Motivation

- Capabilities of Molecular Communication systems are already addressed in the literature
- However, these models only consider general information theoretic issues
- A nanomachine (or a collection of nanomachines) will have an energy budget available for communication purposes which limits the device’s communication capabilities
Molecular Communication

Communication via Diffusion
Pheremone Signaling
Protein Signaling
Ion Signalling
Microtubule & Molecular Motors

Nanomachines (Unit)

Capabilities
- Power Plant (Mitochondria): Can generate energy from raw materials available in the environment
- Factory (Endoplasmic Reticulum/Ribosome): Can synthesize proteins and vesicles
- Packager (Golgi Apparatus): Can synchronize and communicate with another unit using CvD method
- Internal Communication (Microtubular System): Incorporates an internal communication system
- Protective Shielding (Cell membrane): Wrapped inside a protective shielding layer
Communication via Diffusion (CvD)

- Communication by diffusing molecules to the environment
- Information is sent using a sequence of symbols which are spread over sequential time slots as one symbol in each slot
Propagation Model

- The movement of molecules in the environment can be modeled as Brownian Motion.
- The displacement of the molecule in 1D ($\Delta X$) in step time ($\Delta t$) is a random variable,

$$\Delta X \sim N(0, \frac{K_B T}{3 \pi \eta r_s} \Delta t)$$

- In a 3D environment, the total displacement is found using three independent Brownian motions.
- The molecule hits the receiver with a certain probability depending on the distance and the time,

$$P_{hit}(d, t_s)$$
Propagation Model

- Hit Probability Analysis

Avg. hit times are too high to be appropriate as the time slot values

<table>
<thead>
<tr>
<th>Distance (μm)</th>
<th>Average hit time</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.501</td>
</tr>
<tr>
<td>2</td>
<td>1.661</td>
</tr>
<tr>
<td>4</td>
<td>7.346</td>
</tr>
<tr>
<td>8</td>
<td>31.296</td>
</tr>
<tr>
<td>16</td>
<td>107.283</td>
</tr>
<tr>
<td>32</td>
<td>315.203</td>
</tr>
</tbody>
</table>
Propagation Model

• Hit Probability Analysis
  • The hit time histogram of molecules has a very long tail
  • Thus, instead of using average hit times, we use the maximum hit time of the first 60% of the molecules as the time slot time

<table>
<thead>
<tr>
<th>Distance (μm)</th>
<th>$t_s$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.63</td>
</tr>
<tr>
<td>2</td>
<td>0.11</td>
</tr>
<tr>
<td>4</td>
<td>0.40</td>
</tr>
<tr>
<td>8</td>
<td>1.54</td>
</tr>
<tr>
<td>16</td>
<td>5.9</td>
</tr>
<tr>
<td>32</td>
<td>22.01</td>
</tr>
</tbody>
</table>

• Hit probabilities are recalculated using the time slot values selected
• There is not a significant change in $P_{hit}$ after the second time slot
• Therefore, only the ISI caused by the previous symbol is significant
Channel Model

• The **channel capacity** \( C \) of a CvD channel, can be evaluated by taking the maximum of the **mutual information** \( I(X,Y) \)

\[
C = \max_{\tau} I(X,Y)
\]

\[
= \max_{x} \sum_{y:0,1} \sum_{x:0,1} P_{X,Y}(x,y) \log_{2} \frac{P_{X,Y}(x,y)}{P_{X}(x)P_{Y}(y)}
\]

Channel Model

• Using \( P_{hit} \) and the number of molecules sent \( (n) \), we can calculate the number of molecules hitting at the receiver

\[
N_C \sim Binomial (n, P_{hit}(d,t_s))
\]

• Also, the left over molecules from the previous symbol hit at the receiver

\[
N_p \sim Binomial (n, P_{hit}(d,2t_s)) - Binomial (n, P_{hit}(d,t_s))
\]
Energy Model

• Some of the energy produced in the unit is allocated for communication purposes ($P_{W_C}$)

• This energy constitutes an upper bound for the number of molecules that can be produced and sent in a time slot

• The production and release of messenger molecules occur in 4 steps

1. Synthesis of messenger molecules ($E_s$)
2. Production of vesicle ($E_v$)
3. Carrying the vesicle to the cell membrane ($E_c$)
4. Releasing the vesicle to the environment ($E_e$)
Energy Model

- **Synthesis cost of the messenger molecule**
  - Protein based messenger molecule (Insulin)
  - Cost of forming bonds among amino acids
    \[ E_S = 202.88(n_{aa} - 1) \text{ zJ} \]

- **Production cost of Secretory Vesicle**
  - Messenger molecules are packed inside a vesicle
  - The vesicle is generally composed of phospholipids
  - 5 phospholipid in 1nm² area
    \[ E_v = 83 \times 5 \left( 4 \pi r_v^2 \right) \text{ zJ} \]

Energy Model

- **Carrying cost of a vesicle to cell membrane**
  - The vesicle moves along microtubules
  - At each step (8nm), 83 zJ is consumed
    \[ E_S = 83 \left( \frac{r_{unit}}{2} \right) \text{ zJ} \]

- **Extraction cost of the vesicle to the environment**
  - The vesicle fuses with the cell membrane (membrane fusion)
    \[ E_E = 83 \times 10 \text{ zJ} \]
Energy Model

- Total cost of sending n messenger molecules

\[ E_T = 202.88 \left( n_{mRNA} - 1 \right) n + \left[ \frac{n}{c_v} \right] \left( 83 \times 5 \left( 4 \pi r_v^2 \right) + 83 \left[ \frac{r_{\text{unit}}/2}{8} \right] + 83 \cdot 10 \right) \]

