MOLECULAR CHANNEL MODEL
FOR
COMMUNICATION IN NANONETWORKS

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WHAT IS MOLECULAR COMMUNICATION?

Transmission and reception of information encoded in molecules

transmission   propagation   reception
WHY MOLECULAR COMMUNICATION?

- Drawing an analogy:
  - **Living organism** = biological machine with molecular precision (nanometer scale)
  - **Nanomachine** = artificial machine with molecular precision

- Molecular Communication naturally occurs within living organisms
**WHY MOLECULAR COMMUNICATION?**

- Molecular communication allows
  
  - **Nanomachines to send/receive information to/from living organisms**
    
    - Change living organism behaviors (e.g., intelligent drugs)
    - Obtain information from living organisms otherwise not accessible (e.g., nanoscale diagnosis for health monitoring)

  - **Networks between nanomachines and living entities or among nanomachines = bio-inspired nanonetworks**
WHY MOLECULAR COMMUNICATION?

- Low power consumption
  - Chemical reactions (spontaneous, catalyzed by enzymes, etc.)
  - → Energy saving

- High biological compatibility
  - Bio-inspired approach
  - → Bio-related applications (e.g. intra-body deployment, etc.)

- Possibly deployable on nano-scale
  - Molecules/chemical reactions: nano-metric realm
  - → Nanomachine networking (Nanonetworks)
NANONETWORKS THROUGH MOLECULAR COMMUNICATION

- Molecular Multiple Access
- Molecular Broadcast Channel
- Molecular Relay Channel
HOW TO STUDY MOLECULAR COMMUNICATION?

How do molecules propagate? → 3 architectures

- Walkway-based (e.g., molecular motors)
- Flow-based (e.g., guided fluidic medium, guided carrier entities)
- Diffusion-based (e.g., still, randomly turbulent fluidic medium)

Less spontaneous → More spontaneous
MOLECULAR COMMUNICATION ARCHITECTURES

- **Walkway-based**
  - Molecules follow pre-defined pathways (e.g., molecular motors)
  - Carrier substances (e.g., vesicle, container)

MOLECULAR COMMUNICATION ARCHITECTURES

- **Flow-based**
  - Molecules in a fluidic medium
    - flow and turbulence guided and predictable
      (e.g., hormonal communication)
  - **Carrier entities**
    - motion constrained on average along specific paths
    - random motion component
      (e.g., pheromonal communication in ant colonies)

MOLECULAR COMMUNICATION ARCHITECTURES

- **Diffusion-based**
  - *spontaneous diffusion in a fluidic medium*
    - spontaneous diffusion
    - on-predictable fluid turbulence
  
  (e.g., pheromonal communication, when pheromones are released into a fluidic medium)

... A GLIMPSE OF THE LITERATURE

- Limited research on particle diffusion molecular communication from engineering perspective:
  

  - open questions about nano-scale information theory
  - possible comparisons classical Shannon – molecular communication paradigm
  - No concrete mathematical solution for channel modeling

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... A GLIMPSE OF THE LITERATURE


→ a particle receiver model is developed
→ ligand-receptor binding mechanism from bio-chemistry
→ diffusion process is not captured in terms of molecule propagation theory
... A GLIMPSE OF THE LITERATURE


- good mathematical framework to compute capacity
- the assumptions regarding information encoding and reception reduce the system to a very special case
Physical Channel Model
- How information is transmitted, propagated and received when a molecular carrier is used

Noise Representation
- How can be physically and mathematically expressed the noise affecting information transmitted through molecular communication

Information Encoding/Decoding
- Concentration
- Chemical structure
- Encapsulation
QUESTIONS THAT MAY ARISE

- What type of information?
- How to encode information into molecular entities?
- How to transmit?
- Which propagation architecture to rely on?
- How to receive?
THE MOST GENERAL ARCHITECTURE

- A molecule is a particle:
  - indivisible object
  - can be released to/collected from the vacuum space
  - When a particle is not being released or collected: subject to the diffusion process (laws of diffusion)

- Vacuum space
  - infinite extent in any possible direction
THE MOST GENERAL ARCHITECTURE

- If more than one particle is in the vacuum space
  - Thermal molecular vibrations
  - Elastic collisions (kinetic energy conservation)

- Particles have identical properties in terms of:
  - shape
  - size
Particle Diffusion Communication

- exchange of information encoded in the concentration variations of particles
- Particles diffuse in a biological environment (cellular cytoplasm)

Outcome: physical channel model

- normalized gain
- delay

between two peer entities (TN and RN)
MOLECULE DIFFUSION CHANNEL MODEL

Questions and answers

- What type of information?
  - Any continuous scalar signal

- How to encode information?
  - Transmission signals will be encoded into particle concentration variations

- How to transmit?
  - Transmitter should modulate particle concentration

- How information propagates?
  - Through particle diffusion

- How to receive?
  - Receiver should sense particle concentration → translate into received signal
Molecule diffusion wireless communication:
- **Transmitter**: modulates molecule concentration
- **Propagation**: free diffusion of molecules
- **Receiver**: senses molecule concentration
The transmitter is related to the Emission process, the propagation to the Diffusion process and the receiver to the Reception process.
MOLECULE DIFFUSION CHANNEL MODEL
Particle Emission Process (1/2)

- Release/capture of particles at the transmitter location
- Box with inside molecule concentration and aperture to the outside
  - The inside concentration is varied according to the signal to be transmitted
  - Particle outgoing/ingoing flux stimulated by inside-outside concentration gradient
- Emission modeled according to the laws of particle diffusion.

