Stochastic Simulation of Reaction-Diffusion Systems

Adam Noel

School of Engineering
University of Warwick

WCPM Seminar
26 November, 2018

Presentation Summary

Why are we here?

(Some) comms engineers interested in reaction-diffusion systems

Presentation Summary

Why are we here?

(Some) comms engineers interested in reaction-diffusion systems

What have we done?

- Applied comms engineering to chemical signalling in fluids
- Developed a reaction-diffusion simulator for comms analysis

Presentation Summary

Why are we here?

(Some) comms engineers interested in reaction-diffusion systems

What have we done?

- Applied comms engineering to chemical signalling in fluids
- Developed a reaction-diffusion simulator for comms analysis

Where are we going?

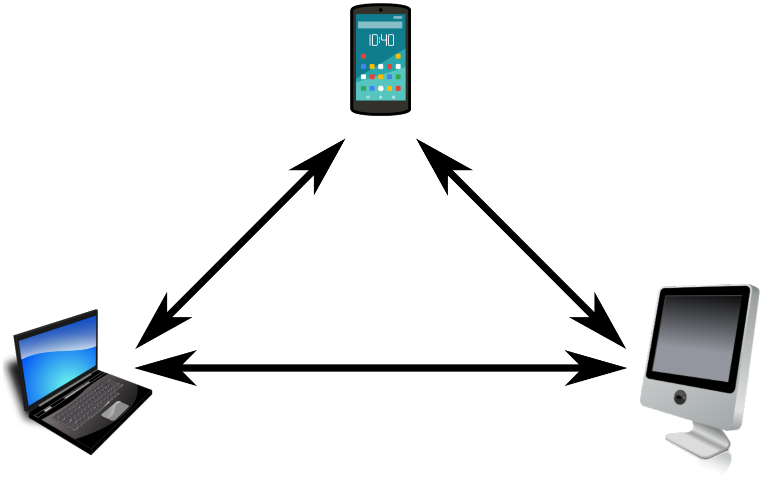
Understand and control communication in “small” natural systems

What is Communications Engineering?

Designing communication systems and measuring their performance

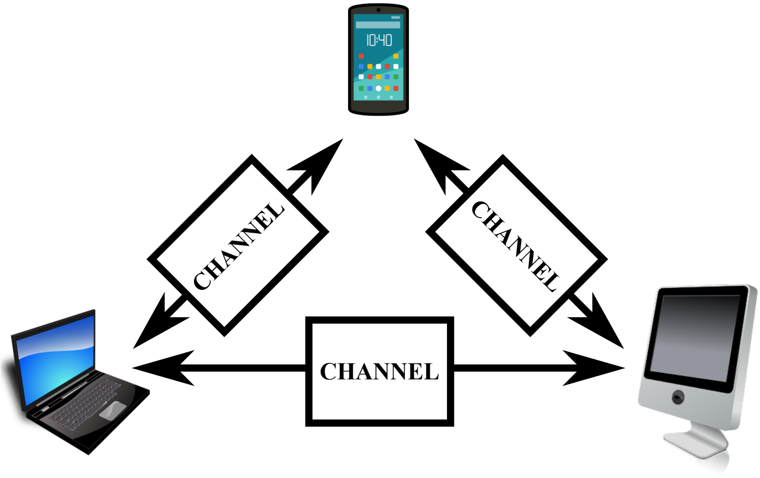
What are Communication Networks?

From conventional networks to molecular communication



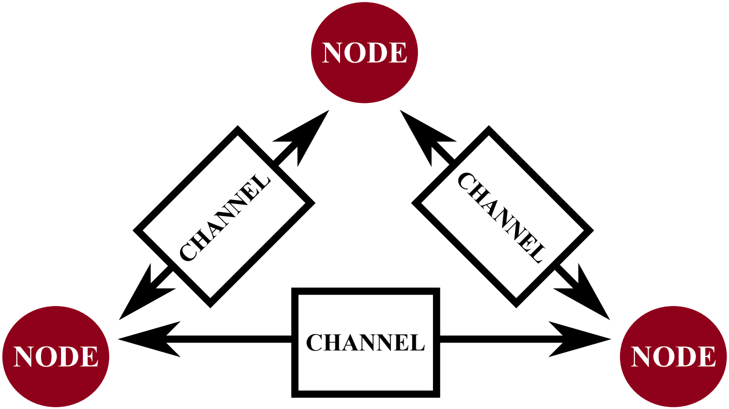
What are Communication Networks?

From conventional networks to molecular communication



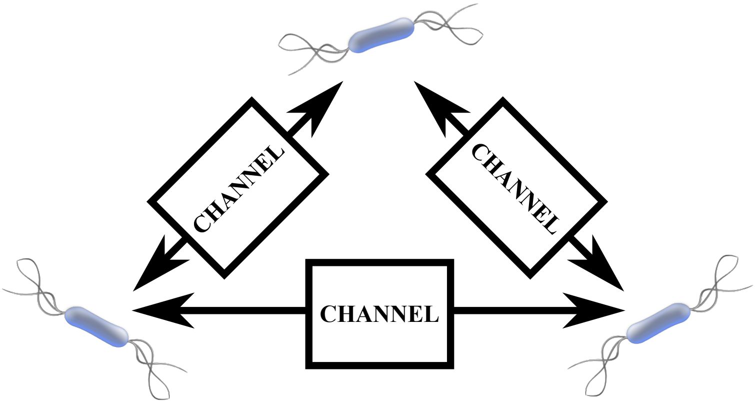
What are Communication Networks?

From conventional networks to molecular communication



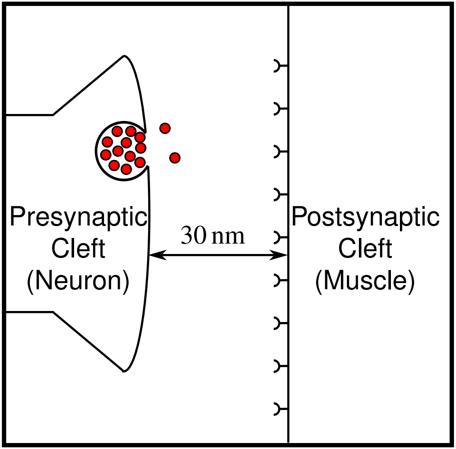
What are Communication Networks?

From conventional networks to molecular communication



Examples of Molecular Communication

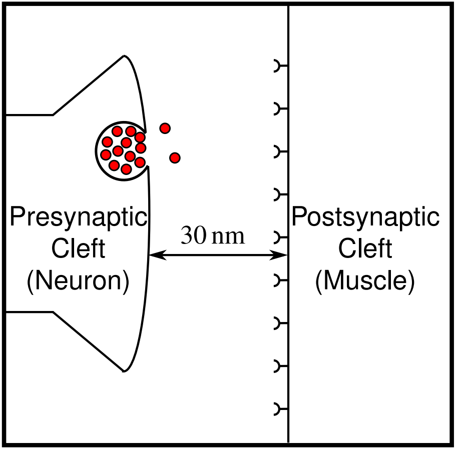
Neuromuscular Junction



Neurons control muscle contraction

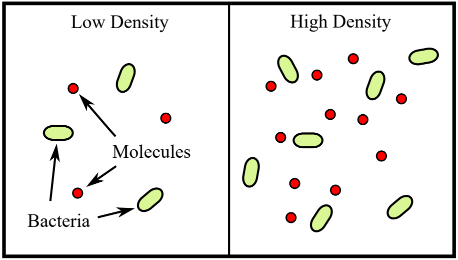
Examples of Molecular Communication

Neuromuscular Junction



Neurons control muscle contraction

Quorum Sensing



Bacteria estimate population density

How Does Engineering Integrate?

Biological Signalling $\Longleftrightarrow$ **Communications and Signal Processing**

Long-Term Question

How to design small systems with living and synthetic devices where we can predict and control behaviour?

