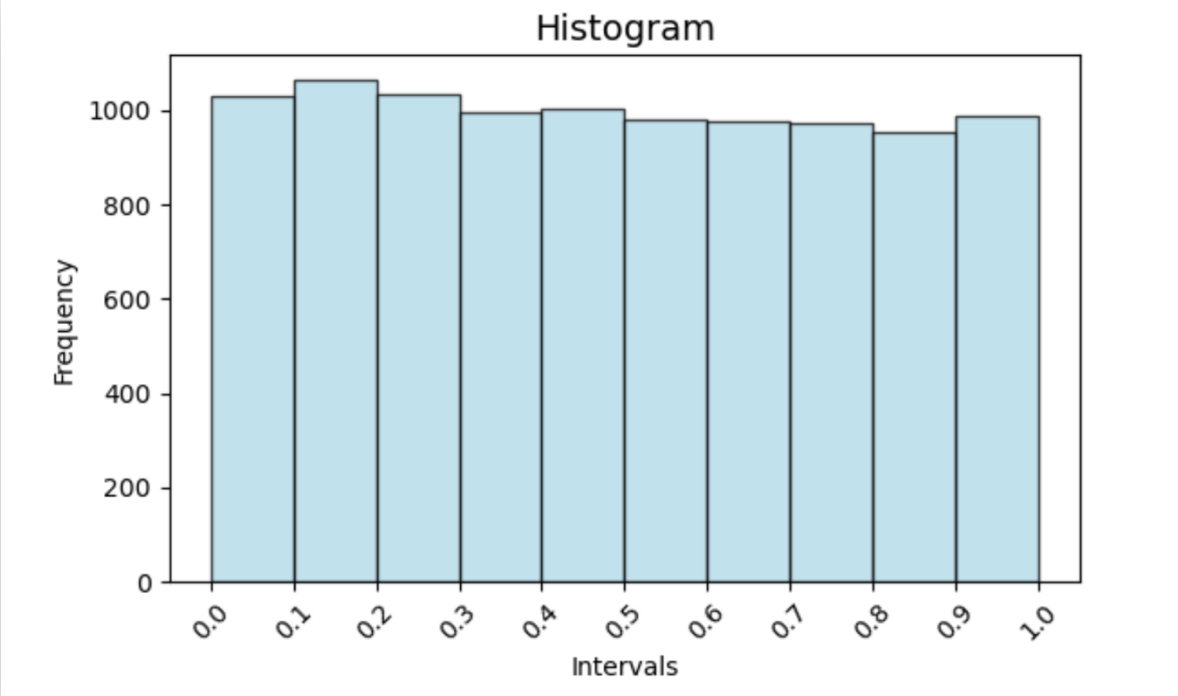

```python
random.uniform(0, 1)
```



Reaction Model

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    else:
        # C → A + B
        # Remove one C, make one A and one B
        ...
```

$$R_1 = 0.1458$$
$$R_2 = 0.09$$

Compute the ratio of $\mathbf{R_1}$ reaction probability relative to the total reaction probability $\mathbf{R_1} + \mathbf{R_2}$

$$\frac{R_1}{R_1 + R_2} = \frac{0.1458}{0.1458 + 0.09} = \frac{0.1458}{0.2358} \cong 0.6183$$

Reaction Model

```python
for step in number_of_steps:

    # Compute concentrations
    V = NA + NB + (2 * NC)
    EA = NA / V
    EB = NB / V
    EC = NC / V

    # Calculate reaction probabilities
    R1 = p * EA * EB
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    if random.uniform(0, 1) < R1 / (R1 + R2):
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        # Remove one A and one B, make one C
        ...
    else:
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        # Remove one C, make one A and one B
        ...
```
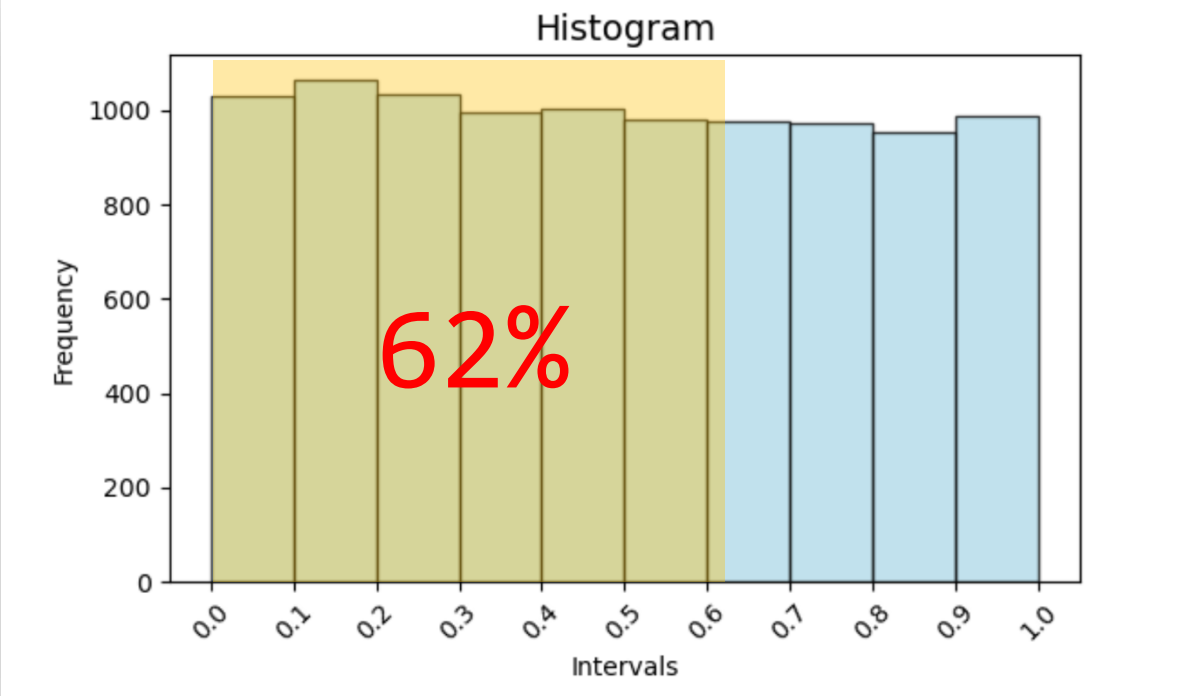
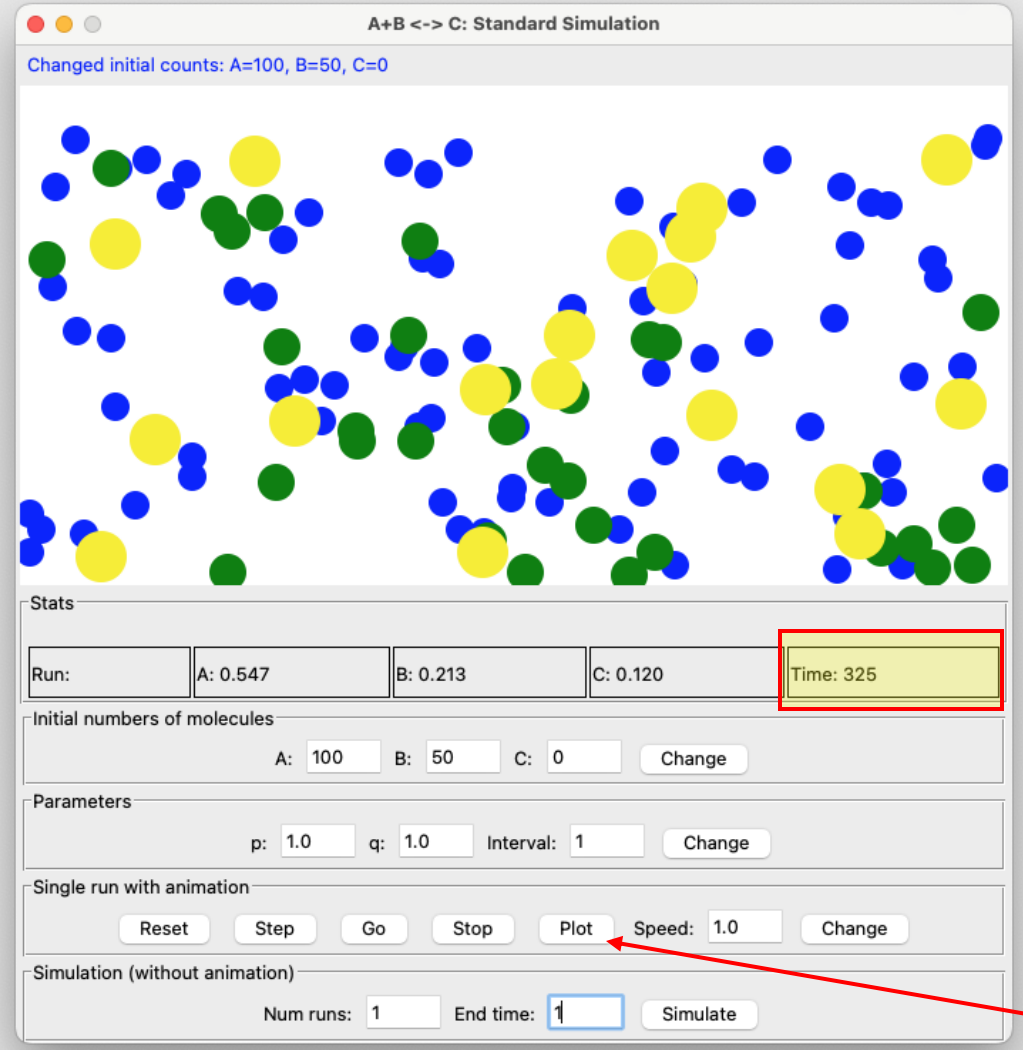

