Simulation Methods for Molecular Communication

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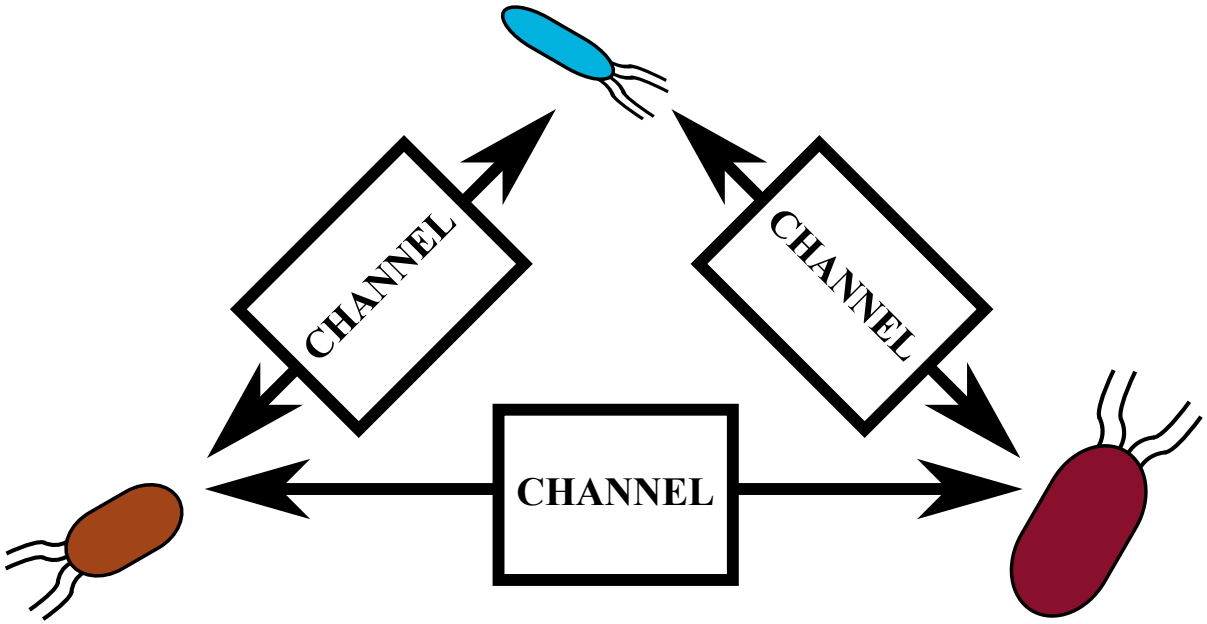
4th Molecular Communications Workshop
Linz, Austria
17 April, 2019

Summary

Learning Objectives

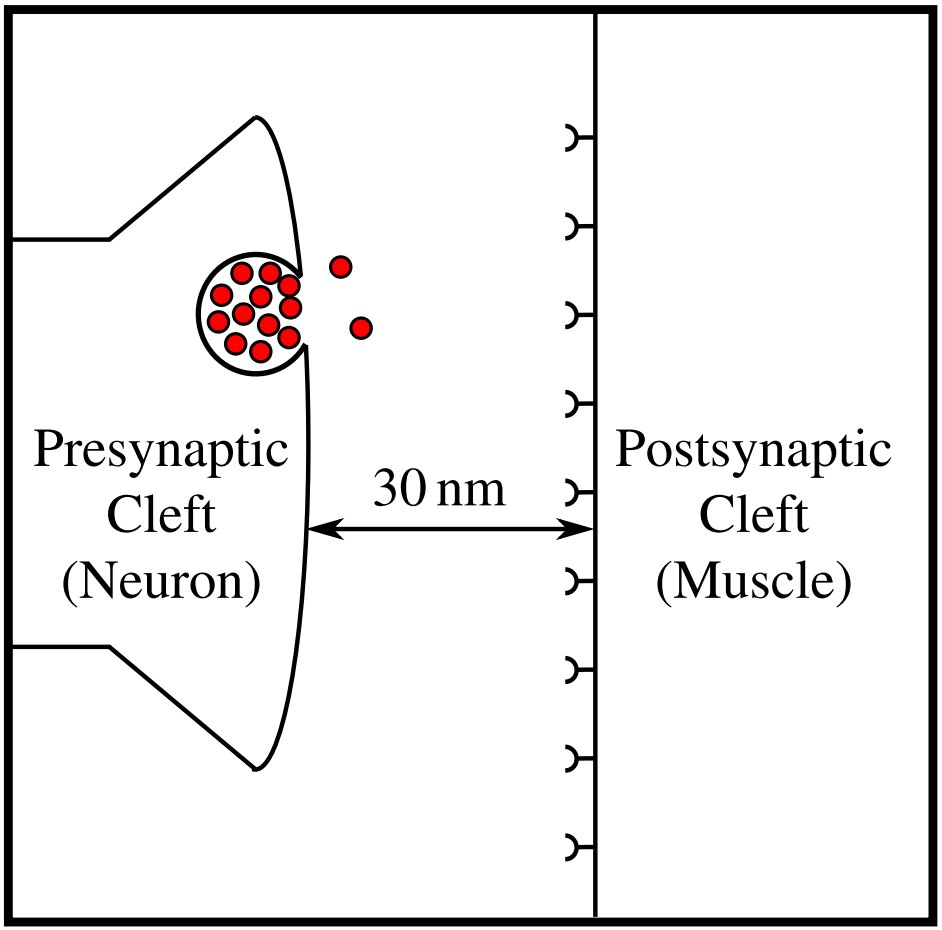
- Introduce molecular communication (MC)
- Understand importance of MC simulations
- Understand the different scales of MC simulation
- Compare different simulation platforms
- Use existing software tools (particularly AcCoRD)

Re-Conceptualizing Communication Networks



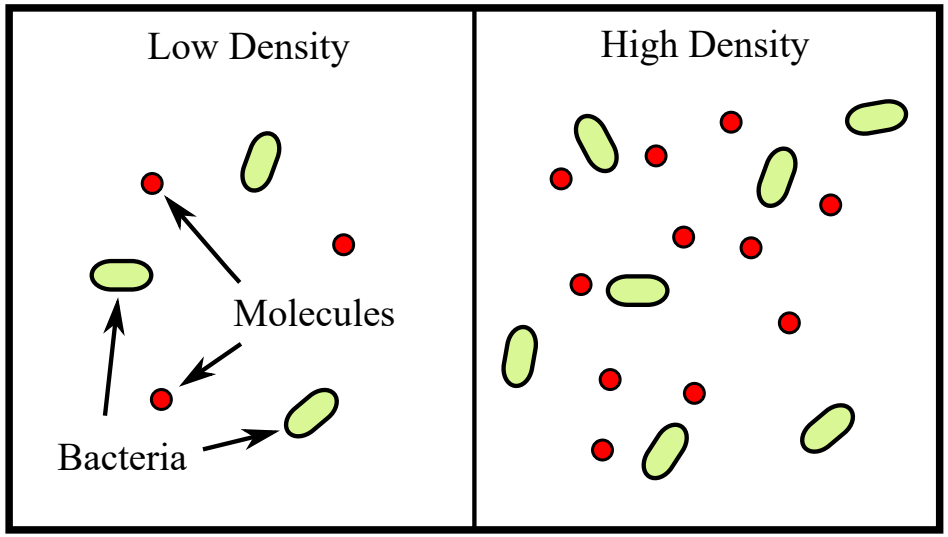
Examples of Natural Molecular Communication

