

Introduction to Molecular Communication

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Why Study Molecular Communications?

Imagine tiny networks with many thousands of devices

- Simple devices working cooperatively to complete challenging tasks
- Ultra-sensitive to changes in the environment
- Fully distributed and ad hoc
- Self-replicating

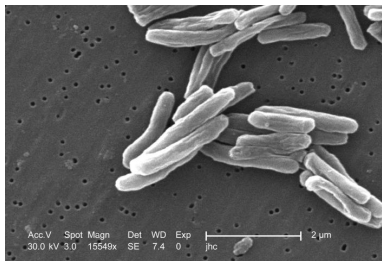
Is this a hopeless fantasy or current reality?

Richard Feynman, Caltech, 1959

“There’s Plenty of Room at the Bottom”

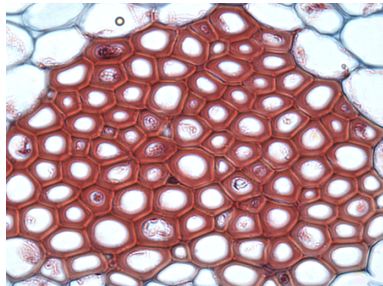
Why Study Molecular Communications?

These networks already exist in biological systems!



Community of Bacteria

Source: US CDC



Eukaryotic Cells in a Tissue

Source: Wikimedia Commons

- Single and multi-celled organisms use communication networks
- How to communicate? **Molecules** are widely used!

Part I: Introduction to Nanoscale Communication

1 Nanometer Devices and Networks

- Nanomachines
- Nanonetworks

2 Molecular Communication

- What is Molecular Communication?
- Design Strategies

Part II: Communicating via Diffusion

- 3 Mathematics of Diffusion
 - Why Diffusion?
 - Fick's Second Law
- 4 Modeling Communication Link
 - System Model
 - Transmitter Design
 - Signal at Receiver
 - Receiver Design
 - External Modification
- 5 Open Problems in Diffusive Communication
 - Physical Environment
 - Transceiver Design

Part III: Reaction-Diffusion Systems

6 Deterministic vs Stochastic Systems

7 Lattice-Based Systems

8 Particle-Based Systems

Part I

Introduction to Nanoscale Communication

- 1 Nanometer Devices and Networks
 - Nanomachines
 - Nanonetworks

- 2 Molecular Communication
 - What is Molecular Communication?
 - Design Strategies

What is a Nanomachine?

How exactly should we define a nanomachine?

- **“Nano”** - nanometre [nm] - 10^{-9} m
- Milli 10^{-3} , Micro 10^{-6} , Pico 10^{-12}
- **“Machine”** - device performing an independent task
- Tasks could be mechanical, chemical, electrical, etc.

First Definition of a Nanomachine

A nanomachine is a machine whose largest dimension is between 1 nm and $1\text{ }\mu\text{m}$

Question - Is this an appropriate definition?

What is a Nanomachine?

What objects are on the order of a nanometre in size?

- Biological cells - most between $1\text{ }\mu\text{m}$ and $100\text{ }\mu\text{m}$
- Single atoms - under 1 nm in diameter
- “Small” molecules - about 1 nm
- Proteins - $5 - 10\text{ nm}$
- Viruses - on the order of 100 nm
- Cellular Organelles (subunits) - $25\text{ nm} - 1\text{ }\mu\text{m}$

A nice visual resource:

<http://learn.genetics.utah.edu/content/begin/cells/scale/>

Another Nanomachine Definition

What is “bad” about first definition?

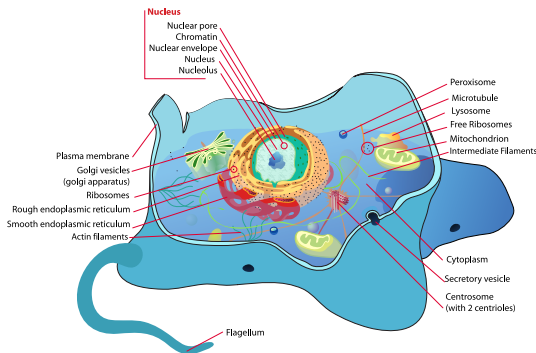
- Entire biological machines at nanoscale are truly small
- Cells are outside scope of definition
- Most subunits of cells are nanoscale

Second Definition of a Nanomachine

A nanomachine is a machine with nanoscale functional components

- This definition includes cells
- We will refer to this definition

What Can a Single Nanomachine Do?



An Animal Cell
Source: Wikimedia Commons

Cells can be very complex structures

- Food Processing, Mobility, Reproduction, Sensing
- **Communication**

What Can a Single Nanomachine Do?

Some options for synthetic nanomachine design:

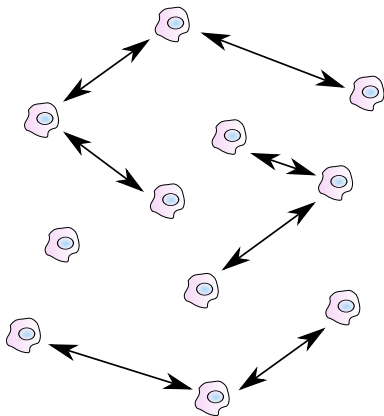
- Modified cells (genetically altered)
- Artificial cells (leave out unnecessary components)
- Downscaled electronic devices

Why consider “bio-hybrid” (e.g. cell-based) designs?