Future Applications of Molecular Communication

Future Applications of Molecular Communication

Drug delivery

Future Applications of Molecular Communication

Drug delivery

In vivo Diagnostics

Future Applications of Molecular Communication

Drug delivery

In vivo Diagnostics

Lab-on-a-chip

Future Applications of Molecular Communication

Drug delivery

In vivo Diagnostics

Lab-on-a-chip

Chemical reactors

Future Applications of Molecular Communication

Drug delivery

In vivo Diagnostics

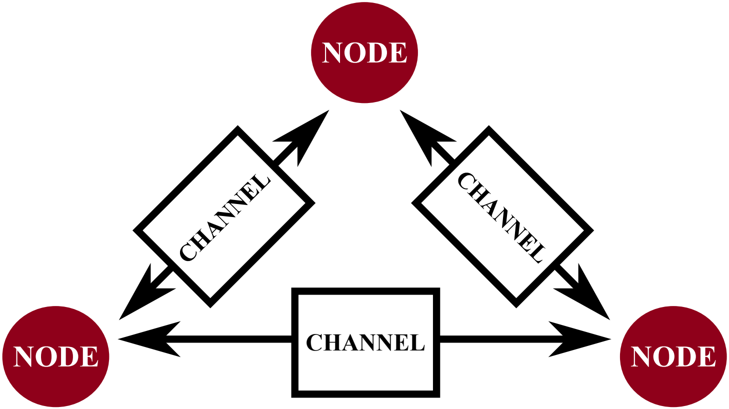
Lab-on-a-chip

Chemical reactors

Pollution monitoring

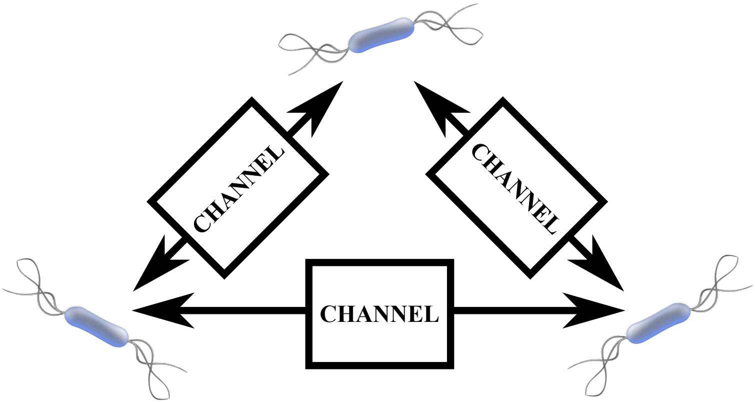
Molecular Communication Channels are Different

Nodes may be simple, molecules must be physically sent



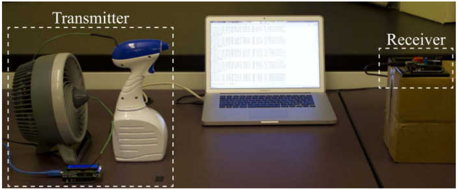
Molecular Communication Channels are Different

Nodes may be simple, molecules must be physically sent



Molecular Communication Experiments

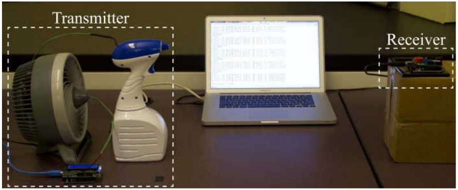
Tabletop Signalling[1]

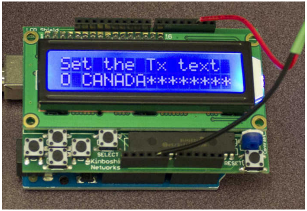


[1] Farsad, Guo, Eckford, *Proc. IEEE INFOCOM Workshops*, Apr. 2014

[2] Krishnaswamy et al., *Proc. IEEE ICC*, Jun. 2013

Tabletop Signalling[1]

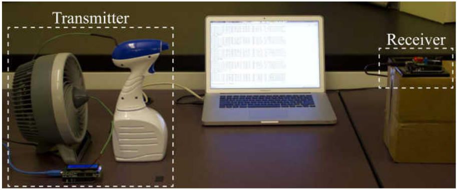


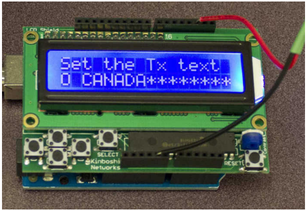


[1] Farsad, Guo, Eckford, *Proc. IEEE INFOCOM Workshops*, Apr. 2014

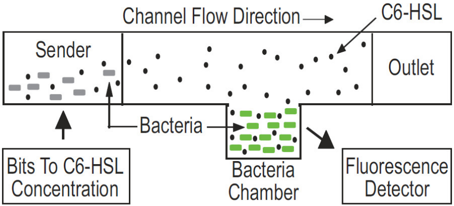
[2] Krishnaswamy et al., *Proc. IEEE ICC*, Jun. 2013

Tabletop Signalling[1]





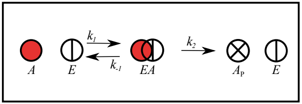
Using Bacteria as Transceivers[2]

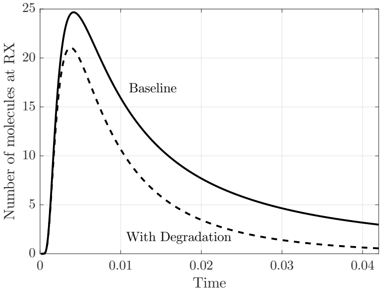


[1] Farsad, Guo, Eckford, *Proc. IEEE INFOCOM Workshops*, Apr. 2014

[2] Krishnaswamy et al., *Proc. IEEE ICC*, Jun. 2013

Molecule Degradation[1]

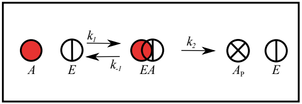


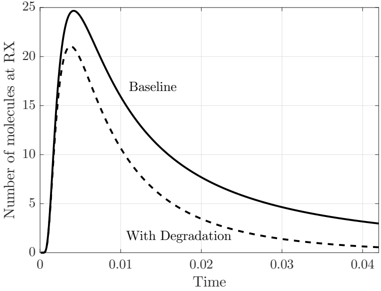


[1]Noel, Cheung, Schober, *IEEE Trans. NanoBiosci.*, Mar. 2014

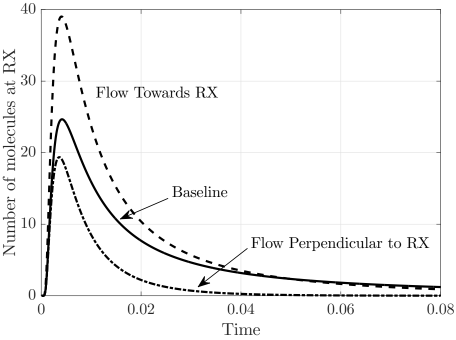
[2]Noel, Cheung, Schober, *IEEE Trans. NanoBiosci.*, Sept. 2014

Molecule Degradation[1]





Bulk Fluid Flow[2]



[1] Noel, Cheung, Schober, *IEEE Trans. NanoBiosci.*, Mar. 2014

[2] Noel, Cheung, Schober, *IEEE Trans. NanoBiosci.*, Sept. 2014

Our Contributions to Channel Modeling

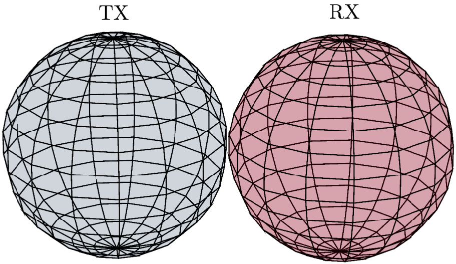
Point-to-Point Model Accuracy

Noel, Cheung, Schober, *Proc. IEEE ICC MoNaCom*, Jun. 2013

Noel, Makrakis, Hafid, *Proc. CSIT BSC*, Jun. 2016

Our Contributions to Channel Modeling

Point-to-Point Model Accuracy



Noel, Cheung, Schober, *Proc. IEEE ICC MoNaCom*, Jun. 2013

Noel, Makrakis, Hafid, *Proc. CSIT BSC*, Jun. 2016

Why Simulate Mol Comm Systems?

Generic reasons for simulation:

- Test assumptions
- Verify expected behaviour
  - E.g., Channel response, bit error rate

Why Simulate Mol Comm Systems?

Generic reasons for simulation:

- Test assumptions
- Verify expected behaviour
  - E.g., Channel response, bit error rate

Specifically for Mol Comm:

- Channels can be very complex
  - Physical space
  - Many phenomena
- Understand unfamiliar environments
- We can control/design the channel

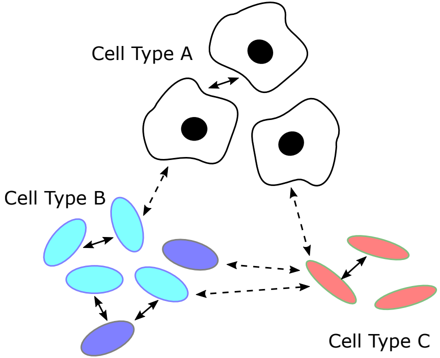
Why Simulate Mol Comm Systems?