Neuromuscular Junction



Neurons control muscle contraction

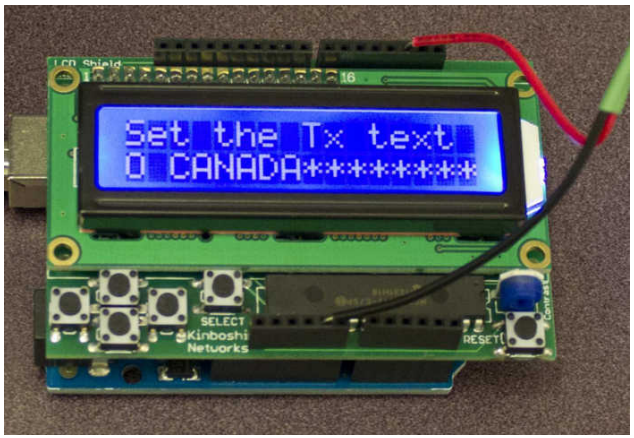
Quorum Sensing



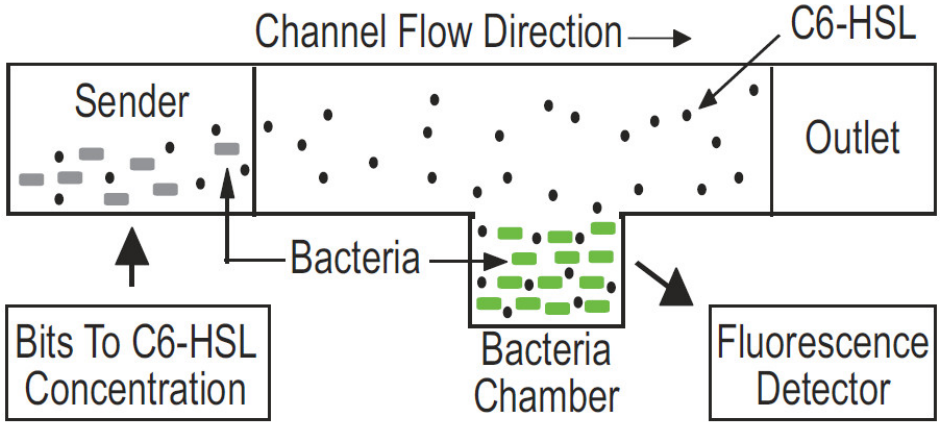
Bacteria estimate population density

Molecular Communication Experiments

Tabletop Signaling[1]



Using Bacteria as Transceivers[2]



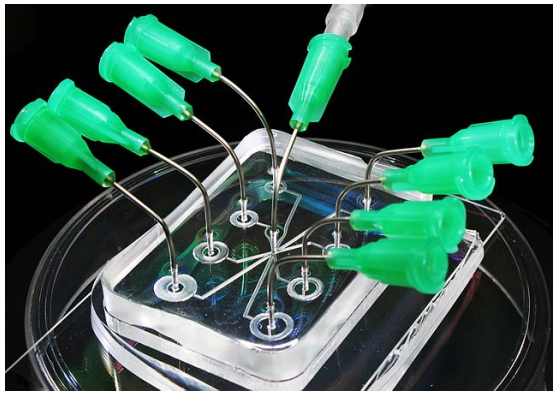
[1] Farsad, Guo, Eckford, *Proc. IEEE INFOCOM Workshops*, Apr. 2014

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

Potential Applications for Molecular Communication

Drug delivery

In vivo diagnostics

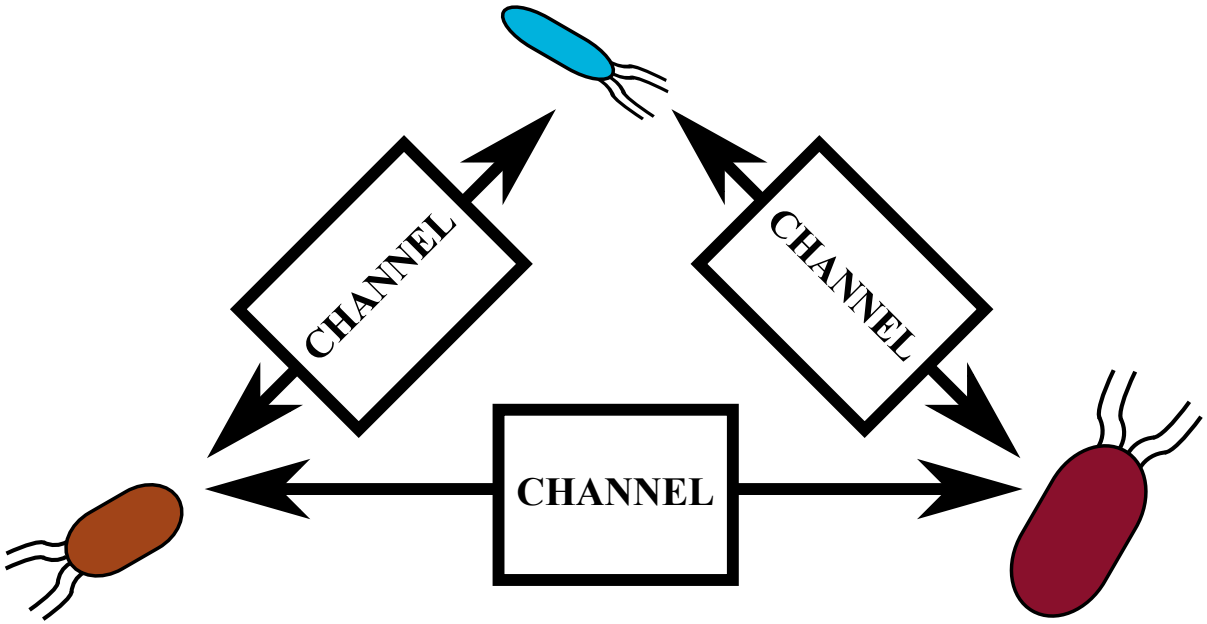


Lab-on-a-chip

Chemical reactors

Pollution monitoring

Can We Directly Apply Communications Tools?



