

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](#)

- 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

- Several technologies have gone into the nano-scale:
 - Chip industry
 - Intel's new 3d 22nm architecture
 - Genetics
 - Materials
 - Graphene
- Increasing research in nanomachines and nanonetworks

RESEARCH ARTICLE

Creation of a Bacterial Cell Controlled by a Chemically Synthesized Genome

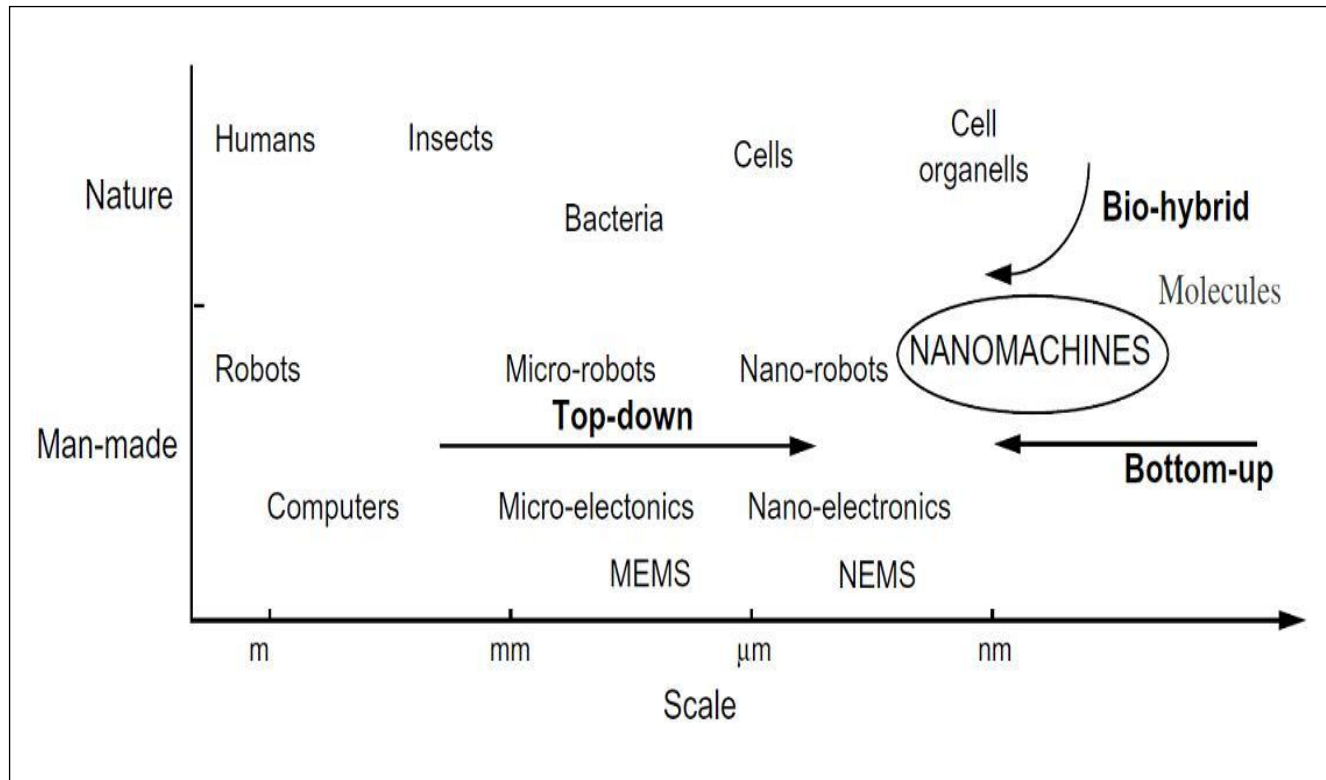
Daniel G. Gibson,¹ John I. Glass,¹ Carole Lartigue,¹ Vladimir N. Noskov,¹ Ray-Yuan Chuang,¹ Mikkel A. Algire,¹ Gwynedd A. Benders,² Michael G. Montague,¹ Li Ma,¹ Monzia M. Moodie,¹ Chuck Merryman,¹ Sanjay Vashee,¹ Radha Krishnakumar,¹ Nacyra Assad-Garcia,¹ Cynthia Andrews-Pfannkoch,¹ Evgeniya A. Denisova,¹ 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 Venter^{1,2*}