```python
if random.uniform(0, 1) < 0.6183:
```

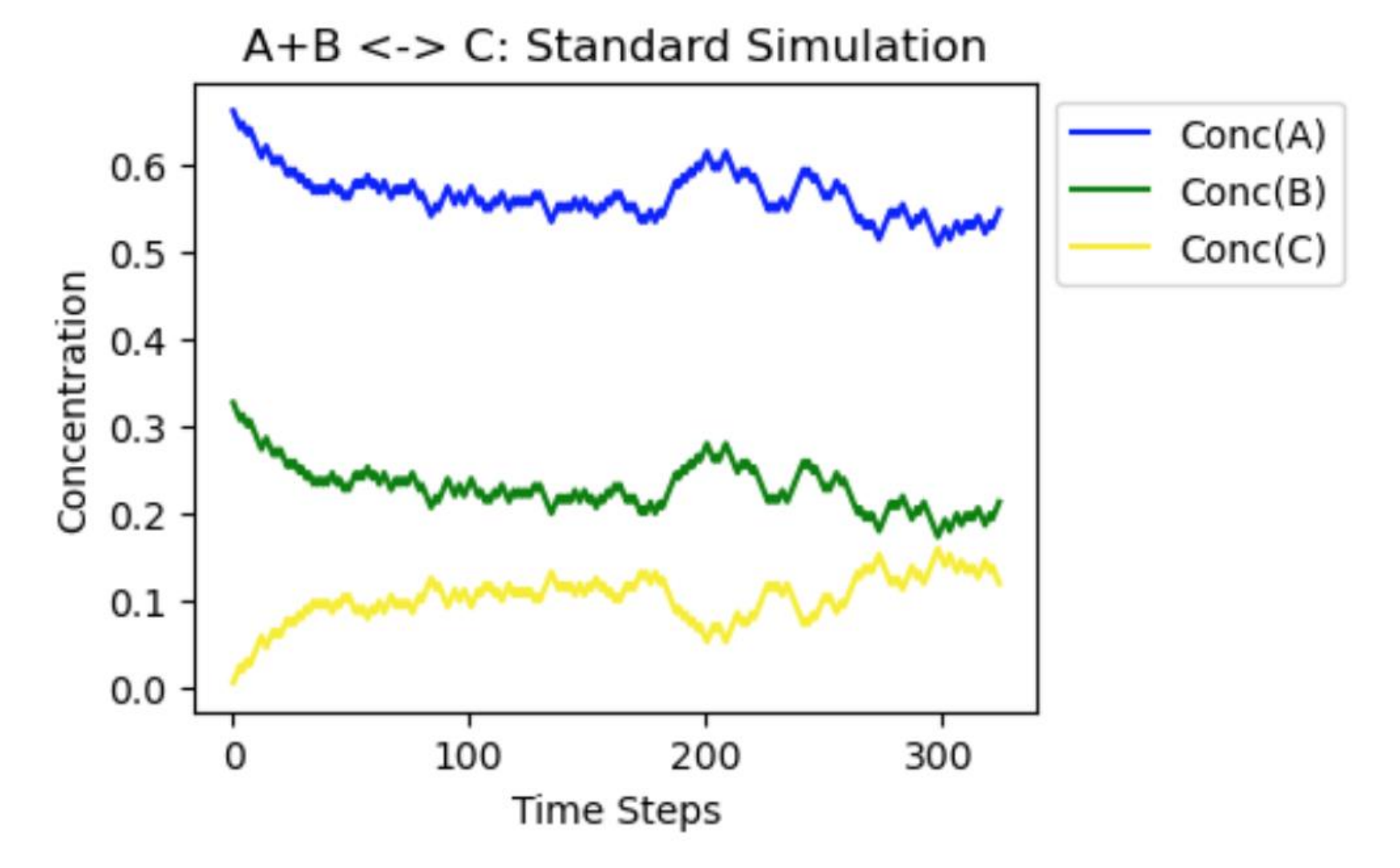


Long-Term Behavior



Click “Plot”

Long-Term Behavior



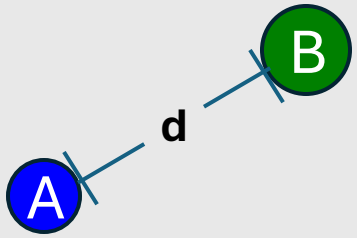
A more detailed model

How closely does our model correspond to reality?

Molecules react when they bump into each other, but we did **not** consider *spatial* closeness at all

Model with Spatial Detail

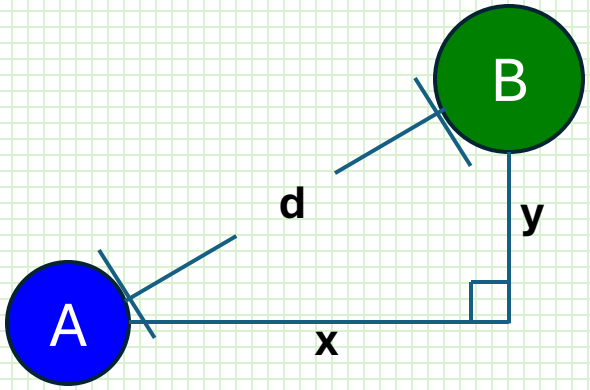
Molecules A and B will
react only if close enough



We'll use a *distance* parameter that we can vary to decide what's "close enough"

Two Ways to Calculate Distance

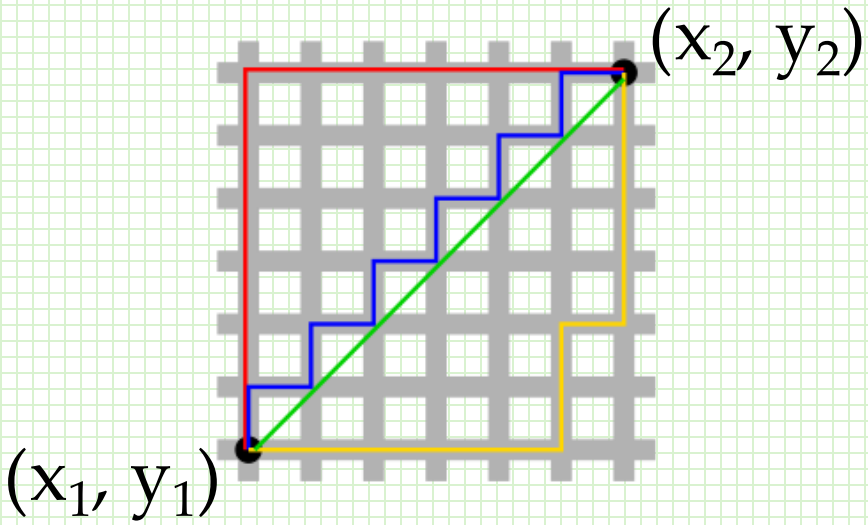
Euclidian Distance



$$distance = \sqrt{x^2 + y^2}$$

Two Ways to Calculate Distance

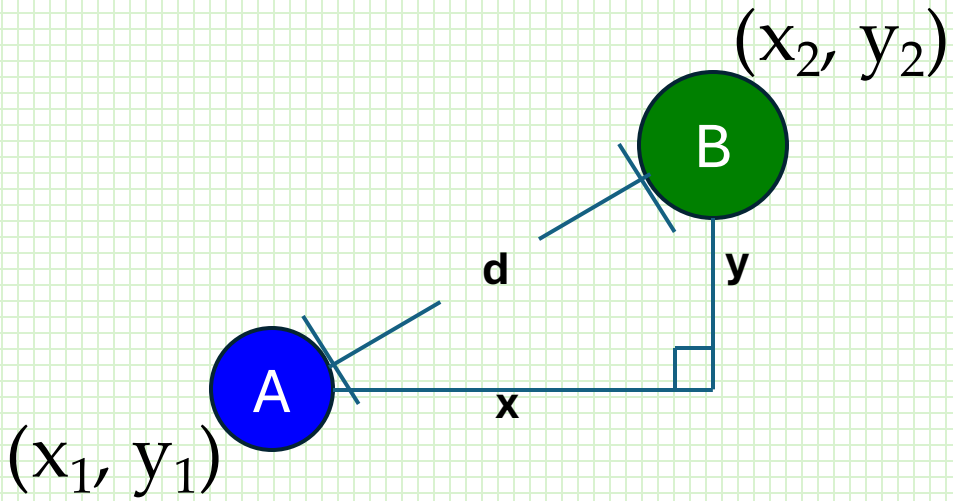
Manhattan Distance



$$distance = |x_2 - x_1| + |y_2 - y_1|$$

Squared Distance

Euclidian Distance



$$distance = \sqrt{(x_2 - x_1)^2 + (y_2 - y_1)^2}$$

$$distance^2 = (x_2 - x_1)^2 + (y_2 - y_1)^2$$

Using Squared Distance