1. Nodes may be simple (as computational devices)
2. Molecules are physically sent (channels are **very** different)

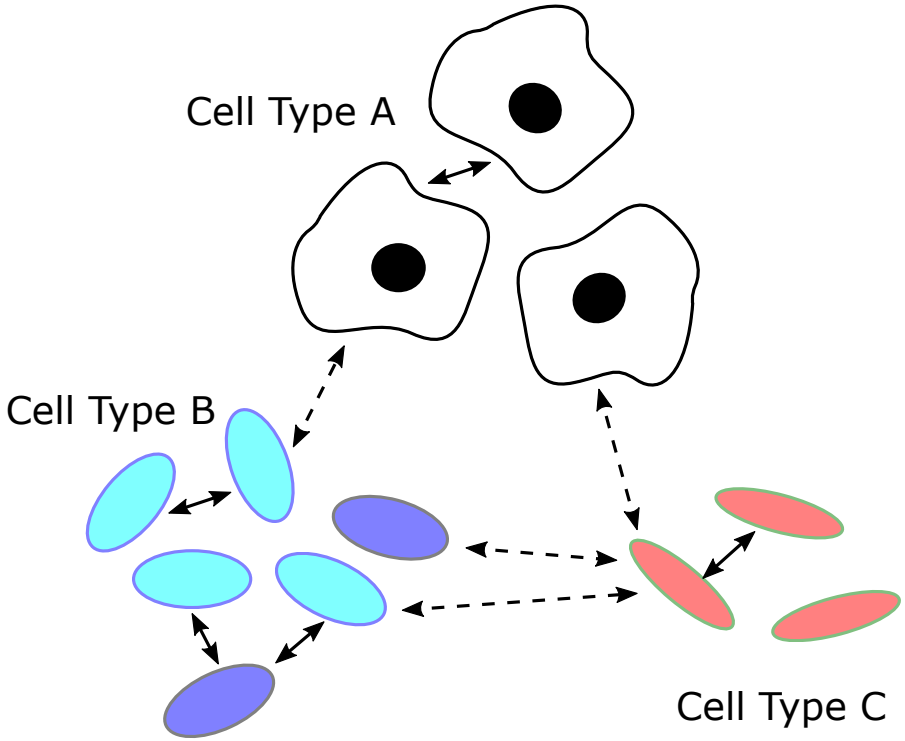
Why Simulate MC Systems?

Generic reasons for simulation:

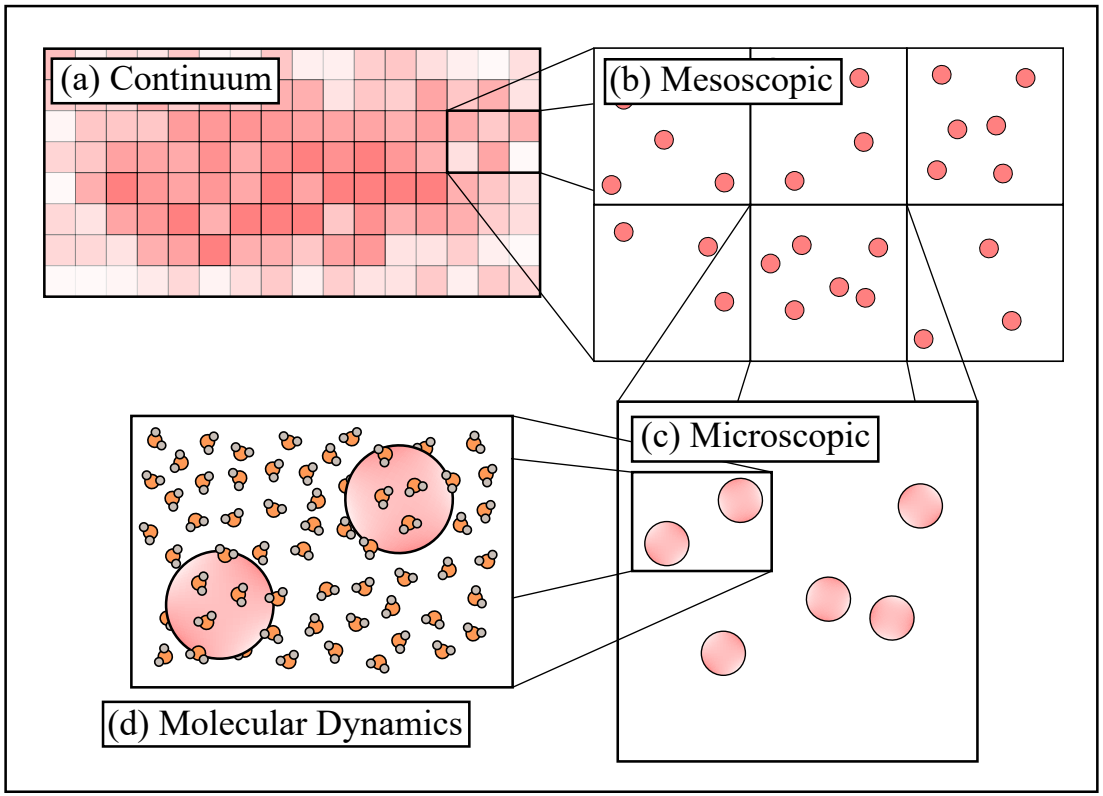
- Test assumptions
- Verify expected behavior
  - E.g., Channel response, BER

Specifically for MC:

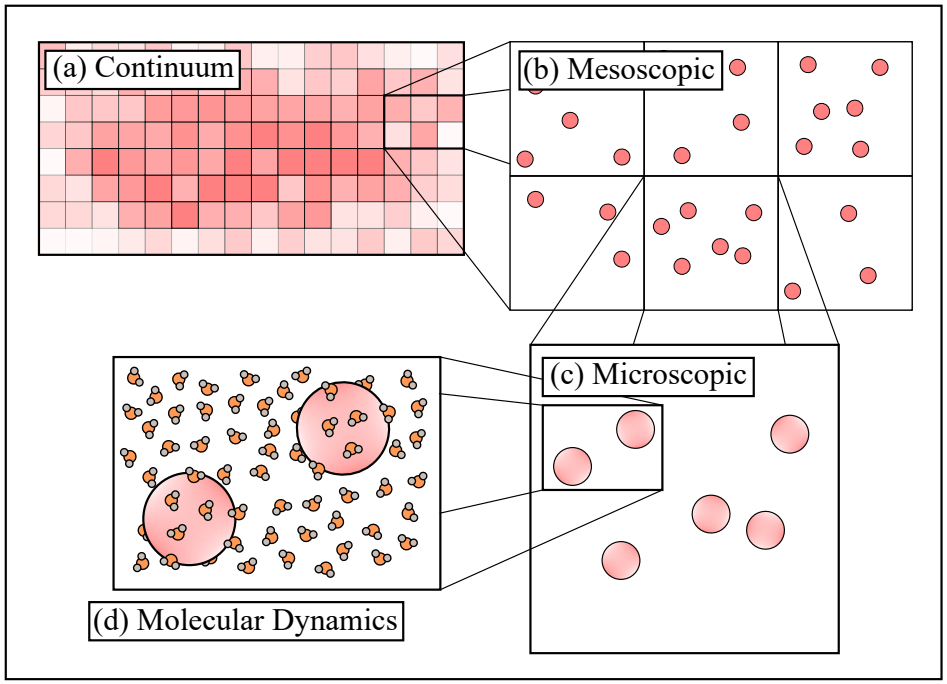
- Channels can be very complex
  - Physical space
  - Many phenomena
- Understand unfamiliar environments
- We can control/design the channel