- Already a “mature” technology (evolved over billions of years)
- Biocompatibility for devices in living systems
- Improve understanding of biological systems

Cooperation: Making it Happen

Single nanomachines may be complex but limited output

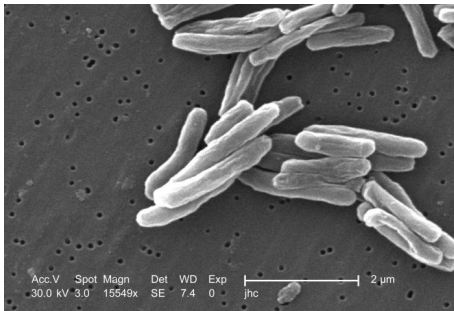


Network of Communicating Cells

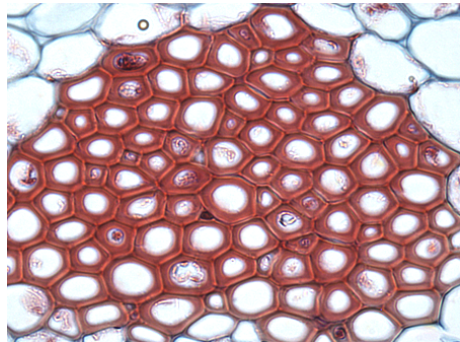
- A **Nanonetwork** is the interconnection of nanomachines
- Cooperate to perform more complex tasks
- Share different local information

Nanonetworks in Nature

Both single- and multi-celled organisms form networks



Community of Bacteria
Source: US CDC

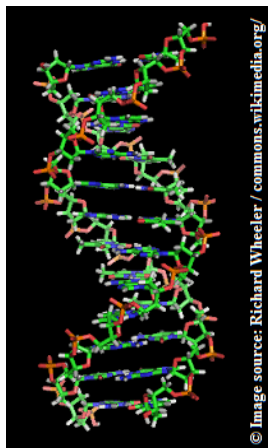


Eukaryotic Cells in a Tissue
Source: Wikimedia Commons

What Could Synthetic Nanonetworks Do?

Biomedical Applications

- Targeted drug delivery - cooperatively release medication
- Health monitoring - identify presence of toxic substances
- Regenerative medicine - rebuild damaged tissues, organs
- Genetic engineering - Manipulate DNA



DNA Double-Helix

What Could Synthetic Nanonetworks Do?

Environmental Applications

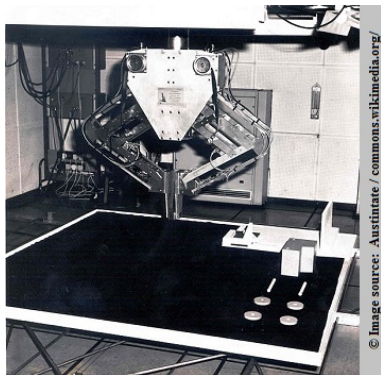


- Environmental monitoring - detection of pollutants or toxins
- Degradation - safe conversion of undesired materials

What Could Synthetic Nanonetworks Do?

Manufacturing

- Quality control - identification of product defects
- Bottom-up formation - precise construction of components
- New functionality - integrate nanonetworks into new products



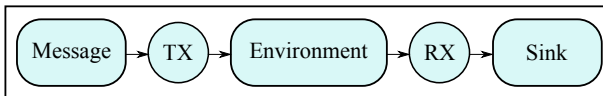
Nanonetworking for Communications Engineers

We want communication systems that are:

- **Reliable** - low probability of receiver error
- **Realistic** - achievable with current/future technology
- **Really fast** - transmit as much data as possible

Aim of Communication Analysis

Robust network design that is not application-specific but does consider the envisioned capabilities of nanomachines



- Conventional problem still exists - transmission of information

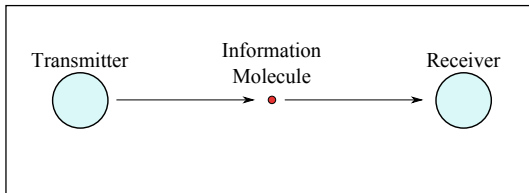
How to Build the Network?