```
# For each molecule A find the closest molecule B
for molecule_A in molecules_type_A:

    # Save the closest molecule B squared distance found so far
    closest_molecule_B_squared_distance = float("inf")

    for molecule_B in molecules_type_B:

        # Use the squared distance to save time/computation.
        squared_distance = (molecule_A.x - molecule_B.x)**2 + (molecule_A.y - molecule_B.y)**2

        # If the squared distance of this molecule B
        # is less than the closest molecule B found so far
        if squared_distance < closest_molecule_B_squared_distance:
            closest_molecule_B_squared_distance = squared_distance
```

Using Squared Distance

```
# For each molecule A find the closest molecule B
for molecule_A in molecules_type_A:

    # Save the closest molecule B squared distance found so far
    closest_molecule_B_squared_distance = float("inf")

    for molecule_B in molecules_type_B:

        # Use the squared distance to save time/computation.
        squared_distance = (molecule_A.x - molecule_B.x)**2 + (molecule_A.y - molecule_B.y)**2

        # If the squared distance of this molecule B
        # is less than the closest molecule B found so far
        if squared_distance < closest_molecule_B_squared_distance:
            closest_molecule_B_squared_distance = squared_distance
```

Reaction Occurs if Close Enough

```
# If the A molecule is close enough to a B molecule then a reaction occurs
if closest_molecule_B_distance < closeness_distance:
    # Select a uniform random number between 0 and 1
    # If the random number is less than the constant p
    # then the first reaction A + B -> C occurs
    if random.uniform(0, 1) < p:
        to_remove_A.append(molecule_A)
        to_remove_B.append(molecule_B)
        # Form a new C at midpoint
        xC = (molecule_A.x + molecule_B.x) / 2
        yC = (molecule_A.y + molecule_B.y) / 2
        to_add_C.append(Molecule(xC, yC))
```

Reaction Occurs if Close Enough

```
# If the A molecule is close enough to a B molecule then a reaction occurs
if closest_molecule_B_distance < closeness_distance:
    # Select a uniform random number between 0 and 1
    # If the random number is less than the constant p
    # then the first reaction A + B -> C occurs
    if random.uniform(0, 1) < p:
        to_remove_A.append(molecule_A)
        to_remove_B.append(molecule_B)
        # Form a new C at midpoint
        xC = (molecule_A.x + molecule_B.x) / 2
        yC = (molecule_A.y + molecule_B.y) / 2
        to_add_C.append(Molecule(xC, yC))
```

Reaction Occurs if Close Enough

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        to_remove_B.append(molecule_B)
        # Form a new C at midpoint
        xC = (molecule_A.x + molecule_B.x) / 2
        yC = (molecule_A.y + molecule_B.y) / 2
        to_add_C.append(Molecule(xC, yC))
```

Random Movement of Molecules

The source of randomness in the **standard model** is which of two reactions to choose at each step

What happens in the **spatial model** depends on the random movement of the molecules

More "*chanciness*" and hence more fluctuation

Random Movement of Molecules

```
def move_molecules(molecules_list):

    # Randomly move each molecule
    for molecule in molecules_list:

        # Random chance to change direction
        if random.uniform(0, 1) < theta_change_probability:
            molecule.theta = random.uniform(0, 2 * math.pi)

        updated_x_position = molecule.x + move_length * math.cos(molecule.theta)
        updated_y_position = molecule.y + move_length * math.sin(molecule.theta)
```

Random Movement of Molecules

```
def move_molecules(molecules_list):

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        # Random chance to change direction
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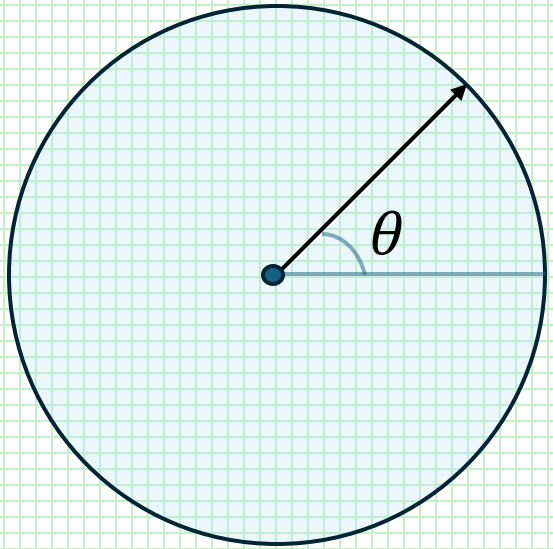
```

Random Movement of Molecules

```
# Random chance to change direction
if random.uniform(0, 1) < theta_change_probability:
    molecule.theta = random.uniform(0, 2 * math.pi)
```



Random angle θ
in radians between 0 and 2π

Random Movement of Molecules

```
def move_molecules(molecules_list):

    # Randomly move each molecule
    for molecule in molecules_list:

        # Random chance to change direction
        if random.uniform(0, 1) < theta_change_probability:
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```

Random Movement of Molecules

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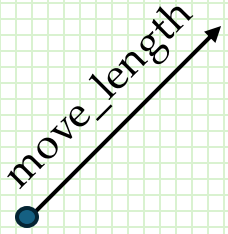
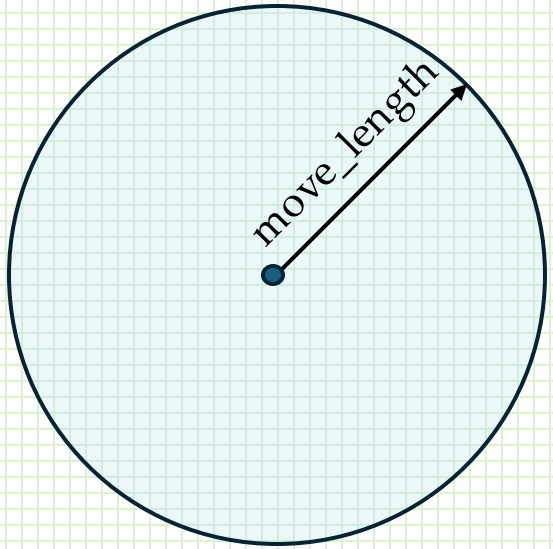
updated_x_position = molecule.x + move_length * math.cos(molecule.theta)
updated_y_position = molecule.y + move_length * math.sin(molecule.theta)
```



Random Movement of Molecules

```
updated_x_position = molecule.x + move_length * math.cos(molecule.theta)
updated_y_position = molecule.y + move_length * math.sin(molecule.theta)
```