Scales of Molecular Simulations



Scale Summary



- **a** Continuum
  - Solves PDEs over grid
  - Need "very large" populations
- **b** Mesoscopic
  - Subvolumes have uniform populations
  - Track changes in composition
- **c** Microscopic
  - Model individual molecules
  - Solvent is a continuum
- **d** Molecular Dynamics
  - Model ALL molecules
  - Handle collisions and intermolecular forces

Generic Simulators

Generic Simulators – Existing platforms from physical chemistry

Advantages:

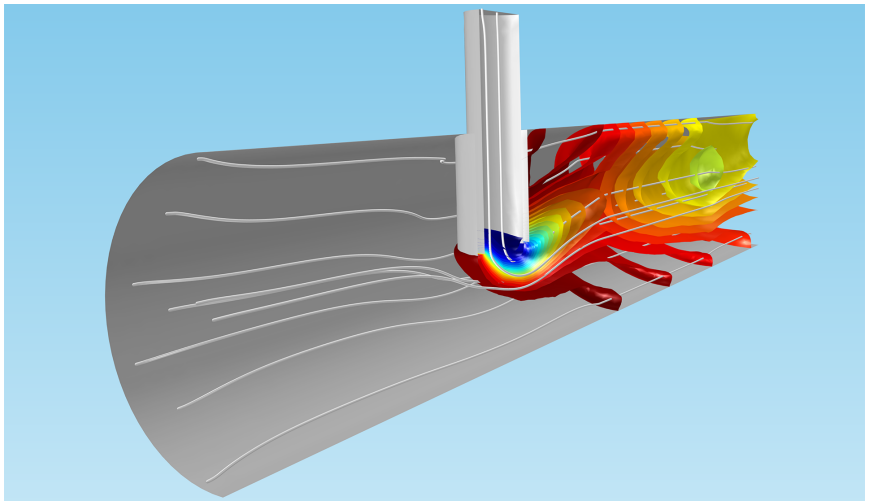
- Advanced "sandbox" tools
- Open source and commercial platforms
- Options for all physical scales
- Many are maturely developed

Disadvantages (for molecular communication):

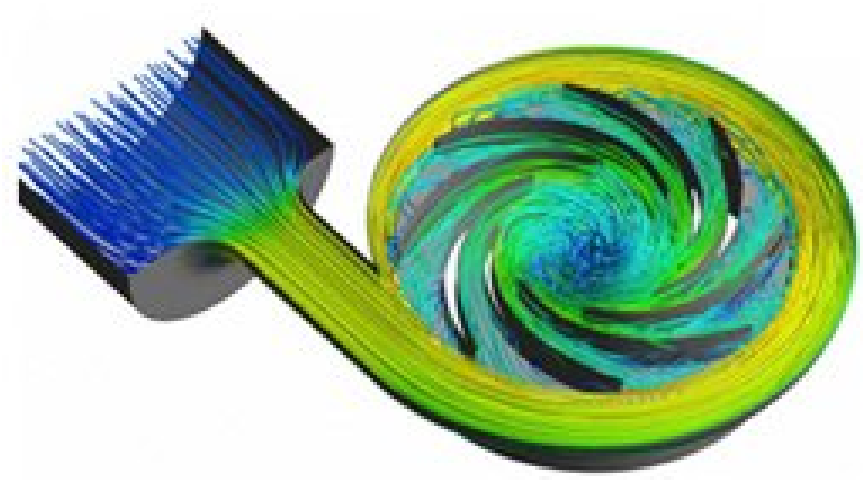
- Not designed for data transmission
- Not designed for channel statistics
- Not always spatially tunable

Popular Generic Simulators

Sample Commercial Platforms



COMSOL Multiphysics (Continuum)[1]



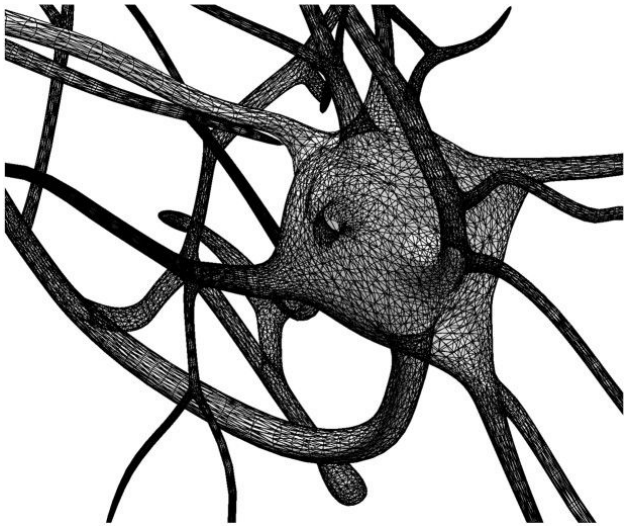
ANSYS (Continuum)[2]

Images: [1]https://uk.comsol.com/multiphysics/what-is-mass-transfer

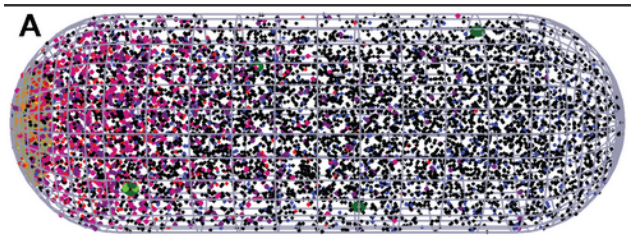
[2]https://www.ansys.com/products/fluids