Two main streams of nanonetwork design consider using either:

- ➊ **Electromagnetic Radiation** - a somewhat top-down design approach
- ➋ **Molecular Communication** - use molecules as information carriers

Molecular communication is a more natural choice for biologically-based nanomachines

Defining Molecular Communication



Molecular Communication

A transmitter emits information molecules that are carried to an intended receiver

Molecular Communication Characteristics

Molecular communication presents the following advantages:

- **Feasibility** - regarded as easier to implement than other approaches in the near term,
- **Scale** - appropriate size for nanomachines
- **Bio-compatibility** - integration with living systems possible (though not guaranteed!)
- **Energy Efficiency** - biochemical reactions have high efficiencies
- **Functional Complexity** - billions of years of evolution

Other advantages depend on the particular implementation

Molecular Communication Characteristics

Molecular communication presents the following challenges:

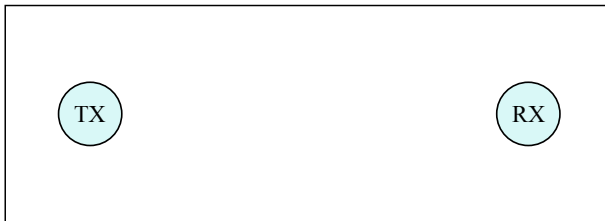
- **Stochasticity** - random propagation of molecules, environmental noise
- **Delay** - propagation times very long compared to speed of light
- **Range** - techniques can have very short practical ranges
- **Fragility** - biological components can be environmentally sensitive (temperature, pH, other reagents)

Candidate Communication Systems

List of “popular” propagation techniques

- Free diffusion
- Gap junctions
- Molecular motors
- Bacterial motors

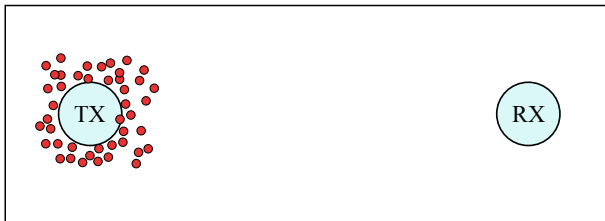
Free Diffusion



- Natural passive process within cell, amongst cells, or between organisms
- Procedure:
 - ① Transmitter floods environment with molecules (emits)
 - ② Molecules motion is entirely random
 - ③ Some molecules reach the receiver
 - ④ Molecules may enter receiver or bind to surface

We will return to diffusion later

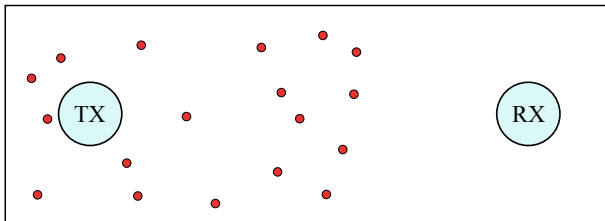
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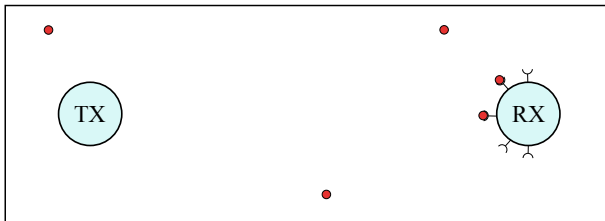
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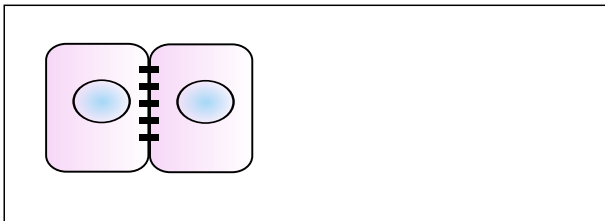
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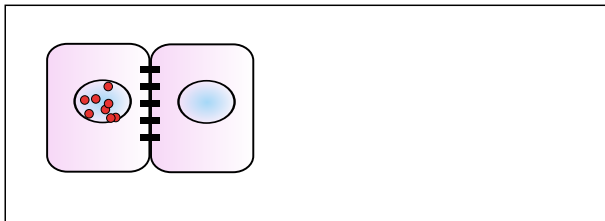
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Diffusion via Gap Junctions



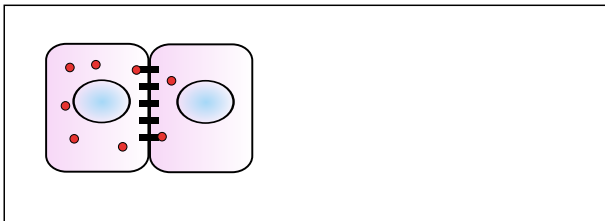
- Gap junctions - channels between adjacent cells
- Procedure:
 - 1 Transmitter creates signalling molecules
 - 2 Some molecules diffuse to adjacent cell
 - 3 Positive feedback reaction amplifies signal
 - 4 Signal can propagate far distances
- Intermediary cells act as relays

Diffusion via Gap Junctions



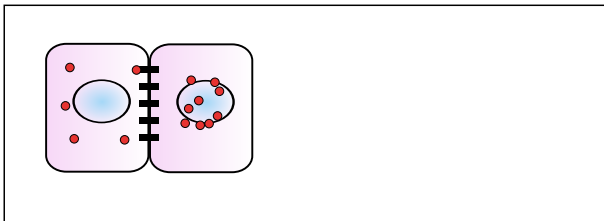
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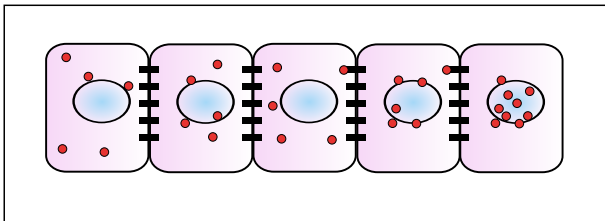
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Molecular Motors