Generic reasons for simulation:

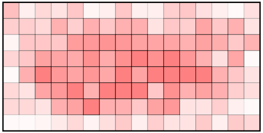
- Test assumptions
- Verify expected behaviour
  - E.g., Channel response, bit error rate

Specifically for Mol Comm:

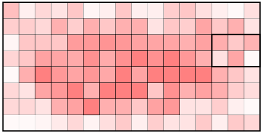
- Channels can be very complex
  - Physical space
  - Many phenomena
- Understand unfamiliar environments
- We can control/design the channel



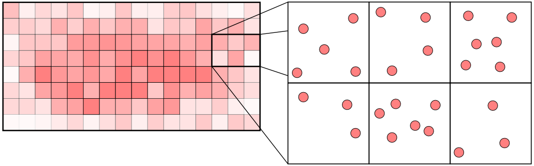
Scales of Molecular Simulations



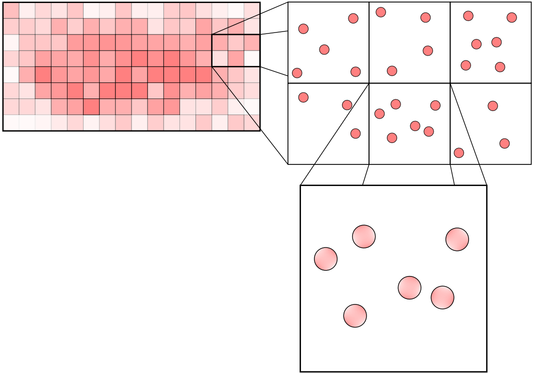
Scales of Molecular Simulations



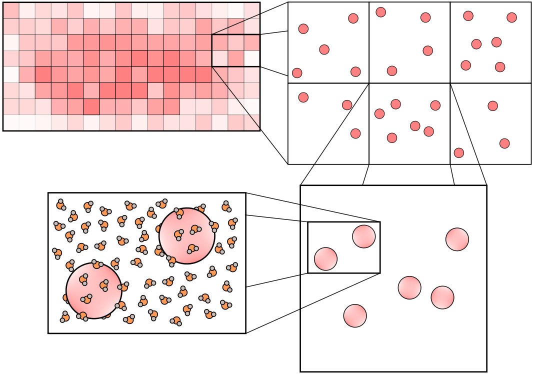
Scales of Molecular Simulations



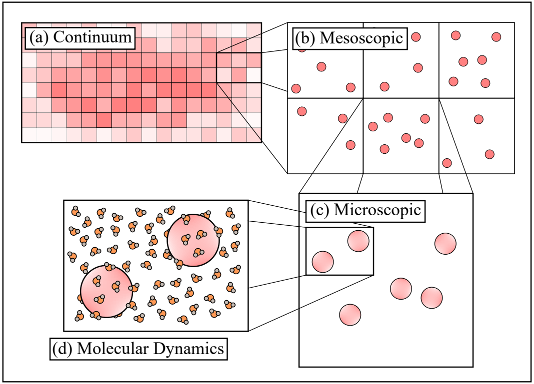
Scales of Molecular Simulations



Scales of Molecular Simulations



Scales of Molecular Simulations



Generic Simulators

Generic Simulators – Existing platforms from physical chemistry

Generic Simulators

Generic Simulators – Existing platforms from physical chemistry

Advantages:

- Advanced “sandbox” tools
- Open source and commercial platforms
- Options for all physical scales
- Many are maturely developed

Generic Simulators

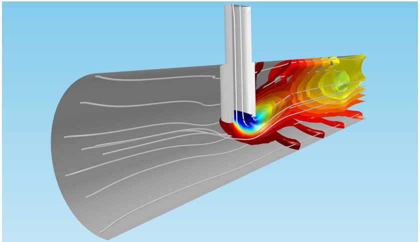
Generic Simulators – Existing platforms from physical chemistry

Advantages:

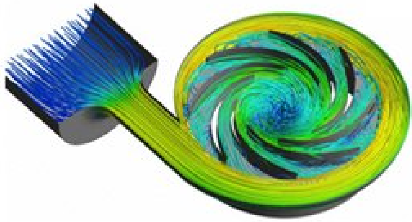
- Advanced “sandbox” tools
- Open source and commercial platforms
- Options for all physical scales
- Many are maturely developed

Disadvantages (for molecular communication):

- Not designed for data transmission
- Not designed for channel statistics
- Not always spatially tunable



COMSOL Multiphysics (Continuum)[1]

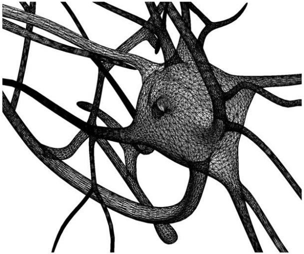


ANSYS (Continuum)[2]

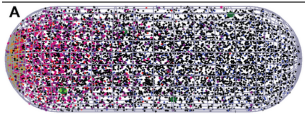
Images: [1]https://uk.comsol.com/multiphysics/what-is-mass-transfer
[2]https://www.ansys.com/products/fluids

Popular Generic Simulators

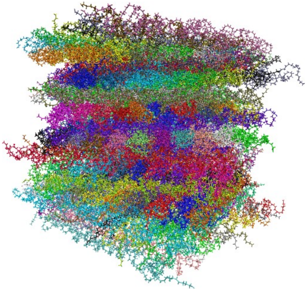
Sample Open Source Platforms



URDME (Mesoscopic)[1]



Smoldyn (Microscopic)[2]



LAMMPS (Mol. Dynamics)[3]

Images: [1]https://doi.org/10.1186/1752-0509-6-76, [2]https://doi.org/10.1371/journal.pcbi.1000705, [3]https://lammps.sandia.gov/prepost.html

Molecular Communication Simulators

Mol Comm Simulators – Developed within MC research community

Molecular Communication Simulators

Mol Comm Simulators – Developed within MC research community

Advantages:

- Designed for data transmission
- Designed for channel statistics
- Free if available

Molecular Communication Simulators

Mol Comm Simulators – Developed within MC research community

Advantages:

- Designed for data transmission
- Designed for channel statistics
- Free if available

Disadvantages:

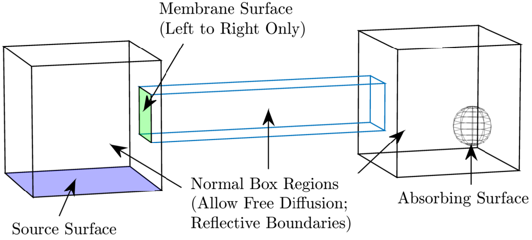
- Most are not generic solvers
  - Implement specific environments
- No options for all scales
  - Development focused on microscopic; some mesoscopic
- Not as maturely developed
- Not all readily accessible

Reaction-Diffusion Sandbox for Communications

`https://www.youtube.com/watch?v=xOGkKG8PsCE`

Noel, Cheung, Schober, Makrakis, Hafid, *Nano Commun. Networks*, Mar. 2017

AcCoRD Simulator



AcCoRD (**Ac**tor-based **Co**mmunication via **R**eaction-**D**iffusion)

- Flexible environmental design (**“sandbox”**)
- Generate *many* independent realizations
- Release molecules based on **modulated data**
- Track **number or locations** of molecules

Noel, Cheung, Schober, Makrakis, Hafid, *Nano Commun. Networks*, Mar. 2017.