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

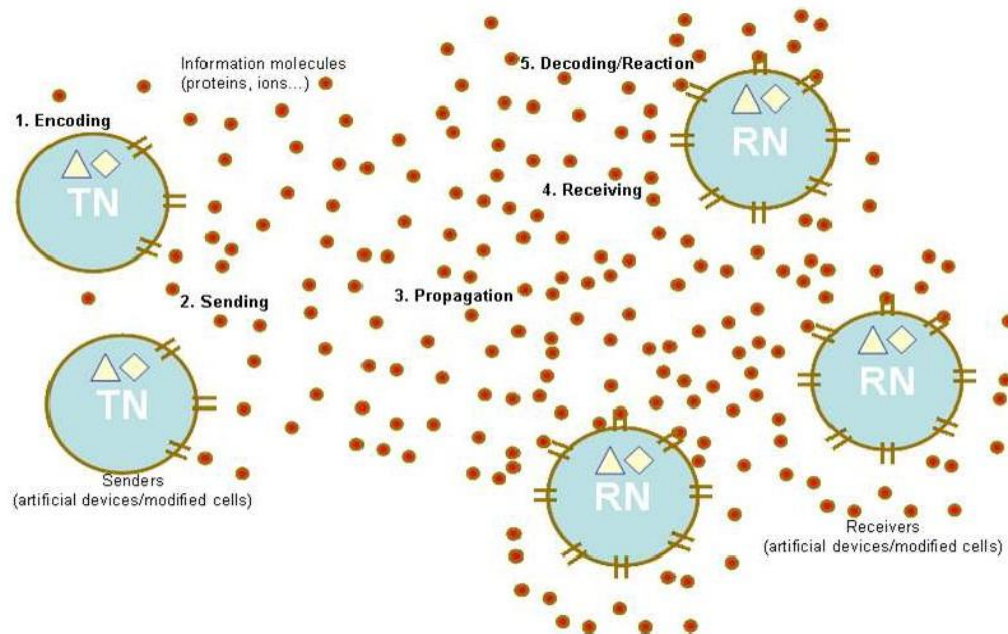
Approaches for the development of nano-machines



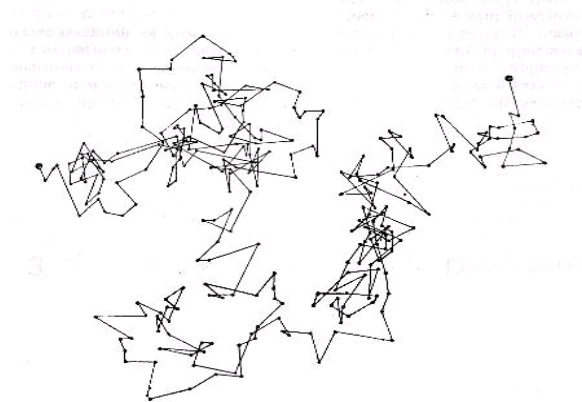
I. F. Akyildiz, F. Brunetti, and C. Blazquez, "Nanonetworks: A new communication paradigm", Computer Networks, vol. 52, no. 12, pp. 2260–2279, 2008.

- 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



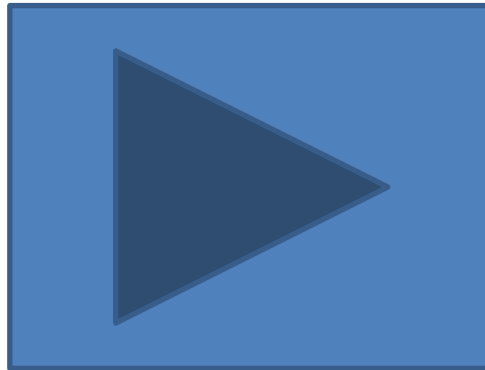
- Fick's Laws (1855) $J = -D \frac{\partial \phi}{\partial x}$
- A. Einstein (1905) $X_{rms} = \sqrt{2Dt}$

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

- Information transport
 - Diffusion
 - Flow
 - Walkway

- 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



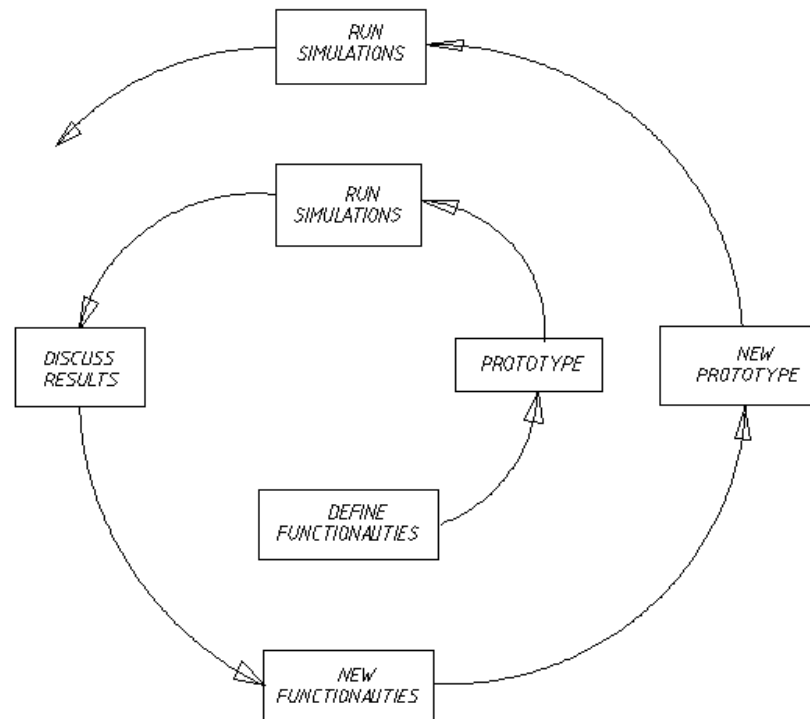
Build a simulator that :