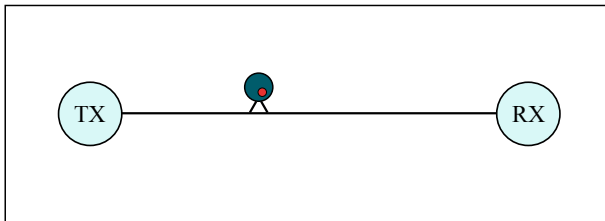
- Commonly used for intracellular transport of larger molecules
- Deploys a generic architecture
- Procedure:
 - 1 Information molecule placed in generic motor container
 - 2 Container travels along rail
 - 3 Container “opened” at receiver

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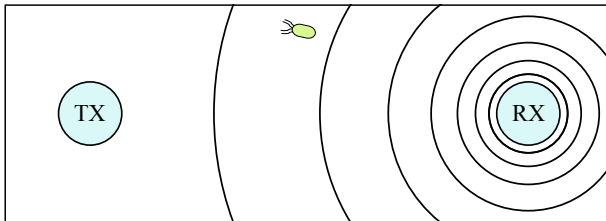
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Bacterial Motors



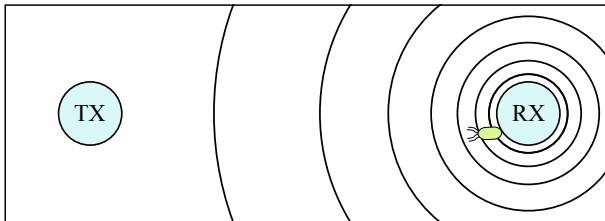
- Bacteria cells have flagella that enable propulsion
- Procedure:
 - 1 Transmitter gives DNA information to bacteria
 - 2 Bacteria runs and tumbles towards receiver
 - 3 DNA information passed to receiver upon contact

Bacterial Motors



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Part II

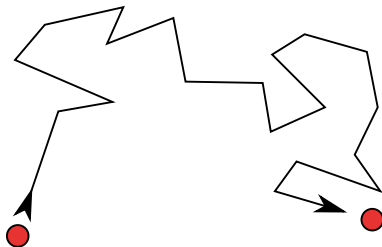
Communicating via Diffusion

- 3 Mathematics of Diffusion
 - Why Diffusion?
 - Fick's Second Law

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Features of Diffusion



- **Random walk** caused by thermal vibrations and collisions
- **Very fast** over short distances ($1\text{ }\mu\text{m}$ in 1 s)
- Bacterial cells rely on diffusion internally
- Rich literature describing diffusive processes (heat transfer, fluid dynamics)
- Most popular method to consider in communications research (thus far)

Foundation of Diffusion

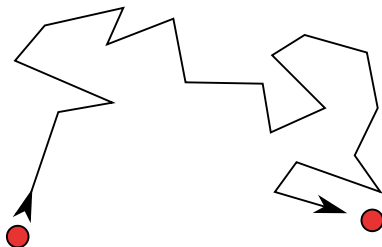
Consider being a “small” molecule immersed in liquid water

- One water molecule is 0.275 nm in diameter
- At 25 °C, water molecules move at over $500 \text{ m/s} = 5 \times 10^5 \text{ nm}/\mu\text{s}$
- There are about 33 water molecules in a 1 nm cube of pure water

A few consequences:

- 1 There are a LOT of collisions
- 2 The “small” molecule we added will be moved randomly
- 3 Gravity is essentially irrelevant at this scale

Foundation of Diffusion



A mathematical description is possible

- Adolf Fick - observed pollen diffusing in a glass
- Fick derived deterministic laws in 1855
- Based on the diffusion coefficient D (m^2/s)

Foundation of Diffusion

Fick's Second Law

$$\frac{\partial C}{\partial t} = D \nabla^2 C$$

Einstein Relation (Spherical particles)

$$D = \frac{k_B T}{6\pi\eta R}$$

- C - concentration of diffusing molecule ($\text{molecule} \cdot \text{m}^{-3}$)
- k_B - Boltzmann constant ($k_B = 1.38 \times 10^{-23} \text{ J/K}$)
- T - temperature in kelvin
- η - solvent viscosity (water, blood, etc.) in $\text{kg} \cdot \text{m}^{-1}\text{s}^{-1}$
- R - radius of diffusing molecule (m)

Diffusion Coefficients

A few more notes on diffusion coefficients:

- Generally not constant but we usually make this assumption
- For small biomolecules, value is on order of $10^{-11} \text{ m}^2/\text{s}$
- Displacement of 1 molecule along one dimension is a **normal random variable** with variance $2Dt$
- Individual molecule motion is random but with known distribution
- Collective motion of many molecules is deterministic

