N3Sim: Simulator for diffusion-based molecular communications in nanonetworks

www.n3cat.upc.edu/n3sim

Degree Project Iñaki Pascual Mariñelarena

Advisors: Albert Cabellos-Aparicio and Ignacio Llatser Martí

Informatics Engineering Degree, Facultat d’Informàtica de Barcelona, Universitat Politècnica de Catalunya, 2011.
OUTLINE

- Intro
  - Molecular Communications (MC)

- N3Sim – Demo

- N3Sim
  - Goals
  - Project Development
  - State of the Art
  - Design & Implementation

- Collision Detection (CD) Algorithm

- Future Work & Conclusions
Molecular Communication
Nanotechnology

Several technologies have gone into nano-scale:
- Chip industry
  - Intel’s new 3d 22nm architecture
- Genetics
- Materials
  - Graphene

Increasing research in nanomachines and nanonetworks
Creation of a Bacterial Cell Controlled by a Chemically Synthesized Genome

Daniel G. Gibson,1 John I. Glass,1 Carole Lartigue,1 Vladimir N. Noskov,1 Ray-Yuan Chuang,1 Mikkel A. Algire,1 Gwynedd A. Benders,2 Michael G. Montague,1 Li Ma,1 Monzia M. Moodie,1 Chuck Merryman,1 Sanjay Vashee,1 Radha Krishnakumar,1 Nacyra Assad-Garcia,1 Cynthia Andrews-Pfannkoch,1 Evgeniya A. Denisova,1 Lei Young,1 Zhi-Qing Qi,1 Thomas H. Segall-Shapiro,1 Christopher H. Calvey,1 Prashanth P. Parmar,1 Clyde A. Hutchison III,2 Hamilton O. Smith,2 J. Craig Venter1,2*

We report the design, synthesis, and assembly of the 1.08-mega-base pair *Mycoplasma mycoides* JCVI-syn1.0 genome starting from digitized genome sequence information and its transplantation into a *M. capricolum* recipient cell to create new *M. mycoides* cells that are controlled only by the synthetic chromosome. The only DNA in the cells is the designed synthetic DNA sequence, including “watermark” sequences and other designed gene deletions and polymorphisms, and mutations acquired during the building process. The new cells have expected phenotypic properties and are capable of continuous self-replication.

www.sciencemag.org/cgi/content/full/science.1190719/DC19
April 2010; accepted 13 May 2010 - Published online 20 May 2010; - 10.1126/science.1190719
Approaches for the development of nano-machines

NanoNetworks, the interconnection of nanomachines

- will allow nanomachines to execute more complex tasks
- will expand nanomachines workspace
Molecular communication is a very common process in nature.

Molecular communication emerges as a new communication paradigm.
Brownian Motion: random endless movement of suspended particles in a fluid

- Fick’s Laws (1855)
  \[ J = -D \frac{\partial \phi}{\partial x} \]

- A. Einstein (1905)
  \[ X_{rms} = \sqrt{2Dt} \]
Molecular Communication

Information codified in
- Molecule’s structure (i.e. ARN)
- Concentration of molecules (i.e. calcium signalling)

Information transport
- Diffusion
- Flow
- Walkway

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Diffusion equations are no longer valid if interactions among suspended particles exist.

Interactions
- Collisions
- Electromagnetic forces
- Chemical

A simulator is needed to model collective diffusion and validate current theories on molecular communications.
N3Sim
N3Sim - Goals

Build a simulator that:

- Allows study of the physical layer:
  - Signal modulation
  - Communication mechanisms
  - Main communication channel metrics

- Implements collective diffusion (Brownian motion + Collisions)

- Is extensible. Future versions may include:
  - Receiver and emitter modules
  - More components of collective diffusion
  - ...

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N3Sim – Requeriments

**Functional Requeriments**
- Multiple Emitters and Receivers
- Custom emission waveform
- Collective Diffusion (Brownian Motion & Collisions)
- Initial background concentration

**Non-functional Requirements**
- Reliability
- Extensibility
- Modifiability
- Usability

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Spiral Development & Rapid Prototyping
N3Sim – Project Development

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Conceptual Model

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3-Layer Architecture & Packages Structure

- User Interface Layer
- Domain Layer
- Data Layer

Packages:
- collision
- simulation
- space
- particles
- emitters
- receivers
- boundaries
- data
- ui
Collision Detection (CD) Algorithm
CD – Problem Statement

- **N-body problem**
  - Time Cost = $O(n^2)$

- **Sequential Process**
  - Each Collision means new Scenario
  - Time Cost = $\#\text{collisions} \times O(n^2)$
  - No significative parallelization

- **Bottleneck**
Well-known problem in graphics, games and simulation software

Some algorithms take advantage of
- Spatial locality
- Temporal locality
Baraff’s Algorithm