Random Movement of Molecules

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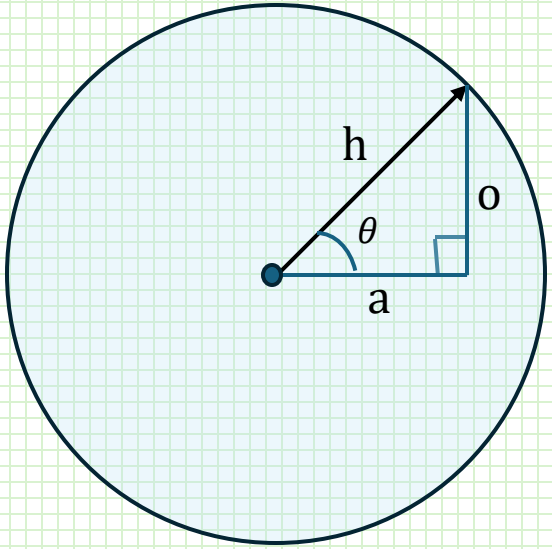
updated_x_position = molecule.x + move_length * math.cos(molecule.theta)
updated_y_position = molecule.y + move_length * math.sin(molecule.theta)
```

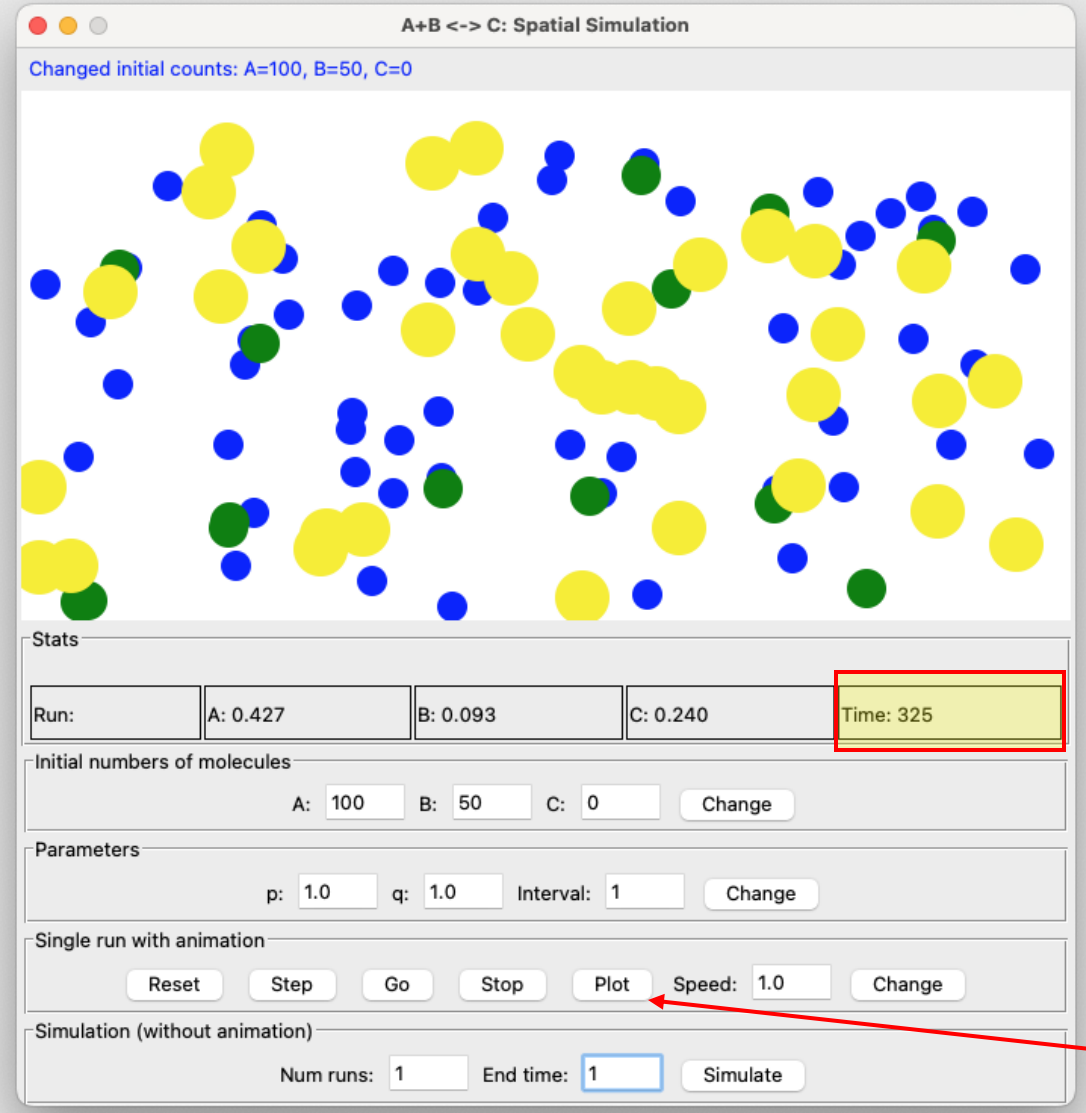


$$\boldsymbol{c}os(\theta) = \frac{\boldsymbol{a}djacent}{\boldsymbol{h}ypotenuse} \qquad \mathbf{s}\mathrm{in}(\theta) = \frac{\boldsymbol{o}pposite}{\boldsymbol{h}ypotenuse}$$

x component: $hypotenuse \times cos(\theta) = adjacent$