Solving Diffusion

Fick's Second Law

$$\frac{\partial C}{\partial t} = D \nabla^2 C$$

- A lot of literature in solving Fick's Second Law
- Solutions depend on the boundary conditions:
 - Shape of environment (infinite, rod, cylinder, sphere, etc.)
 - Source of diffusing molecules (point, surface, steady vs. impulse, etc.)
- Flow of solvent, variable temperature, etc., affects solutions
- **Many** environments have no analytical solution or infinite sums

Sample Solutions

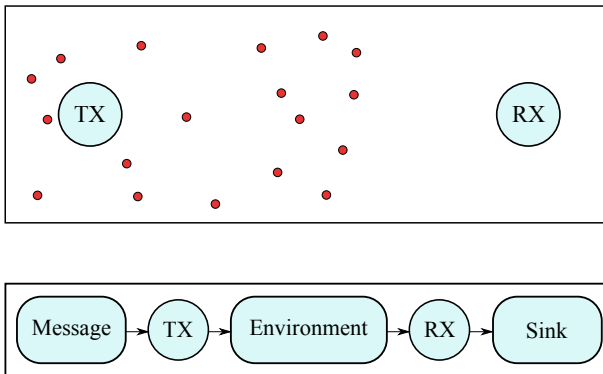
Impulsive Point Source into Infinite Environment

$$C = \frac{N}{(4\pi Dt)^{3/2}} \exp\left(\frac{-|\vec{r}|^2}{4Dt}\right)$$

Impulsive Spherical Source into Infinite Environment

$$\begin{aligned} C(r, t) = & \frac{3}{8\pi r_{obs}^2} \left[\operatorname{erf}\left(\frac{r_{obs} - r}{2\sqrt{Dt}}\right) + \operatorname{erf}\left(\frac{r_{obs} + r}{2\sqrt{Dt}}\right) \right] \\ & + \frac{3}{4\pi r_{obs} r} \sqrt{\frac{Dt}{\pi}} \left[\exp\left(-\frac{(r_{obs} + r)^2}{4Dt}\right) \right. \\ & \left. - \exp\left(-\frac{(r_{obs} - r)^2}{4Dt}\right) \right] \end{aligned}$$

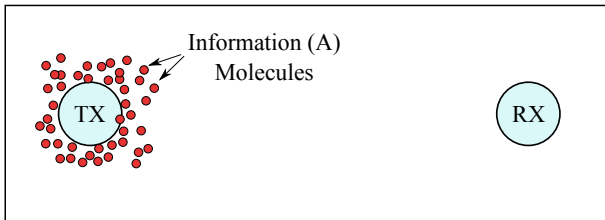
Basic Communication Model



Now we will

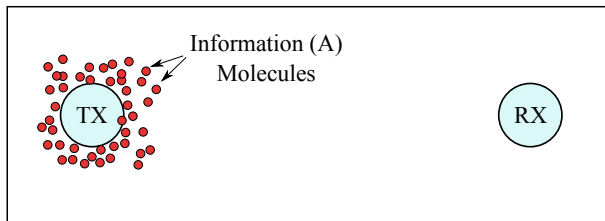
- Assume transmitter (TX) has binary message for receiver (RX)
- Highlight analysis in a diffusive communication link
- Discuss practical challenges

How Are Molecules Released?



- Cells build large containers called **vesicles**
- Biological processes can bring information molecules into vesicles
- When triggered, vesicles can be fused to cell surface
- Fusion releases contents
- Alternatively - immediate release of information molecules as they are created

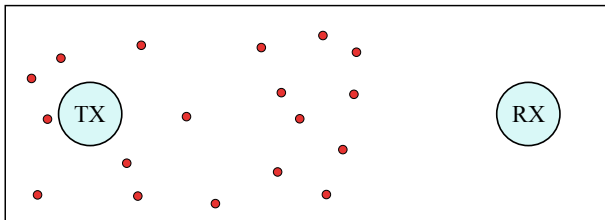
How to Modulate?



Modulation dimensions include:

- Type of molecule (A vs B molecules)
- Number of molecules (i.e., pulse amplitude modulation)
- Time of release
- Pulse-shaping

Factors Influencing # of Molecules at Receiver



- TX modulation scheme
- Environmental shape
- Diffusion coefficient, presence of flow
- Whether information molecules can be added or removed from environment

Basic Receiver Signal

Let's consider the simplest modulation in simplest environment

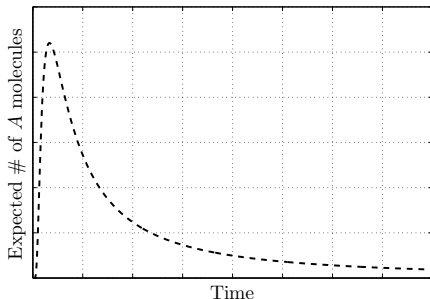
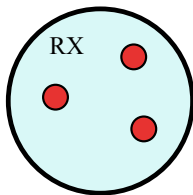
- TX emits impulse of N molecules
- Unbounded 3-dimensional environment
- Constant diffusion and no constant flow
- No change in number of molecules (i.e., no reactions)