- Proven, efficient, easy to implement
- Spatial & Temporal Locality

Time Cost
- First collision $O(n^2)$
- Next collisions $O(n \log n)$
Baraff’s Algorithm

A *posteriori* algorithm

May lose collisions
CD – Implementation

Baraff’s \((a \ posteriori)\)  

N3Sim \((a \ priori)\)
## CD – N3Sim CD Algorithm

<table>
<thead>
<tr>
<th>Stage</th>
<th>Operation</th>
<th>Time Cost</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td><strong>Pre-processing</strong></td>
<td></td>
</tr>
<tr>
<td>1a</td>
<td>Sort Sphere List</td>
<td>O(nlogn)</td>
</tr>
<tr>
<td>1b</td>
<td>Create collisions queue</td>
<td>O(n²logn)</td>
</tr>
<tr>
<td>2</td>
<td><strong>Processing</strong></td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>While collisions queue is not empty</td>
<td>nc iterations</td>
</tr>
<tr>
<td>2a</td>
<td>Obtain first collision</td>
<td>O(1)</td>
</tr>
<tr>
<td>2b</td>
<td>Solve collision</td>
<td>O(1)</td>
</tr>
<tr>
<td>2c</td>
<td>Sort Sphere List</td>
<td>O(n)</td>
</tr>
<tr>
<td>2d</td>
<td>Delete invalid collisions</td>
<td>O(1)</td>
</tr>
<tr>
<td>2e</td>
<td>Find new collisions</td>
<td>O(nlogn)</td>
</tr>
</tbody>
</table>
Cost (time) = nc * O(nlogn)

Time cost per collision

Number of particles

Cost (time) = nc * O(nlogn)
Future Work
Future Work

- Modify Package Structure
- Implement Electrostatic Forces
- Obstacles

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Conclusions
Conclusions

A simulator has been build that
- Implements collective diffusion (brownian motion + collisions)
- Allows the identification of the molecular communication channel

N3Sim, simulator, source code, user guides and publications available at www.n3cat.upc.edu/n3sim
Conclusions – Outcomes


Conclusions – Channel Identification

- Linear Time-Invariant (LTI) channel
- Particle Counting Noise is a Poisson process
- Modulation: Best performance with OOK pulse
- Channel metrics

<table>
<thead>
<tr>
<th>Metric</th>
<th>EM channel</th>
<th>Molecular channel</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pulse delay</td>
<td>$\Theta(r)$</td>
<td>$\Theta(r^2)$</td>
</tr>
<tr>
<td>Pulse amplitude</td>
<td>$\Theta(1/r^2)$</td>
<td>$\Theta(1/r^3)$</td>
</tr>
<tr>
<td>Pulse width</td>
<td>$\Theta(1)$</td>
<td>$\Theta(r^2)$</td>
</tr>
</tbody>
</table>


Thank you!
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QUESTIONS?

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Mostly educational simulators for Brownian Motion
- Do not include emitters/receivers
- Do not include collective diffusion

NanoNS (June 2010) : module for NS2
- Does not include collective diffusion

Universita di Perugia “A simulation tool for nanoscale biological communication systems”
Block Diagram
Molecular Communication – N3SimVideo
N3Cat – N3Sim Project

www.n3cat.upc.edu
The N3Cat Initiative

During the last years, promising advancements in nanotechnology have attracted tremendous attention in many fields such as in the biomedical field, environmental research or industrial technology because of its potential applications. Nanotechnology is inherently a multidisciplinary field based on the knowledge of diverse scientific areas, and presents challenges in biology, chemistry, physics, computer science and electrical and computer engineering, among others. In nanotechnology, nanomachines are envisioned as the most basic functional unit able to perform very simple tasks at a nanoscale. Nanonetworks are the interconnection of nanomachines, and as such expand the capabilities of a single nanomachine.

The NaNoNetworking Center in Catalonia (N3Cat) has been created as an initiative of Prof. Ian F. Akyildiz and Prof. Josep Sole-Pareta at UPC (Universitat Politècnica de Catalunya) with the main goals of carrying fundamental research on nanonetworks and educating and training the new generation of students.
N3Sim: A Simulation Framework for Diffusion-based Molecular Communication

N3Sim is a complete simulation framework for diffusion-based molecular communications, which allows the evaluation of the communication performance of molecular networks with several transmitters and receivers in an infinite space with a given concentration of molecules. Transmitters encode the information by releasing particles into the medium, thus varying the concentration rate in their vicinity. The diffusion of particles through the medium is modeled as Brownian motion, taking into account particle inertia and collisions among particles. Finally, receivers decode the information by sensing the local concentration in their neighborhood. The benefits of such a simulator are multiple: the validation of existing channel models for molecular communications and the evaluation of novel modulation schemes are just two examples.
Aknowledgements

N3Sim has been developed by:

- Iñaki Pascual
- Nora Garralda
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- Albert Cabellos-Aparicio
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- Massimiliano Pierobon