Sandbox Environment Design with AcCoRD

AcCoRD: Actor-Based Communication via Reaction-Diffusion

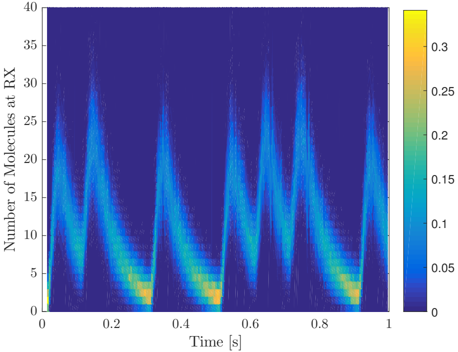
https://www.youtube.com/watch?v=7QcN6eGrC4w

Noel, Cheung, Schober, Makrakis, Hafid, *Nano Commun. Networks*, Mar. 2017

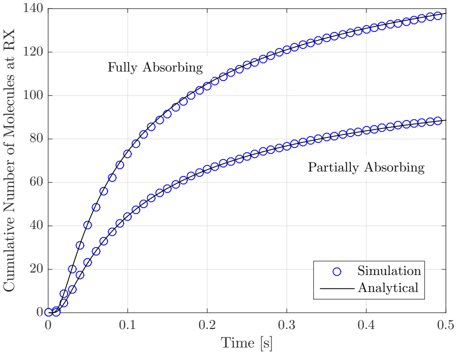
Github page: https://github.com/adamjgnoel/AcCoRD

Sample AcCoRD Results

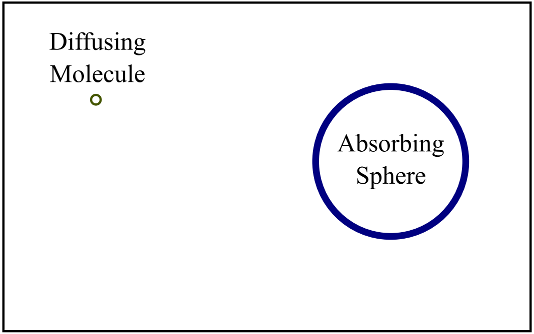
Molecule Observation Distributions



Mean Behaviour



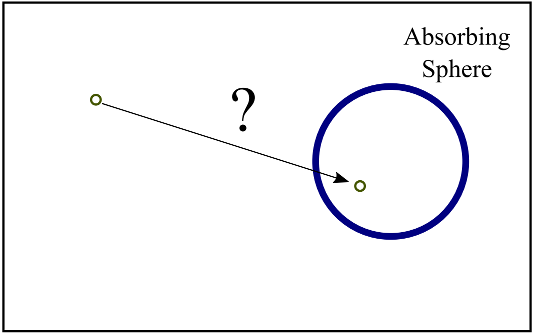
Absorbing Surfaces



- Receivers commonly modelled as absorbing surfaces

Wang, Noel, Yang, submitted to *IEEE Trans. NanoBiosci.*, Aug. 2018

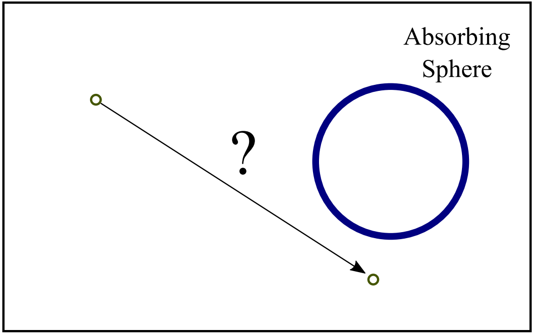
Absorbing Surfaces



- Microscopic simulation - displacements are straight lines
- “Simplistic Monte Carlo” (SMC; Arifler and Arifler, 2017)
- Final point within absorbing object is obvious

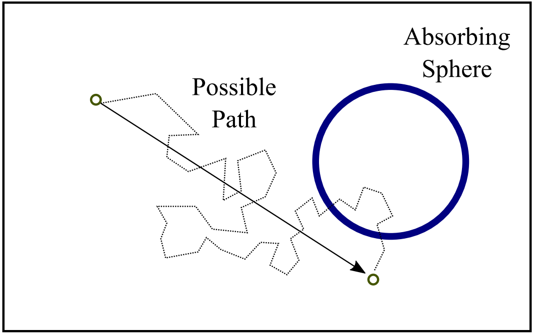
Wang, Noel, Yang, submitted to *IEEE Trans. NanoBiosci.*, Aug. 2018

Absorbing Surfaces



Wang, Noel, Yang, submitted to *IEEE Trans. NanoBiosci.*, Aug. 2018

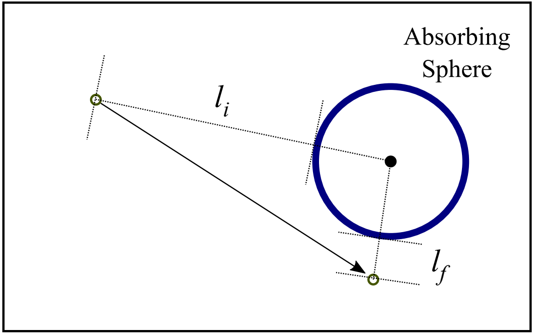
Absorbing Surfaces



- Need small time steps Δt to model path
- Absorption takes **LONG** time to simulate accurately

Wang, Noel, Yang, submitted to *IEEE Trans. NanoBiosci.*, Aug. 2018

Absorbing Surfaces



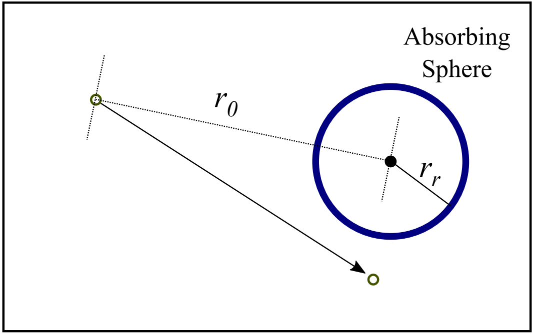
"Refined Monte Carlo" (RMC; Arifler and Arifler, 2017)

- Assume sphere is flat infinite plane and check absorption probability

$$\mathrm{Pr}_{\mathrm{RMC}} = \exp\left(-\frac{l_{\mathrm{i}} l_{\mathrm{f}}}{D\Delta t}\right)$$

Wang, Noel, Yang, submitted to *IEEE Trans. NanoBiosci.*, Aug. 2018

Absorbing Surfaces



"*A priori* Monte Carlo" (APMC)

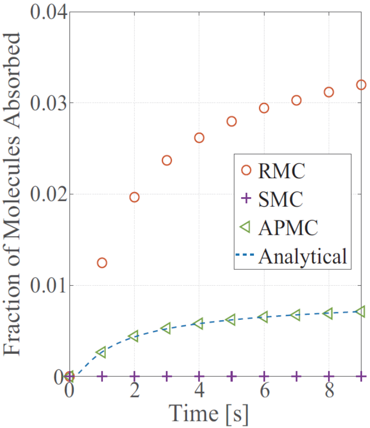
- Check for absorption **BEFORE** diffusing

$$\Pr_{\mathrm{APMC}} = \frac{r_\mathrm{r}}{r_0}\,\mathrm{erfc}\left(\frac{r_0 - r_\mathrm{r}}{\sqrt{4D\Delta t}}\right)$$