Impulsive Point Source into Infinite Environment

$$C = \frac{N}{(4\pi Dt)^{3/2}} \exp\left(\frac{-|\vec{r}|^2}{4Dt}\right)$$

$|\vec{r}|$ - distance from TX

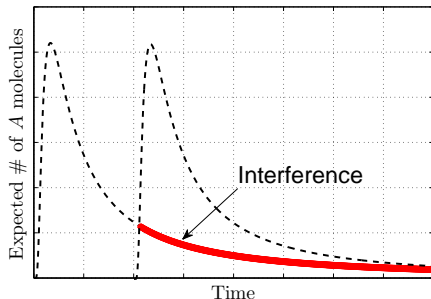
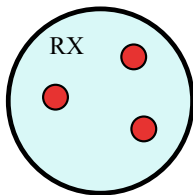
Basic Receiver Signal



Track expected # of molecules at RX when TX emits

- Large # of molecules emitted; only some reach RX
- Increase in propagation time with square of distance
- Long “tail” - long time to diffuse away
- Intersymbol interference (ISI) bottlenecks communication performance

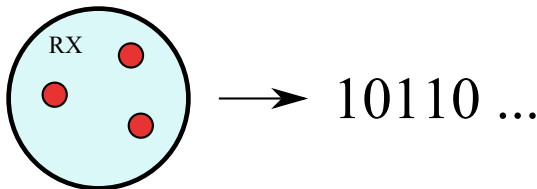
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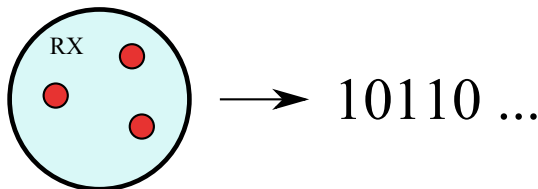
How to Design the Receiver?



Considerations in RX design:

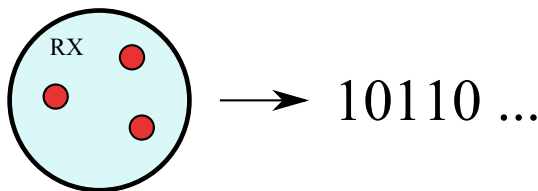
- Is RX synchronized with TX?
 - Synchronization could be achieved via external signal
- How does the RX “see” the signal?
 - Molecules absorbed by a biochemical process?
 - Molecules briefly held, facilitating some other reaction?
 - Practically, some reaction must take place
- What kind of processing is possible?

How to Design the Receiver?



- Local reactions - very difficult to analyze in multiple dimensions
- Assume ideal passive RX
- RX can “count” the # of molecules that go by
- Counting over time gives discrete samples

Receiver Analysis



What to do with the samples?

- Detection scheme needed
- Use maximum likelihood for lower bound on error probability
- Tradeoff in complexity vs. practicality

Sample Communication Scheme

Consider following scheme

- TX sequence $\mathbf{W} = \{W[1], W[2], \dots, W[B]\}$
- ON/OFF keying - N_{AEM} molecules for binary 1
- Constant bit interval T_{int}
- RX makes M samples in a bit interval
- m th sample in j th interval is $s_{j,m}$ at time $t(j, m)$
- $s_{j,m}$ are samples of received signal $N_{Aobs}(t)$
- RX decides sequence $\hat{W}[j]$

Distribution of Received Signal

- $N_{Aobs}(t)$ has time-varying mean $\overline{N_{Aobs}}(t)$
- $\overline{N_{Aobs}}(t)$ can be calculated as function of all prior intervals (additive)
- Samples $s_{j,m}$ are Poisson distributed
- PDF is

$$\Pr(N_{Aobs}(t) = \xi) = \frac{\overline{N_{Aobs}}(t)^\xi \exp(-\overline{N_{Aobs}}(t))}{\xi!}$$

- CDF is

$$\Pr(N_{Aobs}(t) < \xi) = \exp(-\overline{N_{Aobs}}(t)) \sum_{i=0}^{\xi-1} \frac{\overline{N_{Aobs}}(t)^i}{i!}$$

Maximum Likelihood Detection

- From properties of Poisson random variables we can evaluate

$$\Pr(N_{A_{obs}}) = \prod_{j=1}^B \prod_{m=1}^M \Pr(N_{A_{obs}}(t(j, m)) = s_{j,m})$$

where $N_{A_{obs}}$ is the complete set of observations, given sequence \mathbf{W}

- ML detector - evaluate $\Pr(N_{A_{obs}})$ for every possible \mathbf{W}
- Complexity reduced with Viterbi Algorithm, but still large memory and computation requirements
- Importantly, we obtain a bound on the probability of error