Popular Generic Simulators

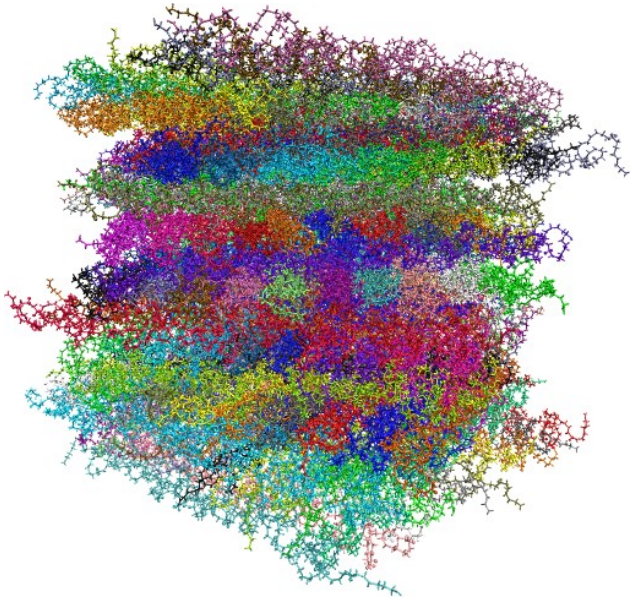
Sample Open Source Platforms



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

Advantages:

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

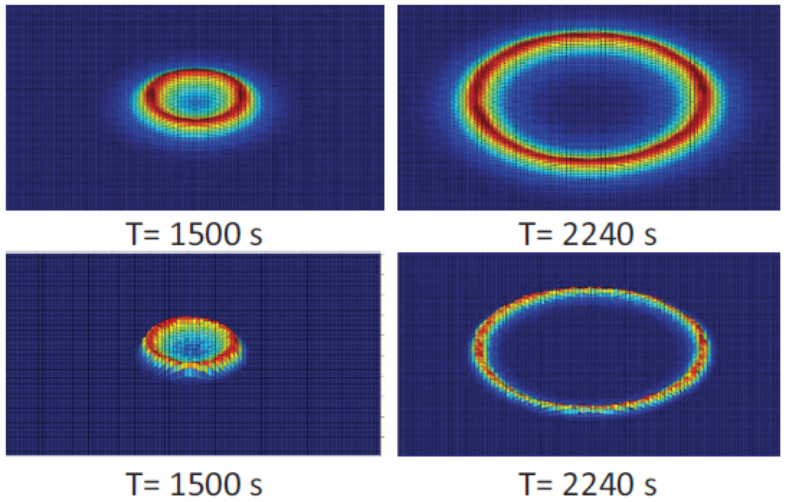
Disadvantages:

- 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

BNSim

Bacterial Network Simulator

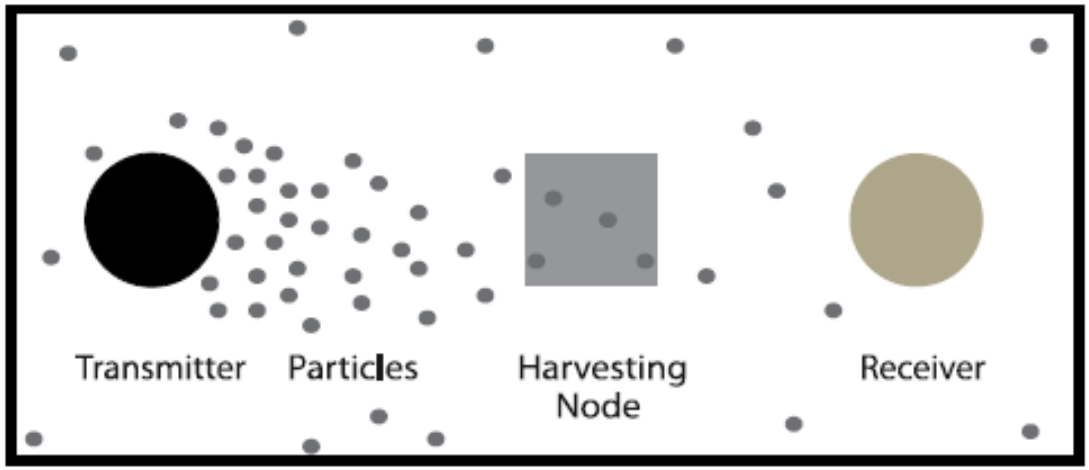
Attractant concentration (top) and bacteria density (bottom)



- Written in java
- Simulate interactions between mobile bacteria
- Multi-scale mesoscopic reaction-diffusion
- No longer in development

Image: https://doi.org/10.1109/JSAC.2013.SUP2.12130019

N3Sim

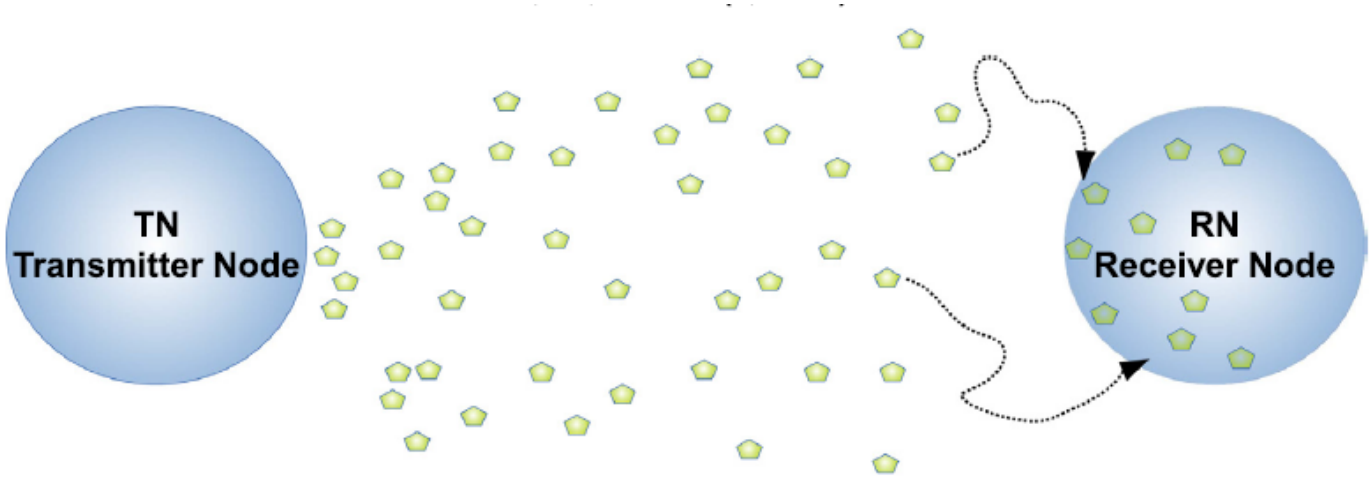


- Written in java
- Simulate within a square or unbounded 3D
- Microscopic diffusion
- Model collisions between diffusing molecules
- Receivers can be transparent or perfectly absorbing
- Detailed user guide and instructions available