Positive rate modulation: \( \frac{d c_{out}}{dt} = r_s(t) > 0 \)

Negative rate modulation: \( \frac{d c_{out}}{dt} = r_s(t) < 0 \)
**MOLECULE DIFFUSION CHANNEL MODEL**

Particle Emission Process (2/2)

- Particle emission model → electrical parallel RC circuit
  - **Input current**: signal to be transmitted
  - **Circuit voltage**: particle inside-outside concentration gradient
  - **Resistor current**: the particle concentration rate stimulated by the transmitter
  - **Resistance**: inversely proportional to the diffusion constant
  - **Capacitance**: unitary value

![Electrical Parallel RC Circuit Diagram]

\[ \begin{align*}
I_{in}(t) & \rightarrow Q_e \\
C_e & \quad V_e \\
I_C(t) & \quad I_{out}(t) \\
R_e &
\end{align*} \]
MOLECULE DIFFUSION CHANNEL MODEL
Particle Diffusion Process (1/4)

Diffusion process

Thermodynamics

Process boundary and starting conditions
Process equilibrium state

Kinetics

Atoms/molecules mechanics
Process rate and evolution

We focused on this
Molecule Diffusion Channel Model
Particle Diffusion Process (2/4)

- Concentration rate signal propagation due to particle free diffusion in space
- Free particle diffusion governed by the diffusion laws
  - The modulated concentration at transmitter location varies with respect to the other space locations
  - Particles move within the space with the trend of homogenizing their concentration → propagation of concentration rate signal
- Emission modeled according to the relativistic laws of diffusion

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MOLECULE DIFFUSION CHANNEL MODEL
Particle Diffusion Process (3/4)

- Particle diffusion model $\rightarrow$ Green’s function $G$ of the laws of diffusion
  - Non-relativistic diffusion (inhomogeneous Fick’s second law)
    \[
    \frac{\partial c(x, t)}{\partial t} = D \nabla^2 c(x, t) + f(x, t)
    \]
    - Problem: allows superluminal propagation of information signals (modulated molecule concentration)
  - Relativistic diffusion (Telegraph equation)
    \[
    \tau_d \frac{\partial^2 c(x, t)}{\partial t^2} + \frac{\partial c(x, t)}{\partial t} = D \nabla^2 c(x, t)
    \]
    - Compliant with Special Relativity and Second Law of Thermodynamics

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Particle Diffusion Process (4/4)

Non-relativistic Diffusion

Relativistic Diffusion

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Particle Reception Process (1/2)

- Sensing of the particle concentration at the receiver location
- N chemical receptors involved in capture/release
  - The outside concentration varies and stimulates complex formation/breaking
  - The particle receiver modulates the output according to number of complexes
- Reception modeled according to the ligand-receptor binding process

\[ \text{ligand} + \text{receptor} \rightarrow \text{complex} \] (particle capture)

\[ \text{complex} \rightarrow \text{ligand} + \text{receptor} \] (particle release)
Particle Reception model $\rightarrow$ electrical series RC circuit

- **Input voltage**: molecule concentration to receiver
- **Circuit current**: particle inside-outside concentration gradient
- **Resistor current**: the molecule concentration rate sensed by the receiver
- **Resistance**: inversely proportional to the ligand-receptor binding/release rates
- **Capacitance**: number of receptors

![RC Circuit Diagram]
MOLECULE DIFFUSION CHANNEL MODEL

Numerical Results (1/4)

- **Model parameters:**
  - **Range:** from 0 micron to 50 micron
  - **Frequency spectrum:** from 0 to 1KHz
  - **Diffusion coefficient:** $D = 10^{-6} \text{ m}^2/\text{sec}$ (calcium molecules diffusing in a biological environment, cellular cytoplasm)
  - **Relativistic relaxation time:** water molecules = $10^9\text{sec.}$
  - **Ligand binding/release rates:** assumed to be $10^8 \text{ 1/(M sec)}$
  - **Number of receptors:** from 20 to 100

- The curves related to higher values of the transmitter-receiver distance show lower values of normalized gain throughout the frequency spectrum range.

- For every curve, each frequency is delayed by a different time → the shape of the channel output signal is distorted with respect to the channel input signal (more pronounced for higher values of the transmitter-receiver distance)
MOLECULE DIFFUSION CHANNEL MODEL
Numerical Results (2/4)
MOLECULE DIFFUSION CHANNEL MODEL
Numerical Results (3/4)
MOLECULE DIFFUSION CHANNEL MODEL
Numerical Results (4/4)
FURTHER RESEARCH CHALLENGES FOR CHANNEL MODEL

- Build a new information theory through the study of:
  - Noise
  - Capacity
  - Throughput

- Study a Molecular Communication system:
  - Max SNR $\rightarrow$ max throughput
  - How to minimize delay
CURRENT RESEARCH: NOISE IN MOLECULE DIFFUSION COMMUNICATION


Diffusion Process (isotropic?) → affects Bw

Chemical change (isotropic?)

Brownian motion (isotropic?)

Turbulence (anisotropic?)

Nano mac 1

Nano mac 2

Nano mac 3

Information mixing (receiver signal processing / adaptive filtering?)

same molecule as
CURRENT RESEARCH: NOISE IN MOLECULE DIFFUSION COMMUNICATION


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<th>Symbol</th>
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Nano mac 1

Nano mac 2

Nano mac 3

Extinction latency

Cross-symbol interference

Symbol usage desynchronizing
Thanks for your attention

QUESTIONS?