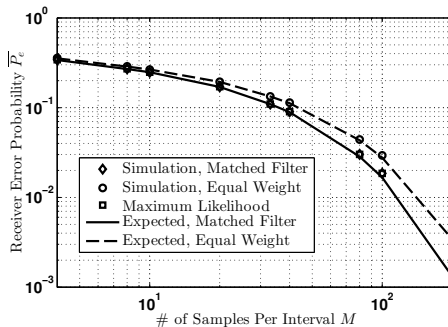
Weighted Sum Detector

- Weighted sum detector is likely more practical
- w_m - the weight of the m th sample
- ξ - decision threshold
- Decision rule is then

$$\hat{W}[j] = \begin{cases} 1 & \text{if } \sum_{m=1}^M w_m N_{Aobs}(t(j, m)) \geq \xi, \\ 0 & \text{otherwise} \end{cases}$$

- Weights scaled to $\overline{N_{Aobs}}(t)$ gives matched filter
- Equal weights are simpler but give poorer performance

Detector Performance



Source: Noel et al., IEEE Trans. on Nanobiosci., submitted Jul. 2013

Other Environmental Influences

Additive Noise Sources

- We can add “noise” sources that generate additional information molecules
- Added noise could be interference from other communication links or just other biochemical processes that create the same molecule
- Straightforward to include impact of noise in current model

Molecule Degradation

- What if environment contains enzymes (molecule destroyers)?
- Enzymes could reduce impact of ISI and make RX design easier

Enzymes in Biology

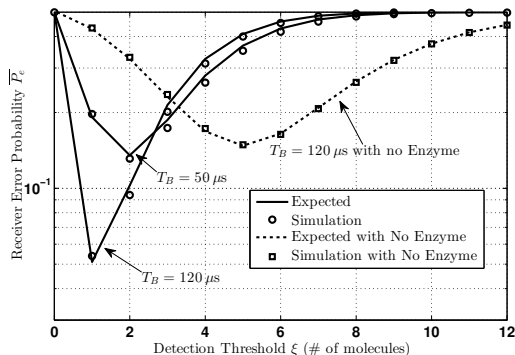


Enzymes in the neuromuscular junction between the terminal axon (T) and muscle fiber (M) reduce ISI

Source: Wikimedia Commons

- Break down information molecules without being consumed (i.e., enzymes are catalysts)
- Improve error probability or increase transmission rate
- No added complexity at the TX or RX

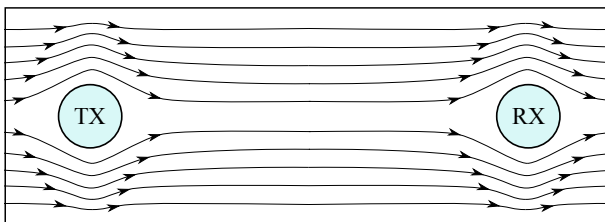
Impact of Enzymes



Source: Noel et al., IEEE Trans. on Nanobiosci., submitted Jan. 2013

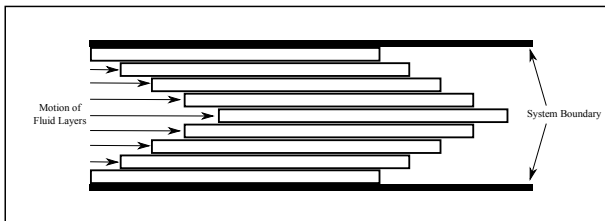
- Consider basic RX (one sample per interval compared to ξ)
- Enzymes enable faster data or less error

Flow Around Objects



- Existing flow models consider flow in one direction
- Presence of obstacles such as the TX and RX themselves can distort how molecules can diffuse

Flow in Restricted Environments

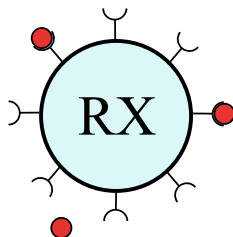


- Very narrow environments alter diffusion
- In narrow blood vessels, flow model changes significantly
- Impact of laminar flow is unstudied but realistic

Other Open Environmental Problems

- Mobility of TX and RX
- Relaying to improve transmission distance
- Multiuser interference
- Recreating environments experimentally

Open Transceiver Problems



- Learning environment (e.g. distance from TX to RX)
- Impact of complex biochemical mechanisms at RX
- Simple but adaptive RX design
- Actual formation and control of transceivers

Part III

Simulating Reaction-Diffusion Systems

6 Deterministic vs Stochastic Systems

7 Lattice-Based Systems

8 Particle-Based Systems

Reaction-Diffusion System

$$\frac{\partial C_A}{\partial t} = D_A \nabla^2 C_A - k_1 C_A C_E + k_{-1} C_{EA}$$

$$\frac{\partial C_E}{\partial t} = D_E \nabla^2 C_E - k_1 C_A C_E + k_{-1} C_{EA} + k_2 C_{EA}$$

$$\frac{\partial C_{EA}}{\partial t} = D_{EA} \nabla^2 C_{EA} + k_1 C_A C_E - k_{-1} C_{EA} - k_2 C_{EA}$$

- These are deterministic equations
- We could numerically solve deterministically
- Deterministic diffusion and reactions