Image: https://doi.org/10.1016/j.simpat.2013.11.004 Software: http://www.n3cat.upc.edu/n3sim

MUCIN

MolecUlar CommunicatIoN



- Entirely in MATLAB; available on File Exchange
- Easy to pick up and modify
- Includes microscopic and Monte Carlo simulations
  - Monte Carlo generates simulations from known channel statistics

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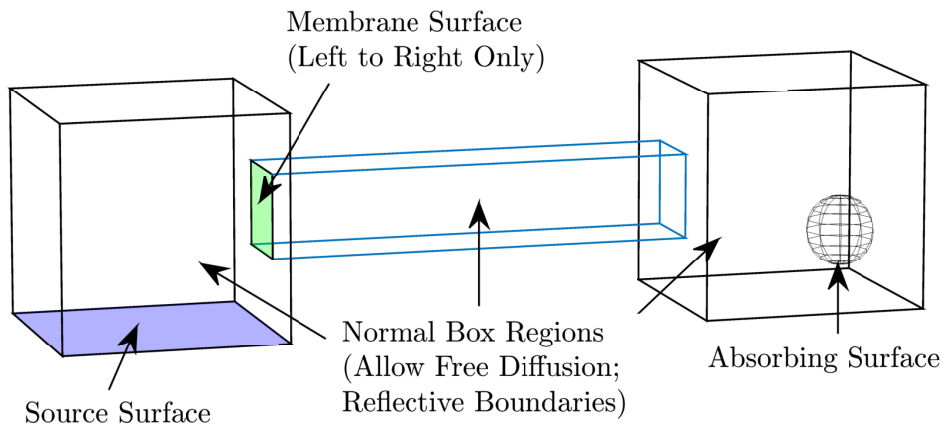
Image: https://doi.org/10.1016/j.simpat.2014.09.002

Software: https://uk.mathworks.com/matlabcentral/fileexchange/46066-molecular-communication-mucin-simulator

AcCoRD

Actor-based Communication via Reaction-Diffusion



- Written in C with utilities in MATLAB
- "Sandbox" environment design with microscopic/mesoscopic hybrid
- Details include: reactions, flow, surfaces, data modulation
- MATLAB utilities for videos and plots
- Public website with user manual
- On-going development (15 releases; most recently **yesterday**)

Image: http://dx.doi.org/10.1016/j.nancom.2017.02.002

Software: www.warwick.ac.uk/adamnoel/software/accord/

Some Other Mol Comm Simulators

BiNS2 (Biological Nanoscale Simulator)

- Developed in java
- Flowing cylindrical environments
- Microscopic reaction-diffusion
- Run time visualization
- On-going development

nanoNS3

- Implemented on top of ns-3
- Continuum simulations of bacteria signaling

BiNS2: http://conan.diei.unipg.it/lab/index.php/product/biological-nanoscale-simulator-bins2

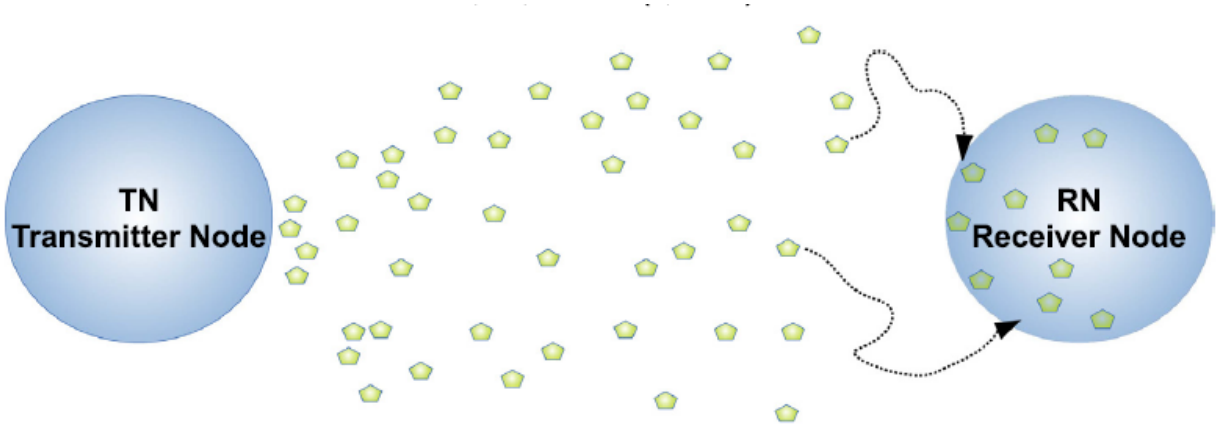
nanoNS3: https://doi.org/10.1145/2967446.2967464

Software Demonstrations

We will go through basic usage of two simulation tools:

1. MUCIN because of ubiquity of MATLAB
2. AcCoRD because of flexibility and resources available
    - And because the developer is presenting!

MUCIN Demo



1. Modify and run sample configuration
2. View simulation output

Image: https://doi.org/10.1016/j.simpat.2014.09.002

Live MUCIN Demo

MUCIN Recap

Advantages for MUCIN:

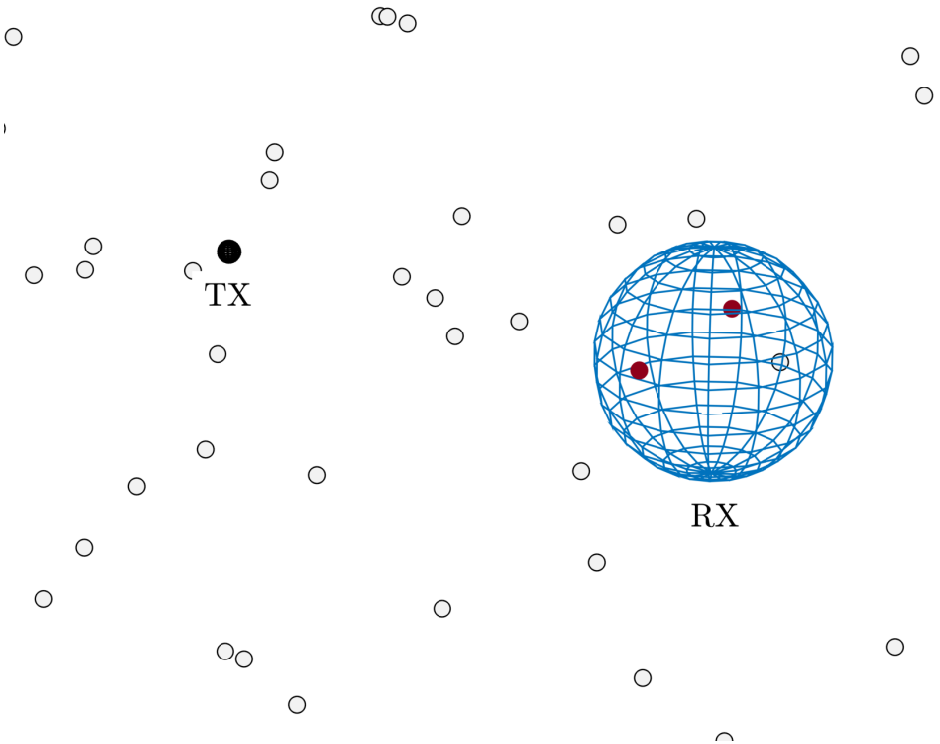
- Having in MATLAB makes it easy to use and modify
- Code is publicly available on MATLAB File Exchange
  - Updated multiple times from 2014-2016
- Good for simple simulations