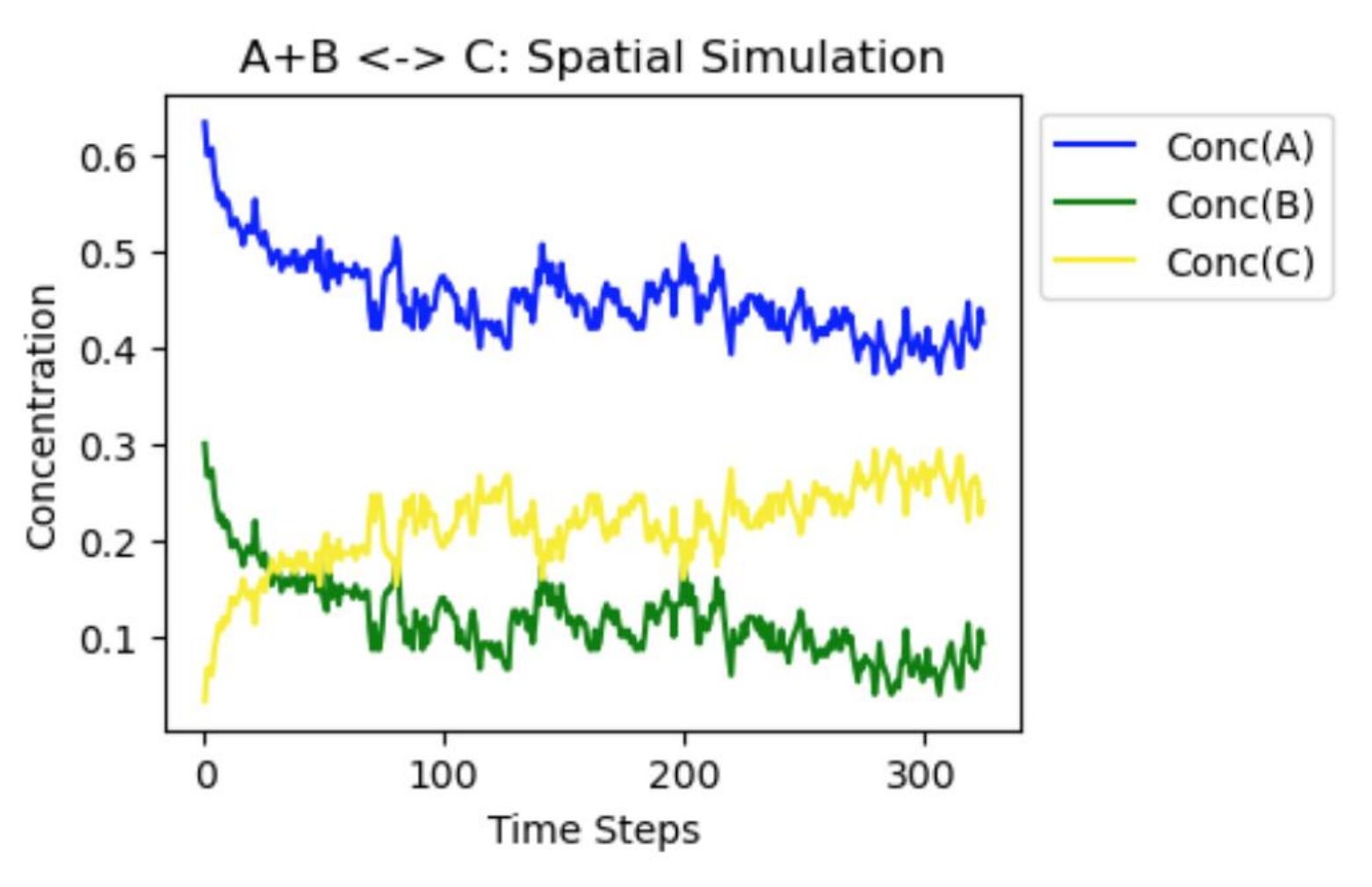
y component: $hypotenuse \times \sin(\theta) = opposite$

Long-Term Behavior

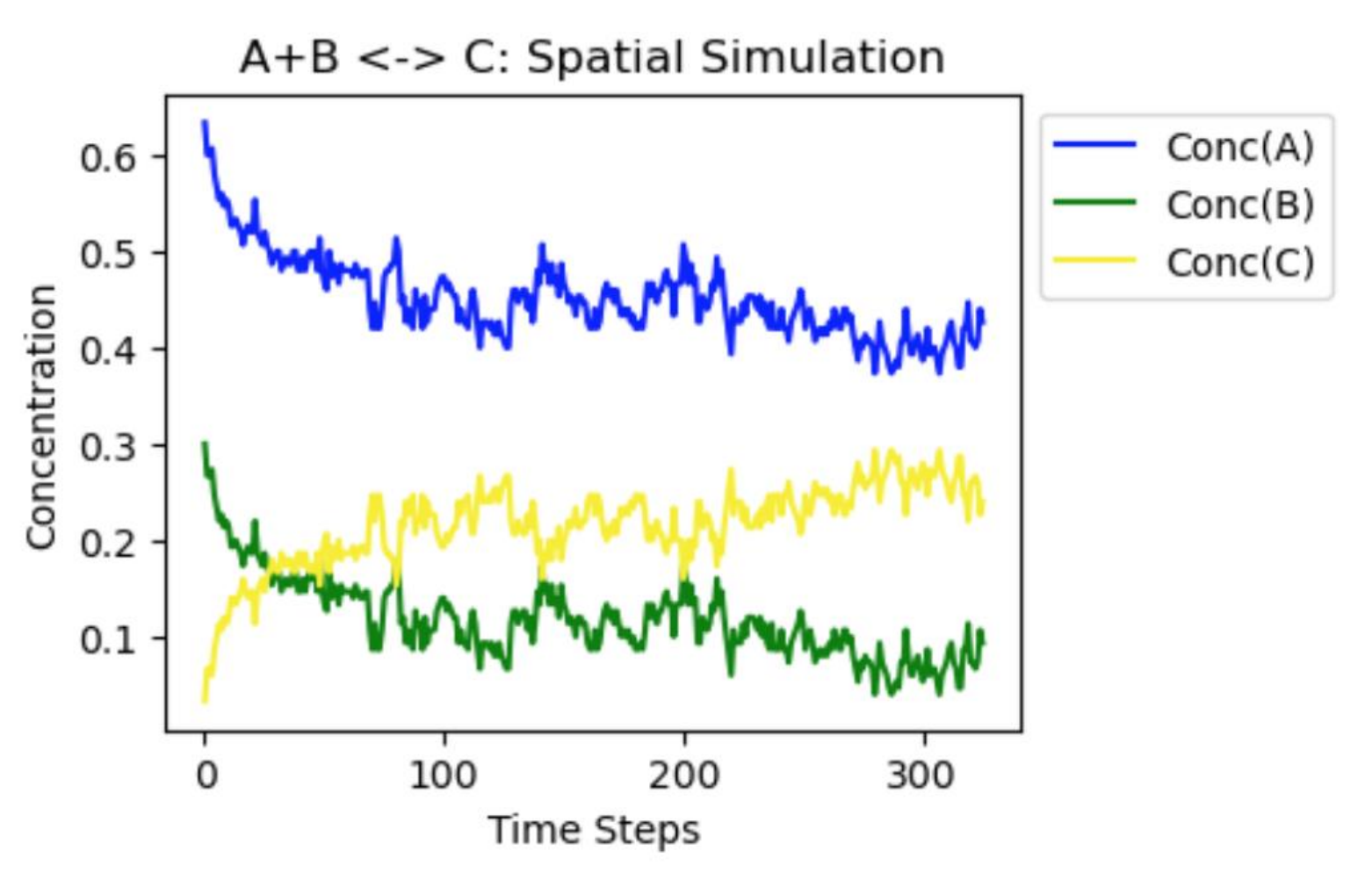


Click “Plot”

Long-Term Behavior

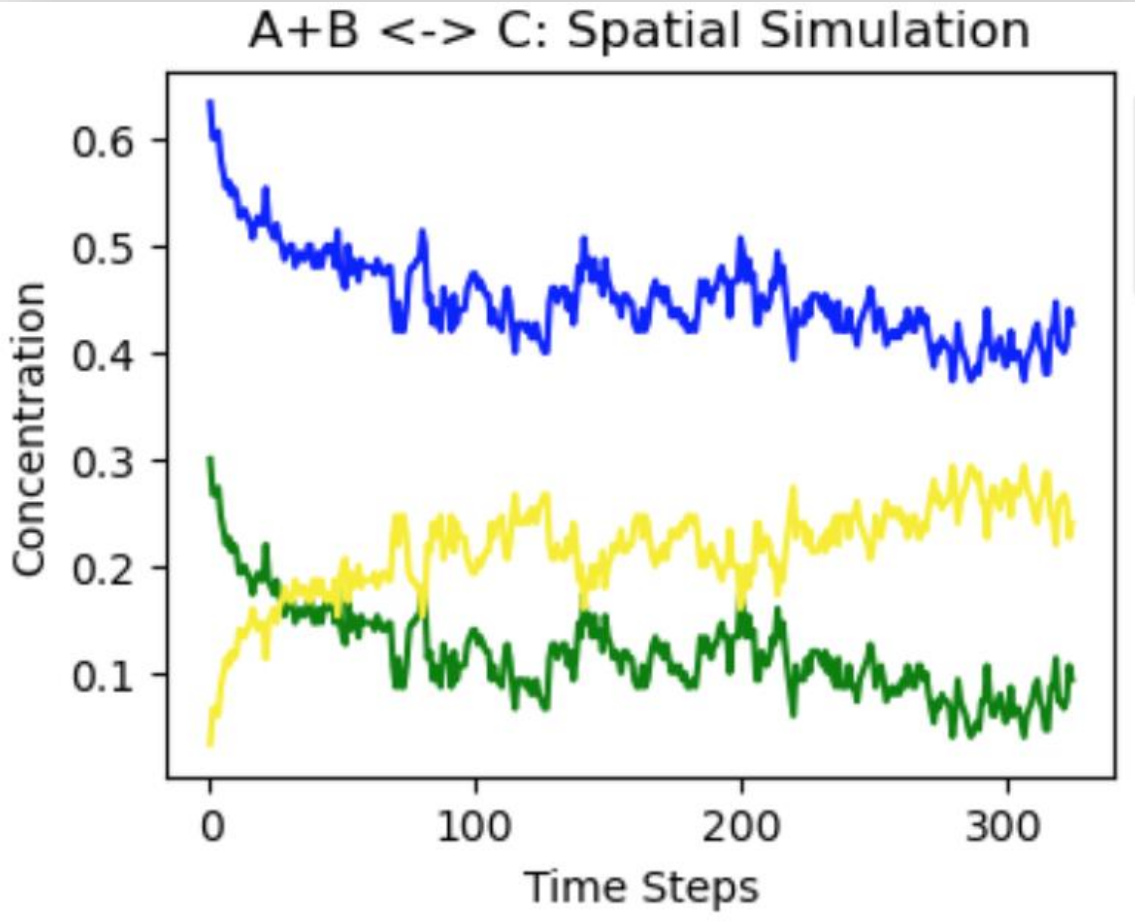


Long-Term Behavior

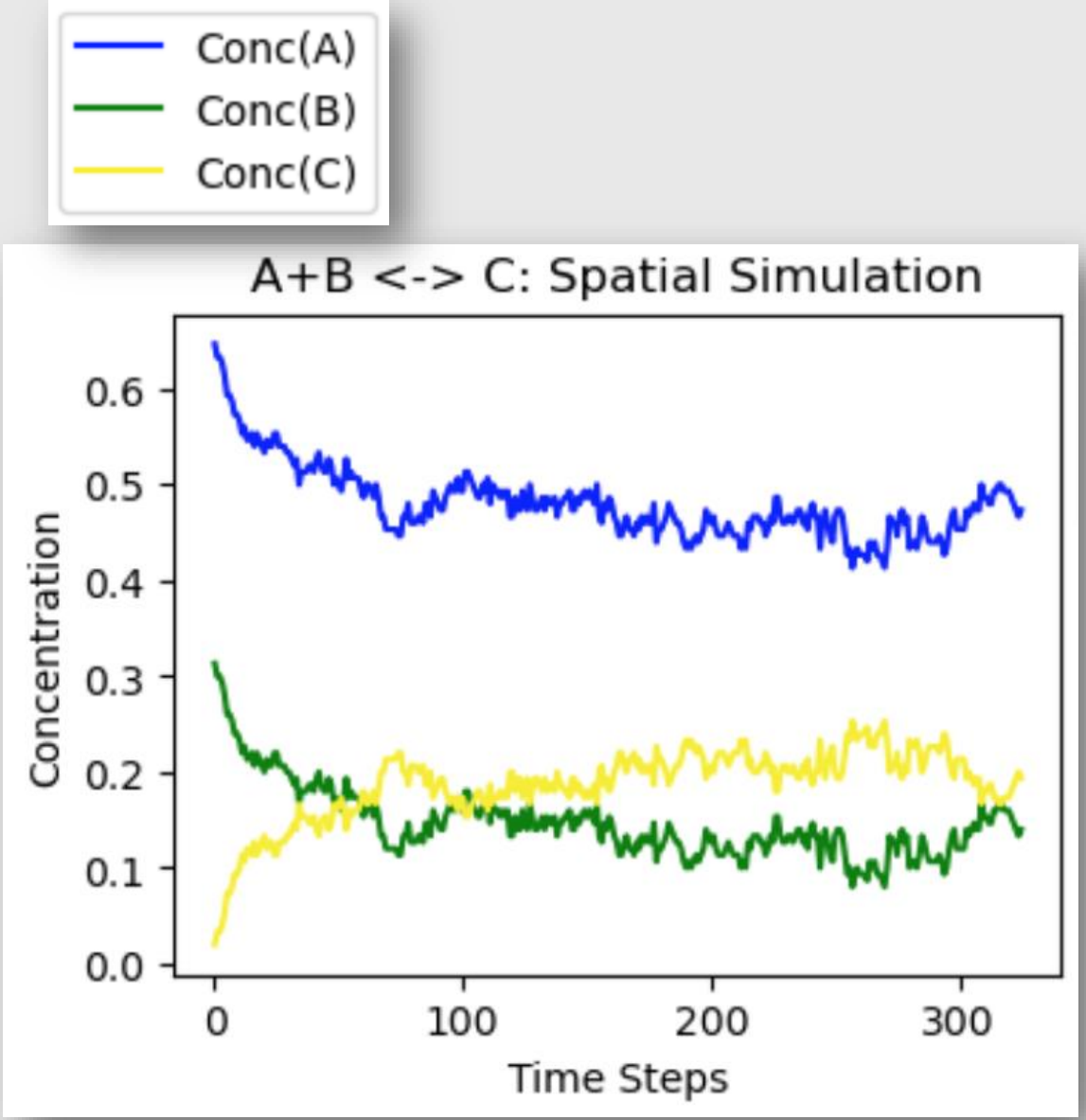