Issue with Deterministic Simulations

There are a few problems with deterministic simulations:

- In practice we have discrete numbers of particles
- Deterministic solutions only valid as # of molecules is very large
- Deterministic solutions have no variance, i.e., no probability of error
- Both diffusion AND reaction are inherently stochastic

Stochastic Reaction-Diffusion

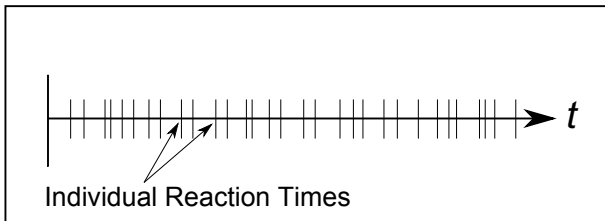
Stochastic Diffusion

Displacement of 1 molecule along one dimension is a **normal random variable** with variance $2Dt$

Stochastic Reaction

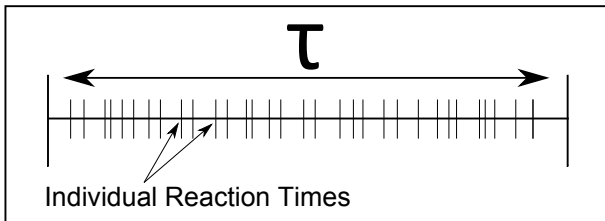
Reaction coefficient k relates to probability of a reaction occurring

Gillespie Algorithm



- Models every individual reaction
- Every execution is a feasible “trajectory”
- Stochastically exact - high accuracy
- Long computation time needed
- Concentrations of reactants must be uniform (no diffusion modeled)

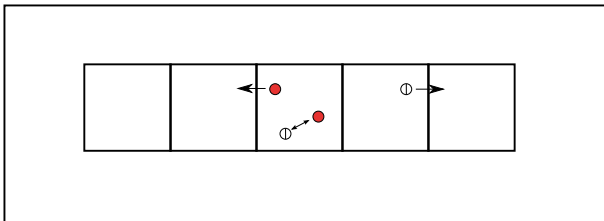
Tau-Leaping



Accelerate simulation time by leaping

- Assume reactant concentrations constant for τ
- Simultaneously execute whatever reactions occur within τ
- Tradeoff accuracy with speed with selection of τ
- Still assumes uniform concentrations (no diffusion)

Lattices in Space



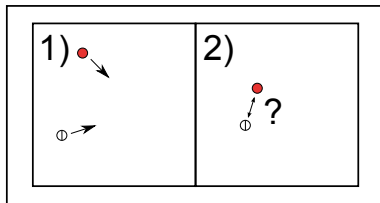
Implement diffusion as a reaction

- Divide environment into “bins”
- Discrete in space
- Diffusion reaction is movement from one bin to an adjacent bin
- Treat diffusion the same as a reaction
- Need uniform concentration in each bin

Introduction of Particle-Based Systems

- With diffusion alone, lattice-based systems are sufficient for molecular communication
- In our model, we cannot satisfy uniform concentration in practical bin sizes
- Must model exact coordinates of every molecule
- Particle-based simulation framework required
- Discrete in time, continuous in space

Workflow of Particle-Based Simulation



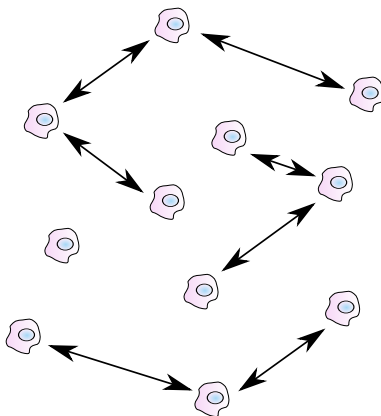
- ➊ Move all molecules based on generation of normal random variables
- ➋ Check whether reactions occur
 - Unimolecular reactions - reaction occurs with probability based on k
 - Bimolecular reactions - If molecules are close enough, then react
- ➌ Advance system time by constant time step

Part IV

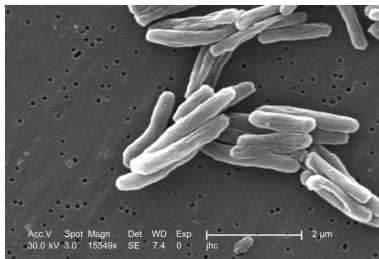
Postlude

9 Conclusions

10 Further Reading



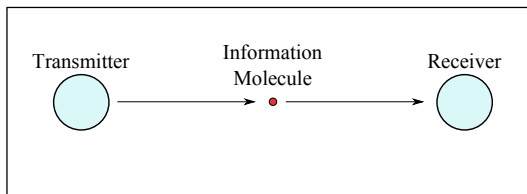
Exciting applications motivate study in the design of synthetic nanonetworks



Community of Bacteria
Source: US CDC

Nature has provided mechanisms to facilitate communication between small, independent devices

Communication Analysis



Molecular communication has many interesting problems for communication engineers

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Introduction to Molecular Communication

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