AcCoRD Demo

AcCoRD Demo Summary:

1. Quick End-to-End Demonstration
2. Installation and Manual
3. **BREAK**
4. Preparing a Simulation
5. Running Simulations
6. Simulation Post-Processing
7. Extra Demo Example
8. Online Resources

AcCoRD Demo Part 1



Part 1: Point to Absorbing Receiver

1. View environment in MATLAB
2. Run Simulation
3. View raw output
4. Import in MATLAB
5. Draw a plot and make a video

Aside: we're using a new algorithm to simulate spherical absorption.

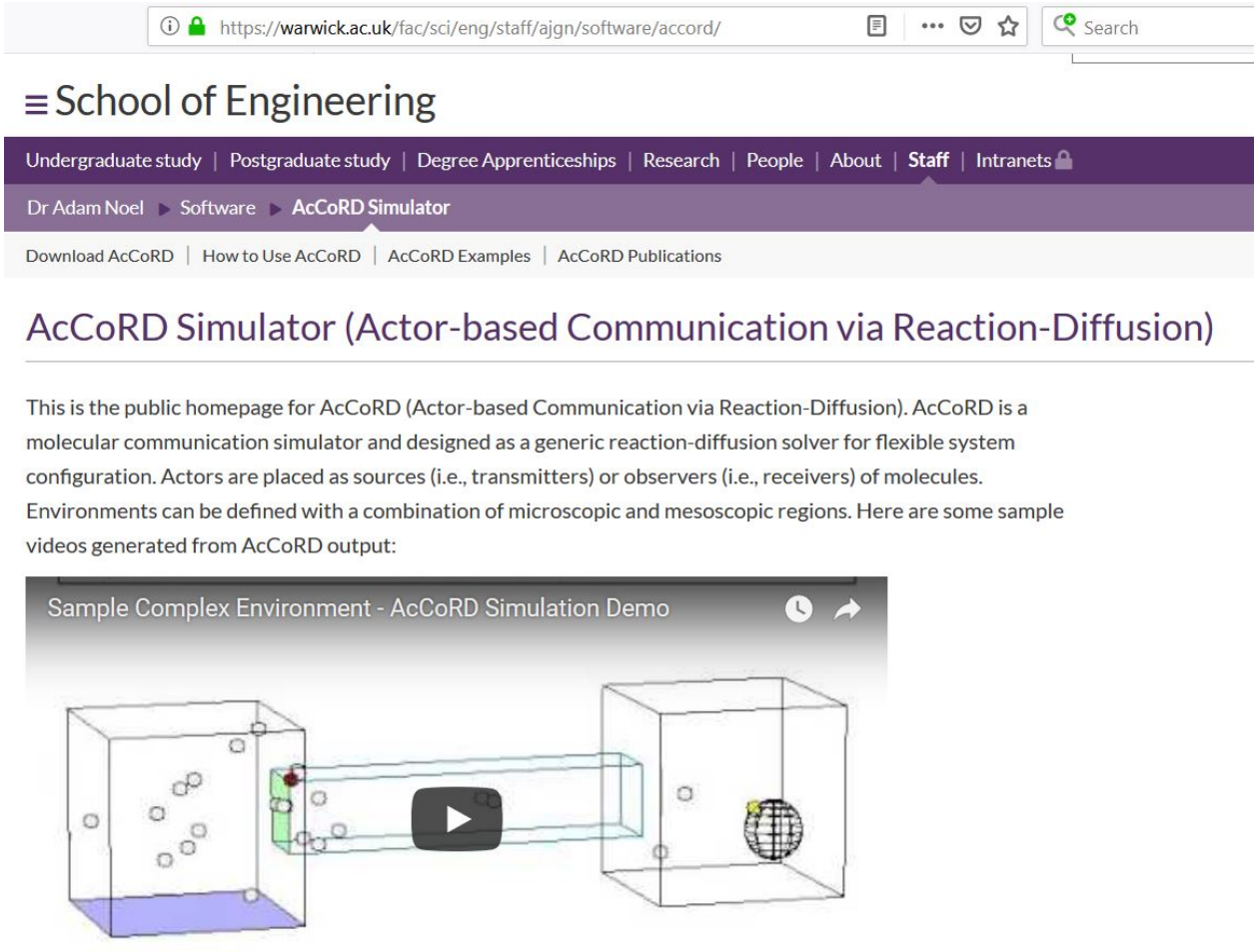
Image: http://dx.doi.org/10.1016/j.nancom.2017.02.002

Algorithm: Wang, Noel, and Yang, *IEEE Transactions on NanoBioscience*, to appear.

AcCoRD Demo Part 2

Part 2: Installation and User Manual

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



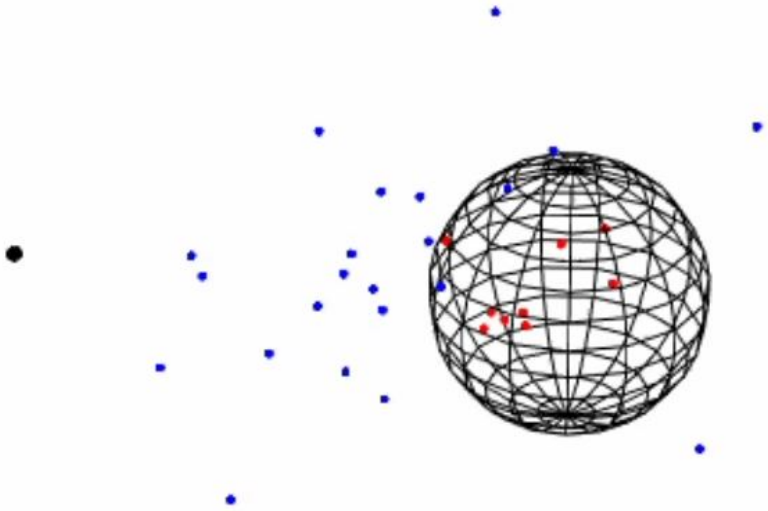
AcCoRD Demo Part 2 Notes

- Pre-compiled for Windows, Linux
  - Just unzip directory to desired folder
- Source code also available
- User manual included with download