```
closeness_distance = 100
```

Long-Term Behavior

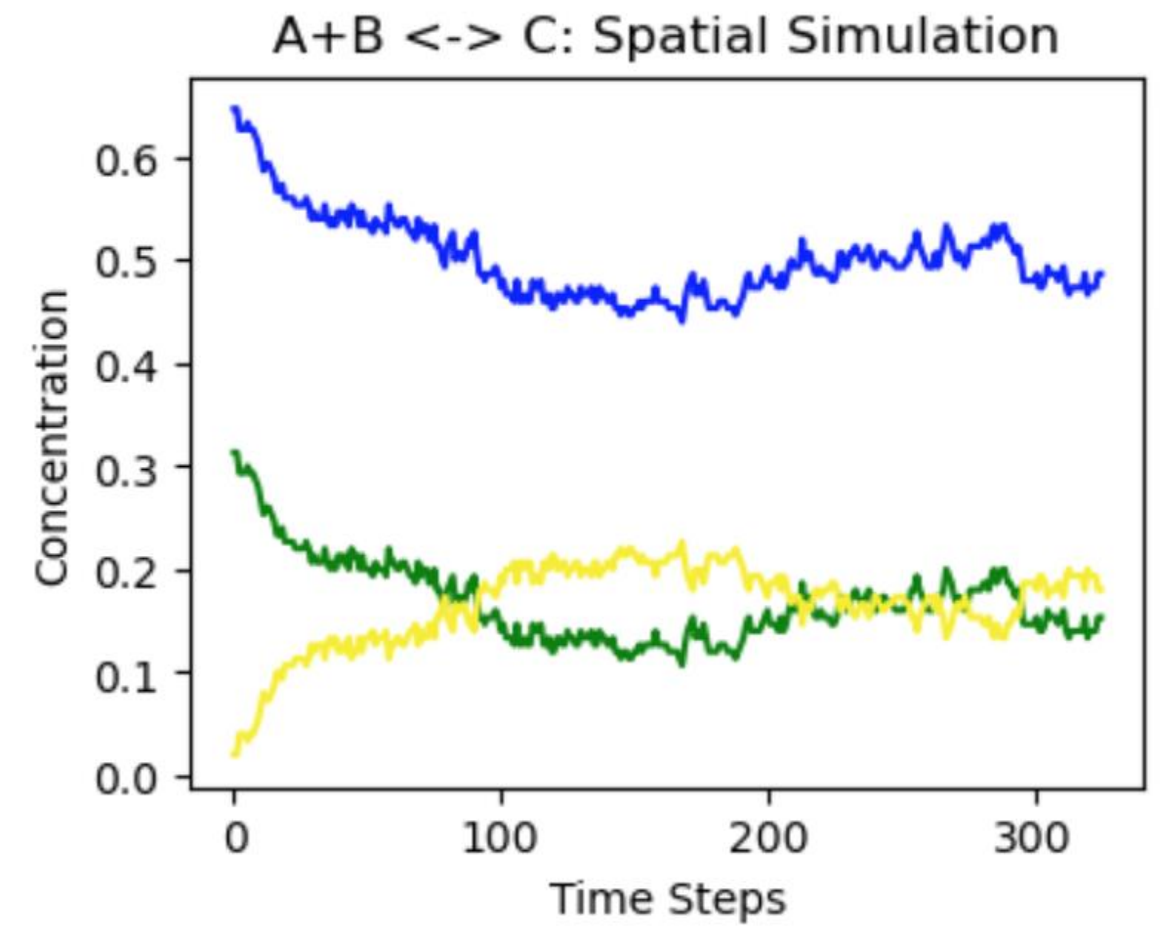