- More accurate for large time steps and when far from receiver

Wang, Noel, Yang, submitted to *IEEE Trans. NanoBiosci.*, Aug. 2018

Absorbing Surfaces
Performance

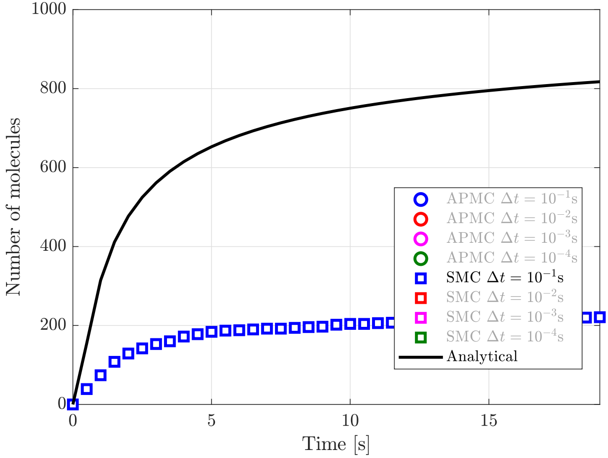


- Distance $r_0 = 50\,\mu$m, receiver radius $r_{\mathrm{r}} = 0.5\,\mu$m

Wang, Noel, Yang, submitted to *IEEE Trans. NanoBiosci.*, Aug. 2018

Absorbing Surfaces

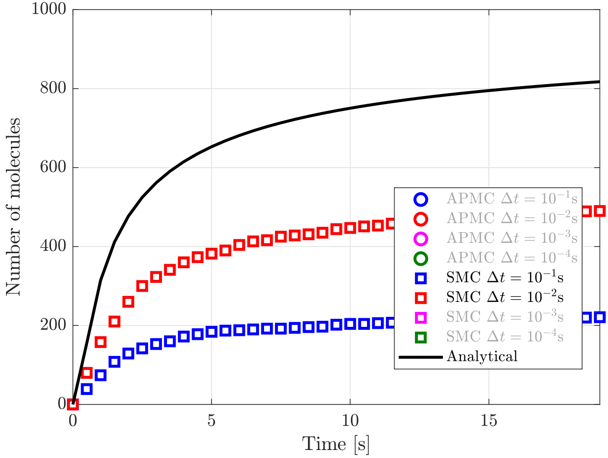
Performance with Different Δt



- Distance $r_0 = 50\,\mu$m, receiver radius $r_\mathrm{r} = 5\,\mu$m

Absorbing Surfaces

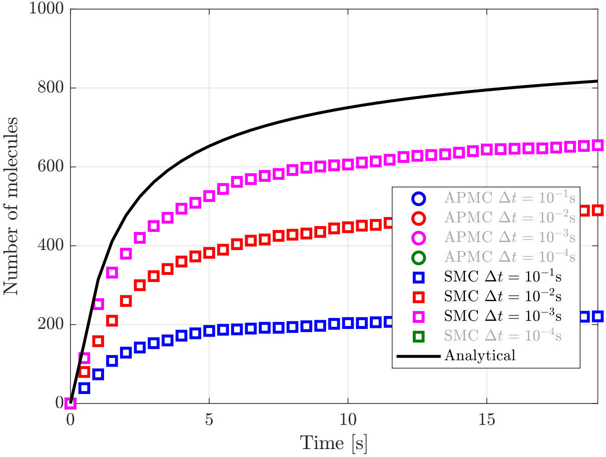
Performance with Different Δt



- Distance $r_0 = 50\,\mu$m, receiver radius $r_\mathrm{r} = 5\,\mu$m

Absorbing Surfaces

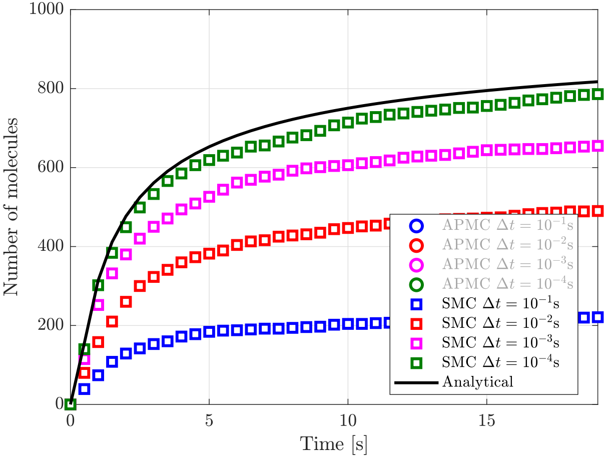
Performance with Different Δt



- Distance $r_0 = 50\,\mu$m, receiver radius $r_\mathrm{r} = 5\,\mu$m

Absorbing Surfaces

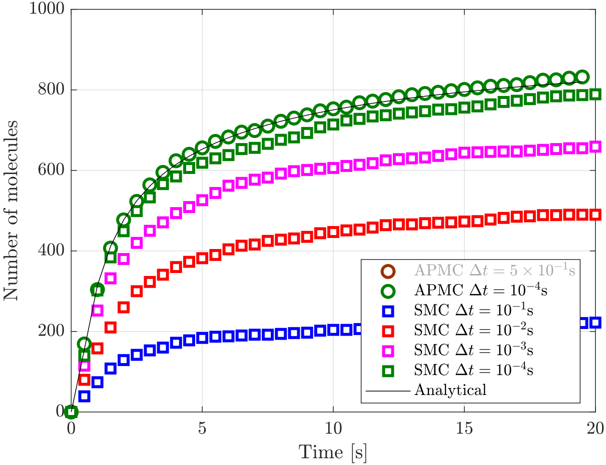
Performance with Different Δt



- Distance $r_0 = 50\,\mu$m, receiver radius $r_{\mathrm{r}} = 5\,\mu$m

Absorbing Surfaces

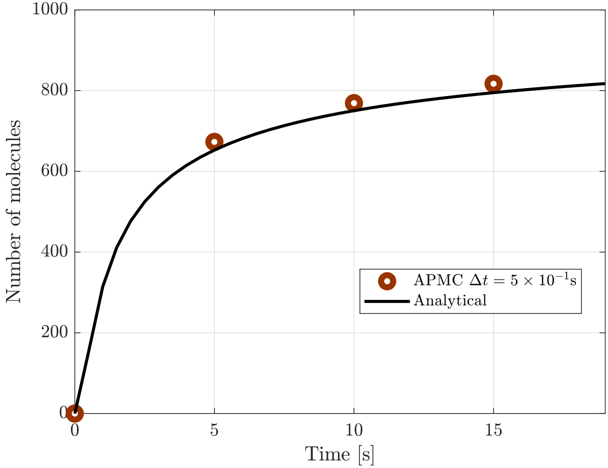
Performance with Different Δt



- Distance $r_0 = 50\,\mu$m, receiver radius $r_r = 5\,\mu$m

Absorbing Surfaces

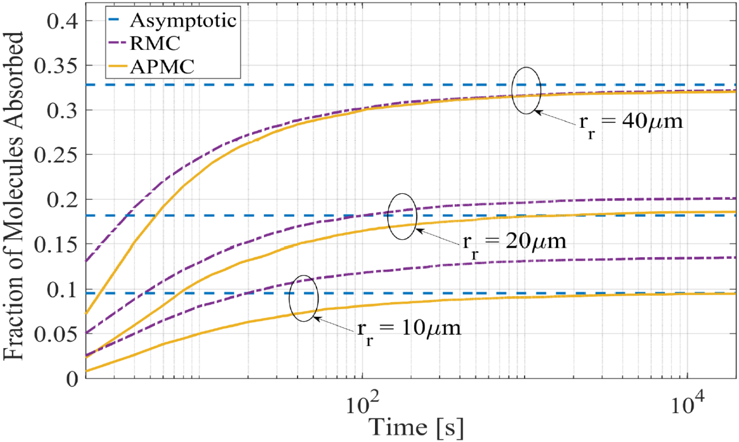
Performance with Different Δt



- Distance $r_0 = 50\,\mu$m, receiver radius $r_r = 5\,\mu$m

Absorbing Surfaces

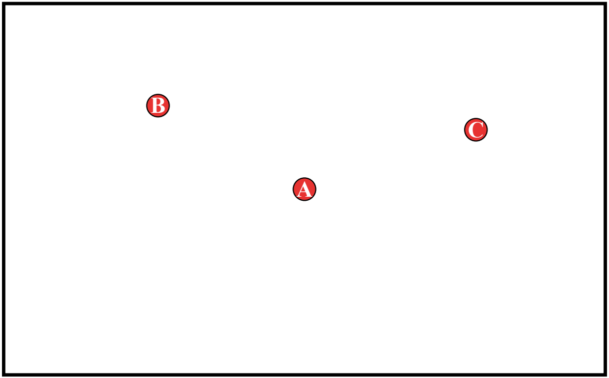
Performance with Multiple Receivers (Limited Analytical Results)



- Distance $r_0 = 100\,\mu$m, $\Delta t = 0.2\,$s

Wang, Noel, Yang, submitted to *IEEE Trans. NanoBiosci.*, Aug. 2018

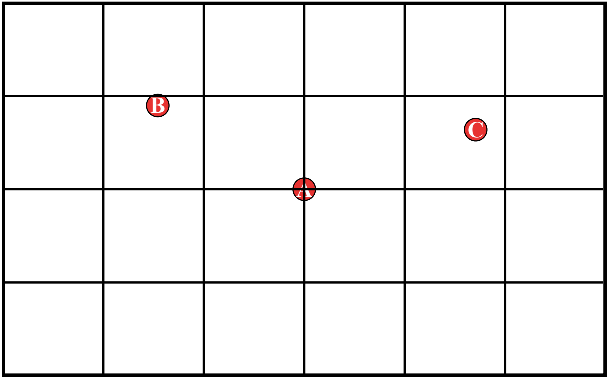
Mesoscopic Model



Divide fluid environment into **virtual subvolumes** (containers)

- Track number of molecules of each type in each subvolume
- Reaction and diffusion events change molecule counts

Mesoscopic Model



Divide fluid environment into virtual subvolumes (containers)