AcCoRD Demo Part 3

Part 3: **BREAK**

AcCoRD Demo Parts 4-6



Parts 4-6: Data from Point to Passive Receiver with Flow, Degradation

1. Part 4: Preparing Simulation
   - Configuration; Viewing
2. Part 5: Running Simulation
   - Execution; Clusters; Output
3. Part 6: Post-Processing
   - MATLAB; Plots; Videos

AcCoRD Demo Part 4 Notes

- Configuration files are in “config” folder
  - JSON format; best to copy and modify existing file
  - User manual has sample configuration file components
- Can use “accordEmptyEnvironmentQuick” MATLAB function to plot

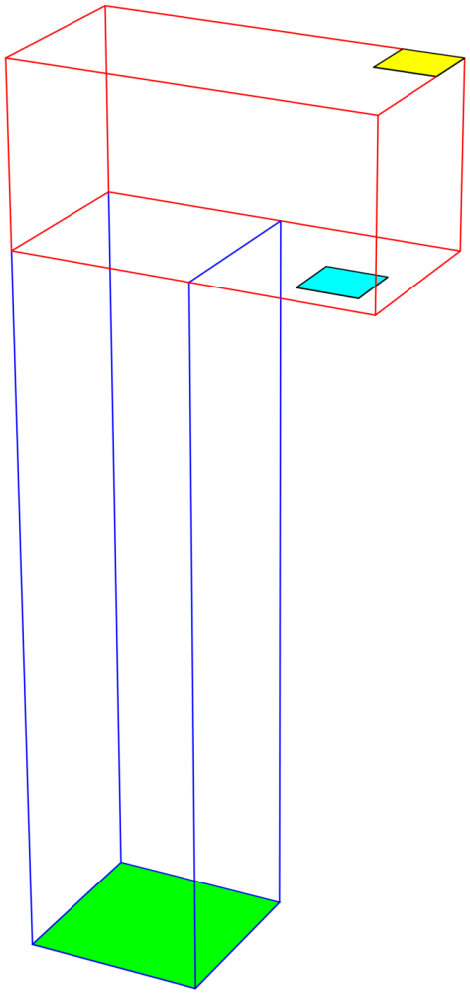
AcCoRD Demo Part 5 Notes

- Call "accord_win.exe" from Windows command line, followed by configuration filename and seed number
- Realizations can be combined from multiple runs that used different random number seeds
- Linux-based optimized versions run faster than the Windows executables
- 2 output files are generated per simulation
  - One file with summary data; one file with raw simulation results
  - Files are readable but better to import in MATLAB

AcCoRD Demo Part 6 Notes

- Import to MATLAB using “accordImport” function
- Quickly plot average time-varying data using “accordQuickPlot” function
- Customized plotting by making your own wrapper for “accordPlotMaker”
- Customized videos by making your own wrapper for “accordVideoMaker”
  - Pre-define camera angles or adjust at runtime

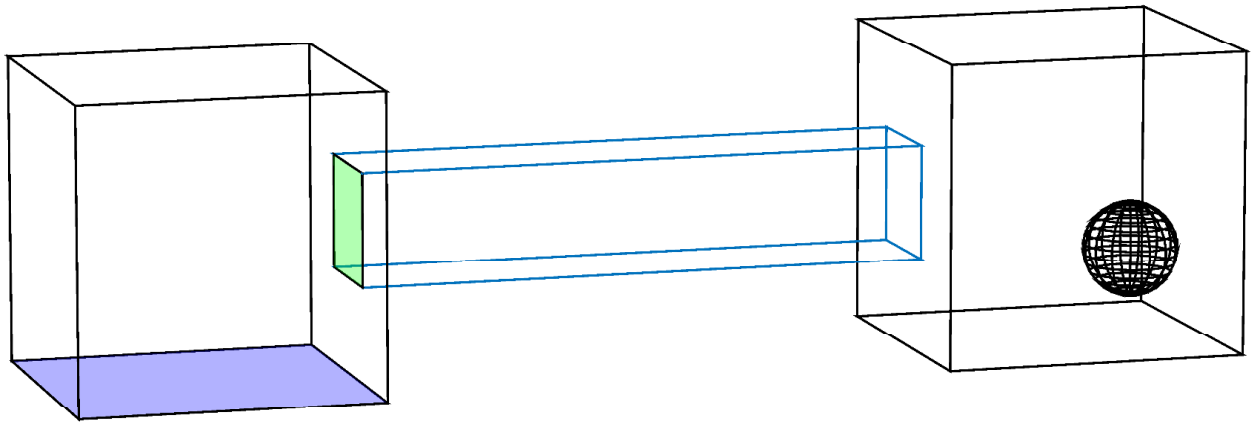
AcCoRD Demo Part 7



Part 7: Surface Reactions in Bounded Environment

- Molecules released from green surface
- Flow carries molecules along blue box
- Reversible absorption to blue and yellow patches

AcCoRD Demo Part 8



Part 8: Resources

- Additional Examples
- Github for code development
  `https://github.com/adamjgnoel/AcCoRD`

Image: http://dx.doi.org/10.1016/j.nancom.2017.02.002

AcCoRD Recap

Advantages for AcCoRD:

- Flexible environment design for molecular communication (components)
- Powerful MATLAB utilities included for videos, distributions, and custom figures
- Detailed user manual with step-by-step instructions
- Many sample configurations
- On-going development

Summary

Recap of Learning Objectives

- Understand importance of simulations
- Understand the different scales of simulation
- Compare different simulation platforms
- Use existing software tools

Conclusions

- Simulations are invaluable – Use them!
- Many existing platforms available

Resources

Molecular Communication Simulators

- AcCoRD
  www.warwick.ac.uk/adamnoel/software/accord/
- MUCIN https://www.mathworks.com/matlabcentral/fileexchange/46066-molecular-communication-mucin-simulator
- BiNS2 http://conan.diei.unipg.it/lab/index.php/product/biological-nanoscale-simulator-bins2
- N3Sim http://www.n3cat.upc.edu/n3sim
- BNSim https://github.com/weiguopeng/BNSim2
- nanoNS3
  http://gnan.ece.gatech.edu/ns-allinone-3.24.zip

Resources

Generic Reaction-Diffusion Solvers

- COMSOL `https://www.comsol.com/multiphysics/`
- ANSYS `https://www.ansys.com`
- URDME (pyURDME) `https://pyurdme.github.io/pyurdme/`
- Smoldyn `http://www.smoldyn.org/`
- LAAMPS `https://lammps.sandia.gov`

The End

Thank you for your time and attention!

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

AcCoRD Simulator:
`www.warwick.ac.uk/adamnoel/software/accord/`