

Modeling molecular biological processes

1. **CREATE** (randomly)
 2. **PERFORM** (randomly)
 3. **REMOVE** (randomly)

1. Create matrix of the probabilities for molecular reactions (Intermolecular collision and intramolecular activity)

	1 molecule <i>single molecule</i>	2 molecules <i>intermolecular</i>	3 molecules <i>intermolecular</i>
1 molecule <i>intramolecular</i>	<p>probability for collision: $0.001 = \frac{0.001 \cdot 1}{1}$</p> <p>possible complete molecular reactions: $\frac{0.001 \cdot 1}{1} = 0.001$</p>	<p>probability for collision: $0.001 = \frac{0.001 \cdot 1}{1}$</p> <p>possible complete molecular reactions: $\frac{0.001 \cdot 1}{1} = 0.001$</p>	<p>probability for collision: $0.001 = \frac{0.001 \cdot 1}{1}$</p> <p>possible complete molecular reactions: $\frac{0.001 \cdot 1}{1} = 0.001$</p>
2 molecules <i>intermolecular</i>	<p>probability for collision: $0.001 = \frac{0.001 \cdot 1}{1}$</p> <p>possible complete molecular reactions: $\frac{0.001 \cdot 1}{1} = 0.001$</p>	<p>probability for collision: $0.001 = \frac{0.001 \cdot 1}{1}$</p> <p>possible complete molecular reactions: $\frac{0.001 \cdot 1}{1} = 0.001$</p> <p>no new product</p>	<p>probability for collision: $0.001 = \frac{0.001 \cdot 1}{1}$</p> <p>possible complete molecular reactions: $\frac{0.001 \cdot 1}{1} = 0.001$</p>
3 molecules <i>intermolecular</i>	<p>probability for collision: $0.001 = \frac{0.001 \cdot 1}{1}$</p> <p>possible complete molecular reactions: $\frac{0.001 \cdot 1}{1} = 0.001$</p>	<p>probability for collision: $0.001 = \frac{0.001 \cdot 1}{1}$</p> <p>possible complete molecular reactions: $\frac{0.001 \cdot 1}{1} = 0.001$</p>	<p>probability for collision: $0.001 = \frac{0.001 \cdot 1}{1}$</p> <p>possible complete molecular reactions: $\frac{0.001 \cdot 1}{1} = 0.001$</p> <p>no new product</p>
4 molecules <i>intermolecular</i>	<p>probability for collision: $0.001 = \frac{0.001 \cdot 1}{1}$</p> <p>possible complete molecular reactions: $\frac{0.001 \cdot 1}{1} = 0.001$</p>	<p>probability for collision: $0.001 = \frac{0.001 \cdot 1}{1}$</p> <p>possible complete molecular reactions: $\frac{0.001 \cdot 1}{1} = 0.001$</p> <p>no new product</p>	<p>probability for collision: $0.001 = \frac{0.001 \cdot 1}{1}$</p> <p>possible complete molecular reactions: $\frac{0.001 \cdot 1}{1} = 0.001$</p>

number of species of molecules affected by one molecular reaction: $n = 2$
 number of DNA molecules: $m = 5$
 number of DNA strands: $p = 10 \times 5 = 7 = 20$

2. Select one combination randomly with respect to the probability distribution

3. Determine all possible complete molecular reaction products and select one of them

4. Perform molecular reaction and modify tube contents

1. **CREATE** (randomly)
 2. **PERFORM** (randomly)
 3. **REMOVE** (randomly)
 4. **REMOVE** (randomly)

total tube

Objectoriented Simulation 1991

F Rizvi



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