- Track number of molecules of each type in each subvolume
- Reaction and diffusion events change molecule counts

Mesoscopic Model

0	0	0	0	0	0
0	1	0	0	1	0
0	0	1	0	0	0
0	0	0	0	0	0

Divide fluid environment into virtual subvolumes (containers)

- Track **number of molecules of each type** in each subvolume
- Reaction and diffusion events change molecule counts

Mesoscopic Model

0	0	0	0	0	0
0	1	0	0	1	0
0	0	1	0	0	0
0	0	0	0	0	0

Divide fluid environment into virtual subvolumes (containers)

- Track number of molecules of each type in each subvolume
- Reaction and diffusion **events change molecule counts**

Mesoscopic Model

0	0	0	0	0	0
0	0	1	0	1	0
0	0	1	0	0	0
0	0	0	0	0	0

Divide fluid environment into virtual subvolumes (containers)

- Track number of molecules of each type in each subvolume
- Reaction and diffusion events change molecule counts

Mesoscopic Model

0	0	0	0	0	0
0	0	1	0	1	0
0	0	1	0	0	0
0	0	0	0	0	0

Divide fluid environment into virtual subvolumes (containers)

- Track number of molecules of each type in each subvolume
- Reaction and diffusion events change molecule counts

Mesoscopic Model

0	0	0	0	0	0
0	0	1	0	1	0
0	0	1	0	0	0
0	1	0	0	0	0

Divide fluid environment into virtual subvolumes (containers)

- Track number of molecules of each type in each subvolume
- Reaction and diffusion events change molecule counts

Mesoscopic Model

0	0	0	0	0	0
0	0	1	0	1	0
0	0	1	0	0	0
0	1	0	0	0	0

Divide fluid environment into virtual subvolumes (containers)

- Track number of molecules of each type in each subvolume
- Reaction and diffusion events change molecule counts

Mesoscopic Model

0	0	0	0	0	0
0	0	2	0	1	0
0	0	0	0	0	0
0	1	0	0	0	0

Divide fluid environment into virtual subvolumes (containers)

- Track number of molecules of each type in each subvolume
- Reaction and diffusion events change molecule counts

Mesoscopic Model

0	0	0	0	0	0
0	0	2	0	1	0
0	0	0	0	0	0
0	1	0	0	0	0

Divide fluid environment into virtual subvolumes (containers)

- Track number of molecules of each type in each subvolume
- Reaction and diffusion events change molecule counts

Mesoscopic Model

0	0	0	0	0	0
0	0	2	0	0	0
0	0	0	0	0	0
0	1	0	0	0	0

Divide fluid environment into virtual subvolumes (containers)

- Track number of molecules of each type in each subvolume
- Reaction and diffusion events change molecule counts

Mesoscopic Simulation (Gillespie Method)

Mesoscopic simulations need **rates** to predict when events occur

- Every event has a propensity α
  - α depends on the rate k, i.e., $\alpha = f(k)$
- For transitions between subvolumes, propensity is $\alpha = kU$
  - U – number of molecules of same type within subvolume

Gillespie, *Phys. Chem.*, Dec. 1977; Bernstein, *Physical Review E*, Apr. 2005

Mesoscopic Simulation (Gillespie Method)

Mesoscopic simulations need **rates** to predict when events occur

- Every event has a propensity α
  - α depends on the rate k, i.e., $\alpha = f(k)$
- For transitions between subvolumes, propensity is $\alpha = kU$
  - U – number of molecules of same type within subvolume

Next event time is then

$$t_{\text{next}} = -\frac{\log u}{\alpha}$$

where u is a uniform RV $u \in (0, 1]$

- Different ways to deal with large number of potential events

---

Gillespie, *Phys. Chem.*, Dec. 1977; Bernstein, *Physical Review E*, Apr. 2005

Mesoscopic Rates with Flow

- v – flow speed perpendicular to subvolume face (assume positive)
- D – diffusion coefficient
- k_w – transition rate in direction of flow
- k_a – transition rate against direction of flow

Diffusion Only ($v = 0$)

$$k_\mathrm{a} = k_\mathrm{w} = \frac{D}{h^2}$$

Noel, Makrakis, *IEEE Trans. NanoBiosci.*, Oct. 2018

Mesoscopic Rates with Flow

- v – flow speed perpendicular to subvolume face (assume positive)
- D – diffusion coefficient
- k_w – transition rate in direction of flow
- k_a – transition rate against direction of flow

Diffusion Only ($v = 0$)

$$k_\mathrm{a} = k_\mathrm{w} = \frac{D}{h^2}$$

"Naive" Flow Model

$$k_\mathrm{w} = \frac{D}{h^2} + \frac{v}{h}$$

$$k_\mathrm{a} = \frac{D}{h^2}$$

Noel, Makrakis, *IEEE Trans. NanoBiosci.*, Oct. 2018

Mesoscopic Rates with Flow

- v – flow speed perpendicular to subvolume face (assume positive)
- D – diffusion coefficient
- k_w – transition rate in direction of flow
- k_a – transition rate against direction of flow

Diffusion Only ($v = 0$)

$$k_\mathrm{a} = k_\mathrm{w} = \frac{D}{h^2}$$

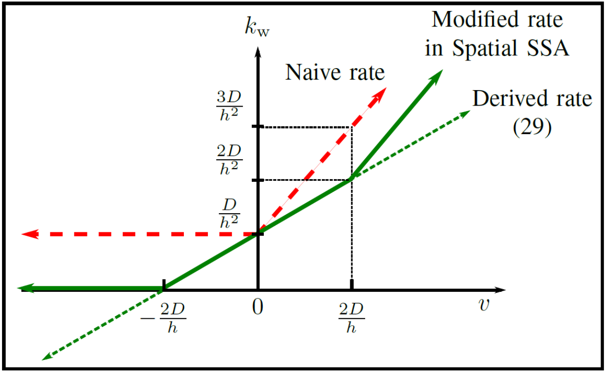
"Naive" Flow Model

$$k_\mathrm{w} = \frac{D}{h^2} + \frac{v}{h}$$
$$k_\mathrm{a} = \frac{D}{h^2}$$

Proposed Flow Model

$$k_\mathrm{w} = \frac{D}{h^2} + \frac{v}{2h}$$
$$k_\mathrm{a} = \frac{D}{h^2} - \frac{v}{2h}$$

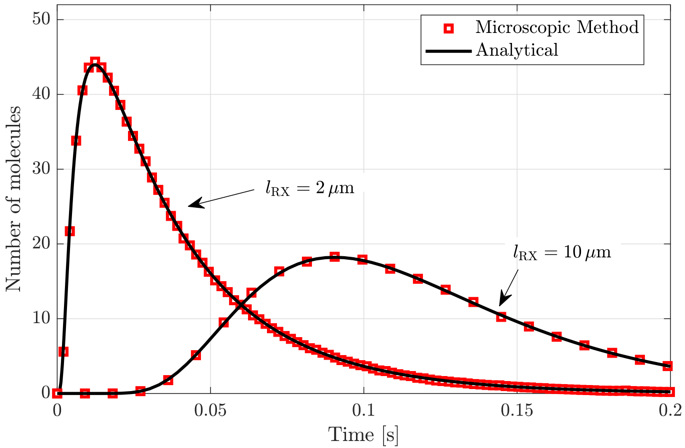
Noel, Makrakis, *IEEE Trans. NanoBiosci.*, Oct. 2018



- Need to make sure transition rates aren't negative

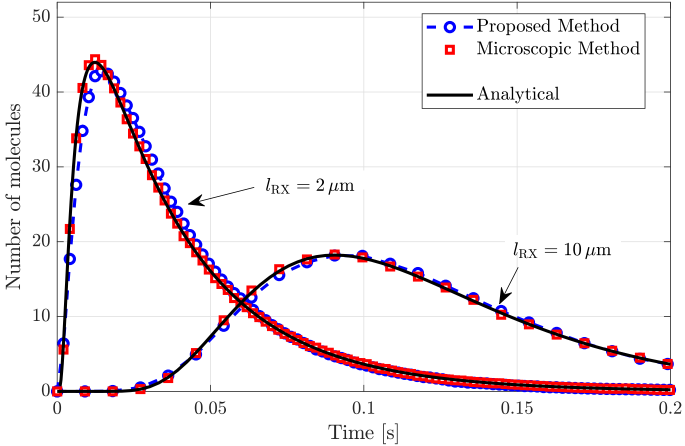
Noel, Makrakis, *IEEE Trans. NanoBiosci.*, Oct. 2018