- This cost must be less than or equal to the energy produced (in 1 time slot)

\[ P_{WC} t_s \geq 202.88 \left( n_{mRNA} - 1 \right) n + \left[ \frac{n}{c_v} \right] \left( 83 \times 5 \left( 4 \pi r_v^2 \right) + 83 \left[ \frac{r_{\text{unit}}/2}{8} \right] + 83 \cdot 10 \right) \]

**Molecular Diversity**

- Instead of using 1 type of molecule in a time step, use different types of molecules
- Each molecule type represents 1-bit information
- Different molecules do NOT affect each other in the environment -> independent channels

- How many independent channels can be opened considering energy constraints?

\[ P_{WC} t_s \geq n_s \left( 202.88 \left( n_{mRNA} - 1 \right) n + \left[ \frac{n}{c_v} \right] \left( 83 \times 5 \left( 4 \pi r_v^2 \right) + 83 \left[ \frac{r_{\text{unit}}/2}{8} \right] + 83 \cdot 10 \right) \right) \]
Optimization Problems

- Maximizing Mutual Information

\[
\begin{align*}
\text{maximize } & \quad I(X,Y) \\
\text{subject to } & \quad n_\theta \leq n_{\text{max}}(P_{w_0}, T_{m_0}, t_\theta, 1), \quad n_\theta \in \mathbb{Z}^+ \\
& \quad t_\theta = \alpha_1 \\
& \quad d = \alpha_2 \\
& \quad P_X(x = 0) = \alpha_3
\end{align*}
\]

Optimization Problems

- Maximizing data rate

\[
\begin{align*}
\text{maximize } & \quad \left( \frac{C \cdot n_t}{t_s} \right) \\
\text{subject to } & \quad n_s \cdot n_t \leq n_{\text{max}}(P_{w_0}, T_{m_0}, t_s, n_t), \quad n_s, n_t \in \mathbb{Z}^+ \\
& \quad t_s = \alpha_1 \\
& \quad d = \alpha_2 \\
& \quad P_X(x = 0) = \alpha_3
\end{align*}
\]
Evaluation

- Simulation Parameters

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td># of amino-acids ($n_{ba}$)</td>
<td>51</td>
</tr>
<tr>
<td>Stokes’ radius of insulin ($r_s$)</td>
<td>2.86 nm [18]</td>
</tr>
<tr>
<td>Radius of insulin molecule ($r_{ins}$)</td>
<td>2.5 nm [11]</td>
</tr>
<tr>
<td>Viscosity of the fluid ($\eta$)</td>
<td>0.001 $\frac{kg}{m}$</td>
</tr>
<tr>
<td>Temperature ($T$)</td>
<td>310°K</td>
</tr>
<tr>
<td>Drug constant ($b$)</td>
<td>5,391 $10^{-11}$</td>
</tr>
<tr>
<td>Diffusion coefficient ($D$)</td>
<td>79.4 $\frac{m^2}{s}$</td>
</tr>
<tr>
<td>Radius of the receiver</td>
<td>10 $\mu m$ [2]</td>
</tr>
<tr>
<td>Radius of the vesicle ($r_v$)</td>
<td>0.05 $\mu m$ [11, 16]</td>
</tr>
<tr>
<td>Capacity of the vesicle ($c_v$)</td>
<td>1549 $Insulin$</td>
</tr>
<tr>
<td>Radius of the transmitter ($r_{trans}$)</td>
<td>10 $\mu m$ [2]</td>
</tr>
<tr>
<td>Energy budget for communication ($P_{cc}$)</td>
<td>4.5 $pW$ [11]</td>
</tr>
</tbody>
</table>

Evaluation

- Analysis of Mutual Information (Optimization Prob. 1)

$n_{\text{max}} = 100$

$n_{\text{max}} = 500$
Evaluation

• Analysis of Mutual Information (Optimization Prob. 1)
  • As the distance increases, the capacity drops
  • Threshold value, which maximizes the capacity, decreases with the distance

<table>
<thead>
<tr>
<th>( n_{\text{max}} )</th>
<th>2 ( \mu \text{m} )</th>
<th>8 ( \mu \text{m} )</th>
<th>32 ( \mu \text{m} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( C )</td>
<td>( \tau^* )</td>
<td>( C )</td>
<td>( \tau^* )</td>
</tr>
<tr>
<td>10</td>
<td>0.642</td>
<td>2</td>
<td>0.542</td>
</tr>
<tr>
<td>50</td>
<td>0.935</td>
<td>15</td>
<td>0.8</td>
</tr>
<tr>
<td>100</td>
<td>0.963</td>
<td>31</td>
<td>0.934</td>
</tr>
<tr>
<td>500</td>
<td>0.999</td>
<td>153</td>
<td>0.999</td>
</tr>
<tr>
<td>1000</td>
<td>0.999</td>
<td>352</td>
<td>0.999</td>
</tr>
</tbody>
</table>

Evaluation

• Analysis of Data Rate (Optimization Prob. 2)
  • Energy cost of a single channel is low compared to the energy budget of a \( \beta \)-cell similar device
Evaluation

- Analysis of Data Rate (Optimization Prob. 2)
  - Distance does not heavily affect the data rate
    - As distance increases, more molecules are required
    - As distance increases, the slot duration also increases, which leads to more energy production in a time slot
  - Energy budget constitutes an upper bound on data rate
  - If the energy budget and the slot duration are too low, the data rate suffers significantly

Conclusion & Future Work

- Energy constraints are not considered in the literature for Molecular Communication
- Energy budget constitutes a limit to data rates
- The effect of energy budget using different modulation techniques might be considered
- Energy models for other Molecular Communication systems (e.g., ion signaling) should be developed
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