```
closeness_distance = 100
```

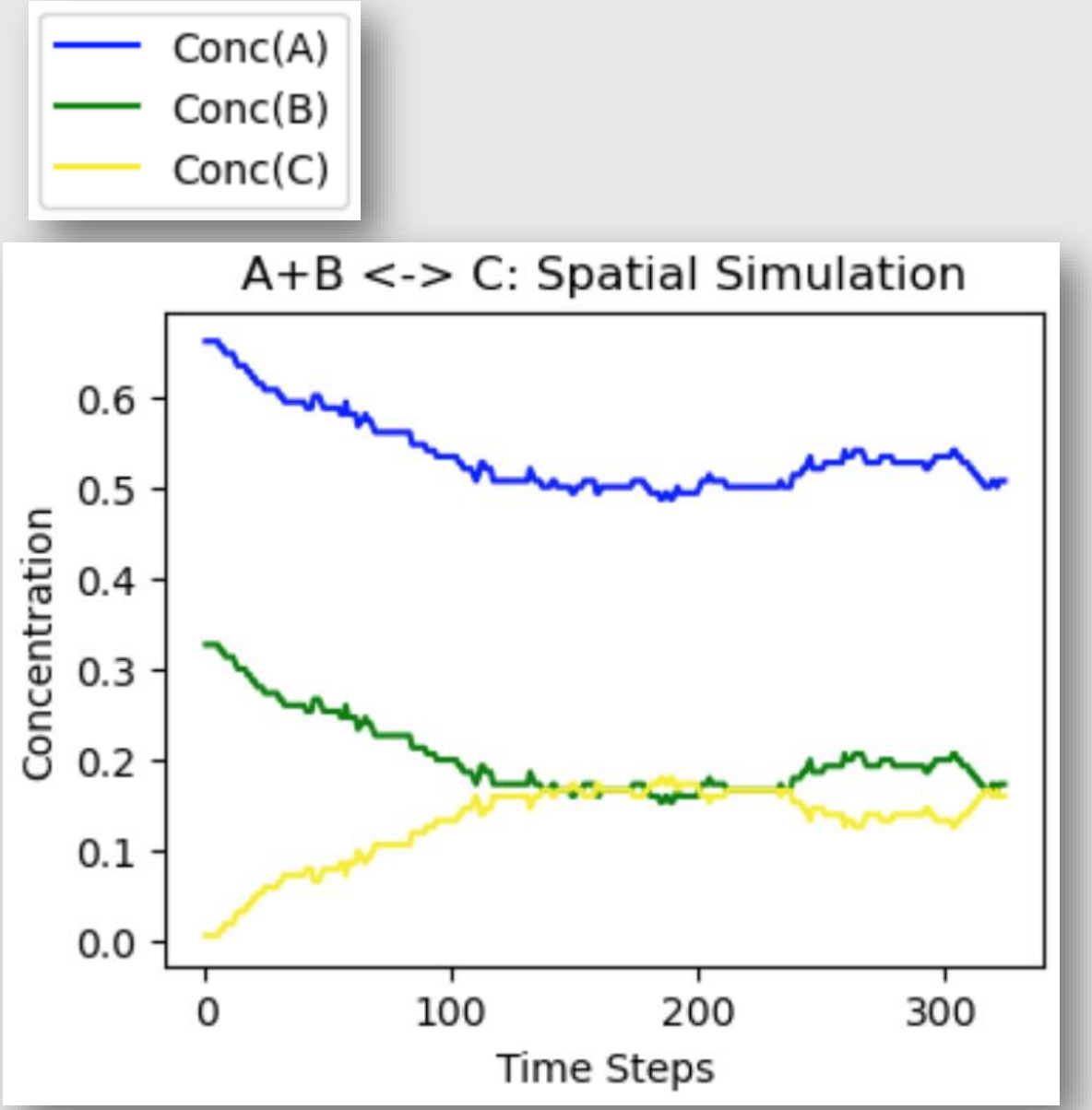



```
closeness_distance = 50
```

Long-Term Behavior




```
closeness_distance = 25
```




```
closeness_distance = 5
```