Mesoscopic Flow
Performance



- Subvolume size $h = 1\,\mu$m, flow speed $v = 0.1$ mm/s

Noel, Makrakis, *IEEE Trans. NanoBiosci.*, Oct. 2018

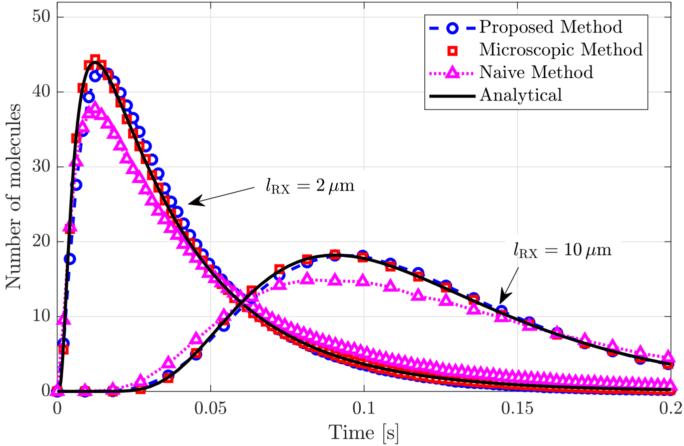


- Subvolume size $h = 1\,\mu$m, flow speed $v = 0.1$ mm/s

Noel, Makrakis, *IEEE Trans. NanoBiosci.*, Oct. 2018

Mesoscopic Flow

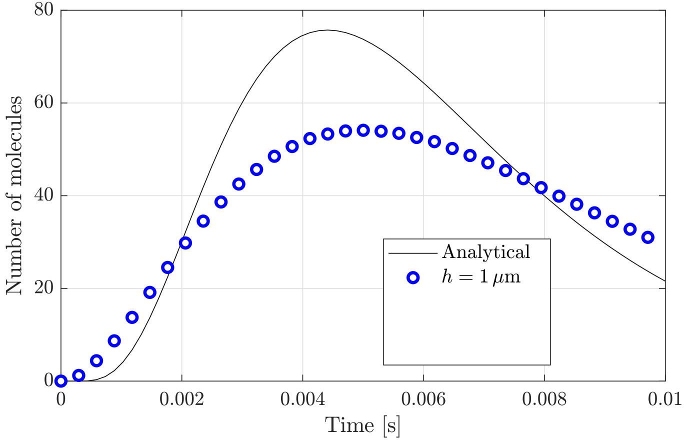
Performance



- Subvolume size $h = 1\,\mu$m, flow speed $v = 0.1$ mm/s

Noel, Makrakis, *IEEE Trans. NanoBiosci.*, Oct. 2018

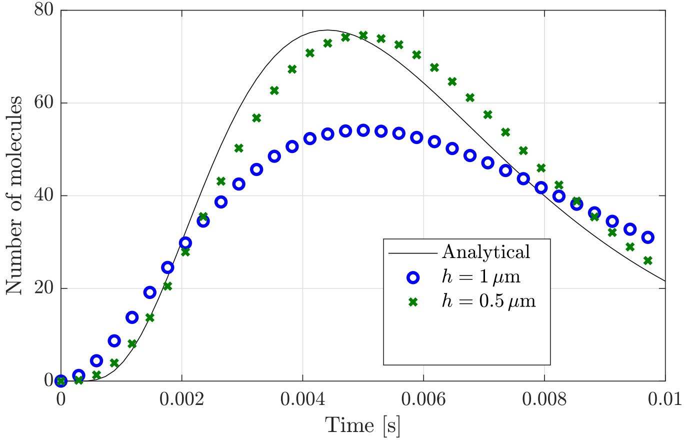
Mesoscopic Flow
Dependence on Subvolume Size



- Flow speed $v = 0.4$ mm/s, distance $l_{\mathrm{RX}} = 2\,\mu$m

Noel, Makrakis, *IEEE Trans. NanoBiosci.*, Oct. 2018

Mesoscopic Flow
Dependence on Subvolume Size



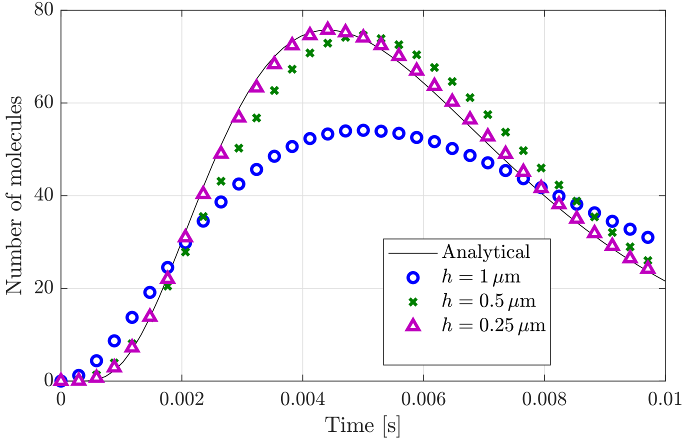
- Flow speed $v = 0.4$ mm/s, distance $l_{\mathrm{RX}} = 2\,\mu$m

---

Noel, Makrakis, *IEEE Trans. NanoBiosci.*, Oct. 2018

Mesoscopic Flow

Dependence on Subvolume Size

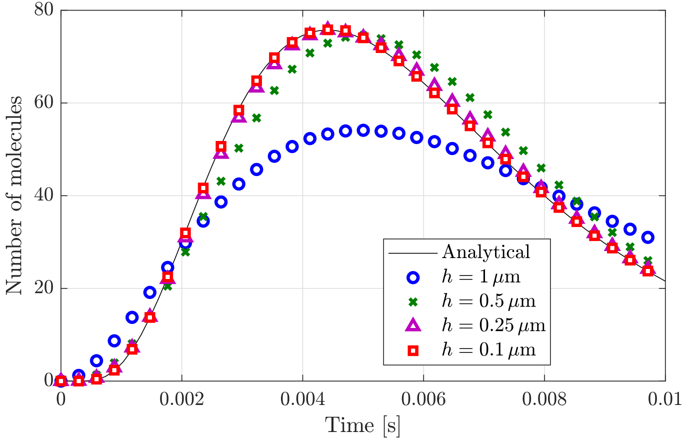


- Flow speed $v = 0.4\,$mm/s, distance $l_{\text{RX}} = 2\,\mu$m

Noel, Makrakis, *IEEE Trans. NanoBiosci.*, Oct. 2018

Mesoscopic Flow

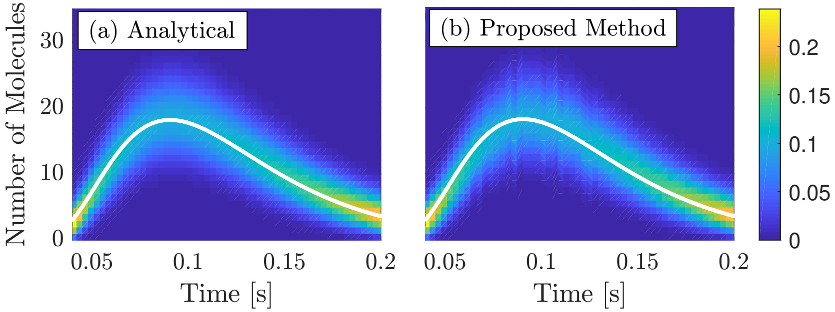
Dependence on Subvolume Size



- Flow speed $v = 0.4$ mm/s, distance $l_{\mathrm{RX}} = 2\,\mu$m

Noel, Makrakis, *IEEE Trans. NanoBiosci.*, Oct. 2018

Mesoscopic Flow
Time-Varying Statistics



- Flow speed $v = 0.1$ mm/s, distance $l_{\mathrm{RX}} = 10\,\mu$m

Noel, Makrakis, *IEEE Trans. NanoBiosci.*, Oct. 2018

Long Term Objectives

Question

How to design small systems with both living and synthetic devices where we can predict and control behaviour?

Biology

Communications and Signal Processing

Long Term Objectives

Question

How to design small systems with both living and synthetic devices where we can predict and control behaviour?

Biology

Communications and Signal Processing

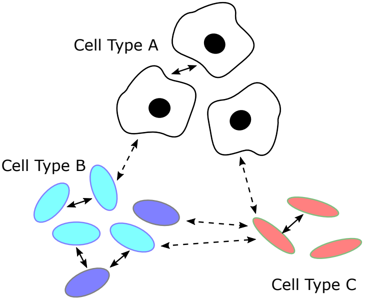
On-going topics

Use communications and signal processing tools to model:

- **Behavioural dynamics** of the system
- Devices' ability to **share information** (including living "devices")

Behaviour in Microscopic Cellular Populations

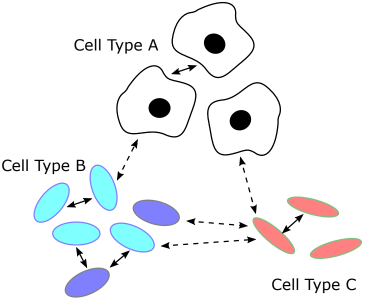
Heterogeneous Quorum Sensing



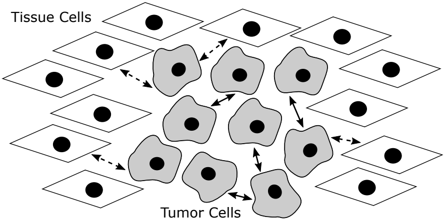
Noel, Fang, Yang, Makrakis, Eckford, https://arxiv.org/abs/1711.04870

Behaviour in Microscopic Cellular Populations

Heterogeneous Quorum Sensing



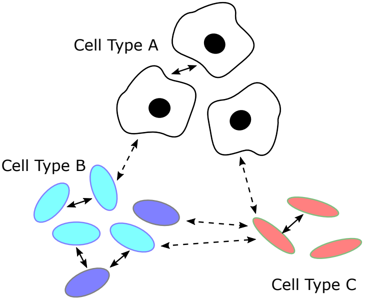
Tumour Growth and Development



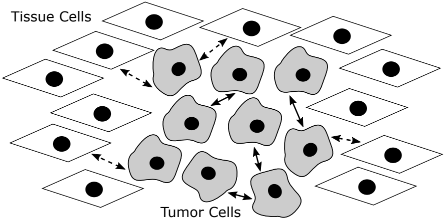
Noel, Fang, Yang, Makrakis, Eckford, https://arxiv.org/abs/1711.04870

Behaviour in Microscopic Cellular Populations

Heterogeneous Quorum Sensing



Tumour Growth and Development



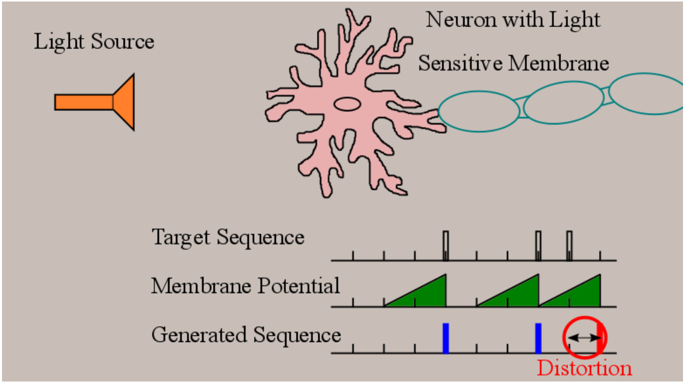
The Idea

Noisy signalling contributes uncertainty for us to mitigate or enhance

Noel, Fang, Yang, Makrakis, Eckford, https://arxiv.org/abs/1711.04870

Information Theory in Biochemical Processes

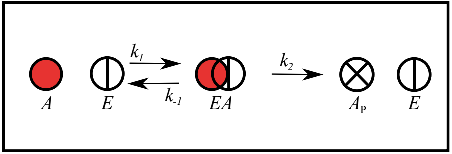
How much information is there?



- **Optogenetics** lets us externally stimulate neurons
- What are the limits to generate **any kind of spike train**?
- We are constrained by a neuron's membrane potential dynamics

Noel, Makrakis, Eckford, *IEEE Trans. Biomed. Eng.*, Dec. 2018

Information Transfer in Chemical Reactions



- Biochemical reactions occur with **significant randomness**
  - Gillespie method initially intended for chemical reactions
- **How much information can be transmitted** in a reaction?
- How well can we **statistically characterize the evolution** of a chemical reaction?

Conclusions

Communications engineering can be applied to reaction-diffusion modelling

Conclusions

Communications engineering can be applied to reaction-diffusion modelling

We want to predict and control behaviour in small natural environments

Conclusions

Communications engineering can be applied to reaction-diffusion modelling

We want to predict and control behaviour in small natural environments

Going Forward

Many open questions in behavioural dynamics and information transfer

Acknowledgements

- Primary collaborators on simulation work:
  - D. Makrakis (University of Ottawa)
  - J. Yang, Y. Wang (Australian National University)
- Funding
  - Natural Sciences and Engineering Research Council of Canada (NSERC)

The End

Thank you for your time and attention!

Homepage: `www.warwick.ac.uk/adamnoel`

AcCoRD Simulator:

`www.warwick.ac.uk/adamnoel/software/accord/`

Point vs Spherical Receiver

$\overline{N}_{\mathsf{RX}}(t)$ – number of molecules expected at RX as a function of time

3D Point Receiver Observation (Point TX) – "Classical" Result

$$\overline{N}_{\mathsf{RX}}(t) = \frac{NV_{\mathsf{RX}}}{(4\pi Dt)^{3/2}} \exp\left(-\frac{d^2}{4Dt}\right)$$

3D Spherical Receiver Observation (Point TX)

$$\overline{N}_{\mathsf{RX}}(t) = \frac{N}{2}\left[\operatorname{erf}\left(\frac{r_{\mathsf{RX}} - d}{2\sqrt{Dt}}\right) + \operatorname{erf}\left(\frac{r_{\mathsf{RX}} + d}{2\sqrt{Dt}}\right)\right] + \frac{N}{d}\sqrt{\frac{Dt}{\pi}}\left[\exp\left(-\frac{(d + r_{\mathsf{RX}})^2}{4Dt}\right) - \exp\left(-\frac{(d - r_{\mathsf{RX}})^2}{4Dt}\right)\right]$$

Noel, Cheung, Schober, *Proc. IEEE ICC MoNaCom*, Jun. 2013

Point vs Volume Transmitter

1D Receiver Observation (Point TX)

$$\overline{N}_{\mathsf{RX}}(t) = \frac{N}{2}\left(\mathrm{erf}\left(\frac{r_{\mathsf{RX}} + d}{2\sqrt{Dt}}\right) - \mathrm{erf}\left(\frac{d - r_{\mathsf{RX}}}{2\sqrt{Dt}}\right)\right)$$

1D Receiver Observation (Volume TX)

$$\overline{N}_{\mathsf{RX}}(t) = \frac{N}{2r_{\mathsf{TX}}}\left\{\sqrt{\frac{Dt}{\pi}}\left[\exp\left(-\frac{(x_{\mathsf{f}} + r_{\mathsf{RX}})^2}{4Dt}\right) - \exp\left(-\frac{(x_{\mathsf{f}} - r_{\mathsf{RX}})^2}{4Dt}\right) - \exp\left(-\frac{(x_{\mathsf{i}} + r_{\mathsf{RX}})^2}{4Dt}\right) + \exp\left(-\frac{(x_{\mathsf{i}} - r_{\mathsf{RX}})^2}{4Dt}\right)\right] + \frac{1}{2}\left[(x_{\mathsf{f}} + r_{\mathsf{RX}})\,\mathrm{erf}\left(\frac{x_{\mathsf{f}} + r_{\mathsf{RX}}}{2\sqrt{Dt}}\right) - (x_{\mathsf{i}} + r_{\mathsf{RX}})\,\mathrm{erf}\left(\frac{x_{\mathsf{i}} + r_{\mathsf{RX}}}{2\sqrt{Dt}}\right) - (x_{\mathsf{f}} - r_{\mathsf{RX}})\,\mathrm{erf}\left(\frac{x_{\mathsf{f}} - r_{\mathsf{RX}}}{2\sqrt{Dt}}\right) + (x_{\mathsf{i}} - r_{\mathsf{RX}})\,\mathrm{erf}\left(\frac{x_{\mathsf{i}} - r_{\mathsf{RX}}}{2\sqrt{Dt}}\right)\right]\right\}$$

Noel, Makrakis, Hafid, *Proc. CSIT BSC*, Jun. 2016