- 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
 - ...

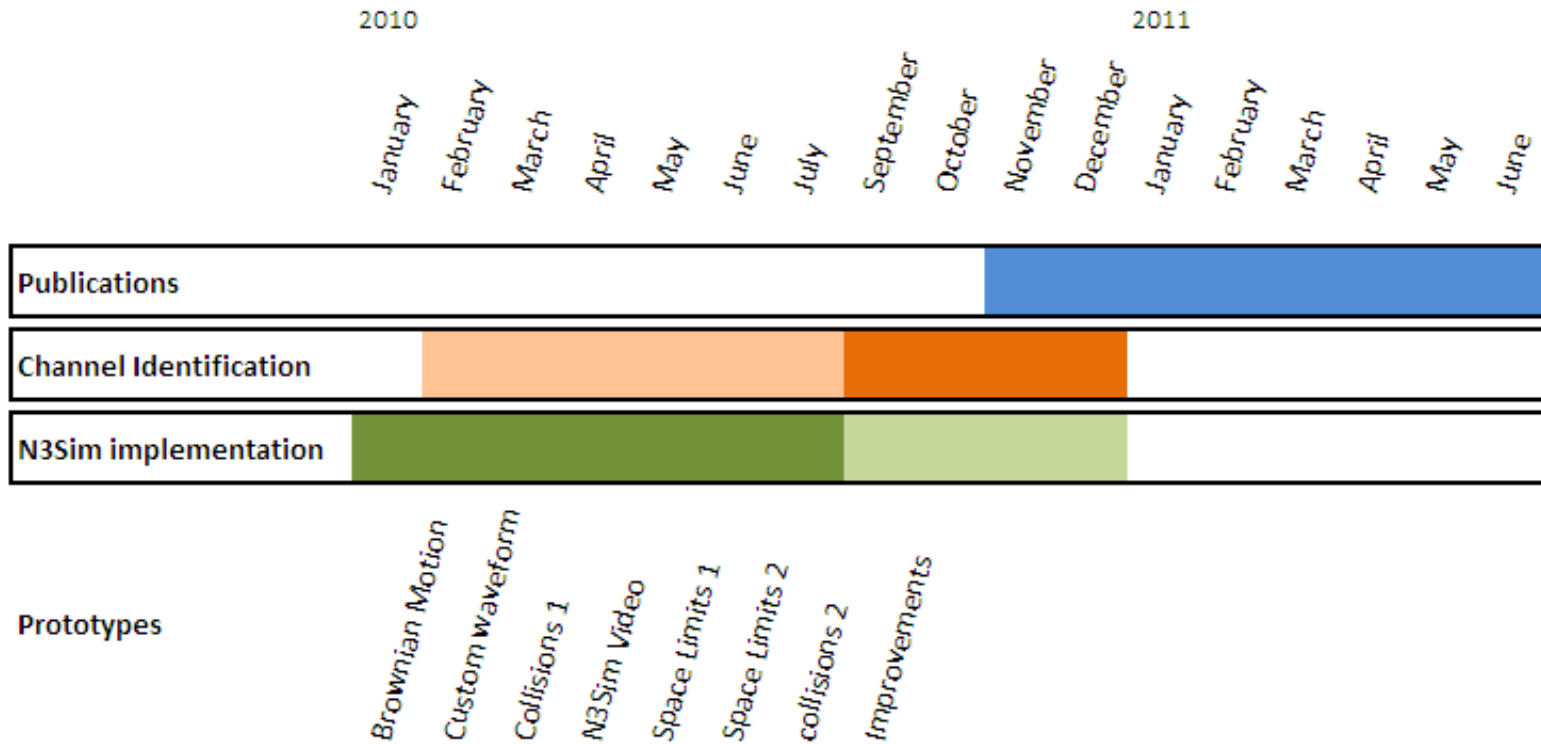
- Functional Requeriments
 - Multiple Emitters and Receivers
 - Custom emission waveform
 - Collective Diffusion (Brownian Motion & Collisions)
 - Initial background concentration

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

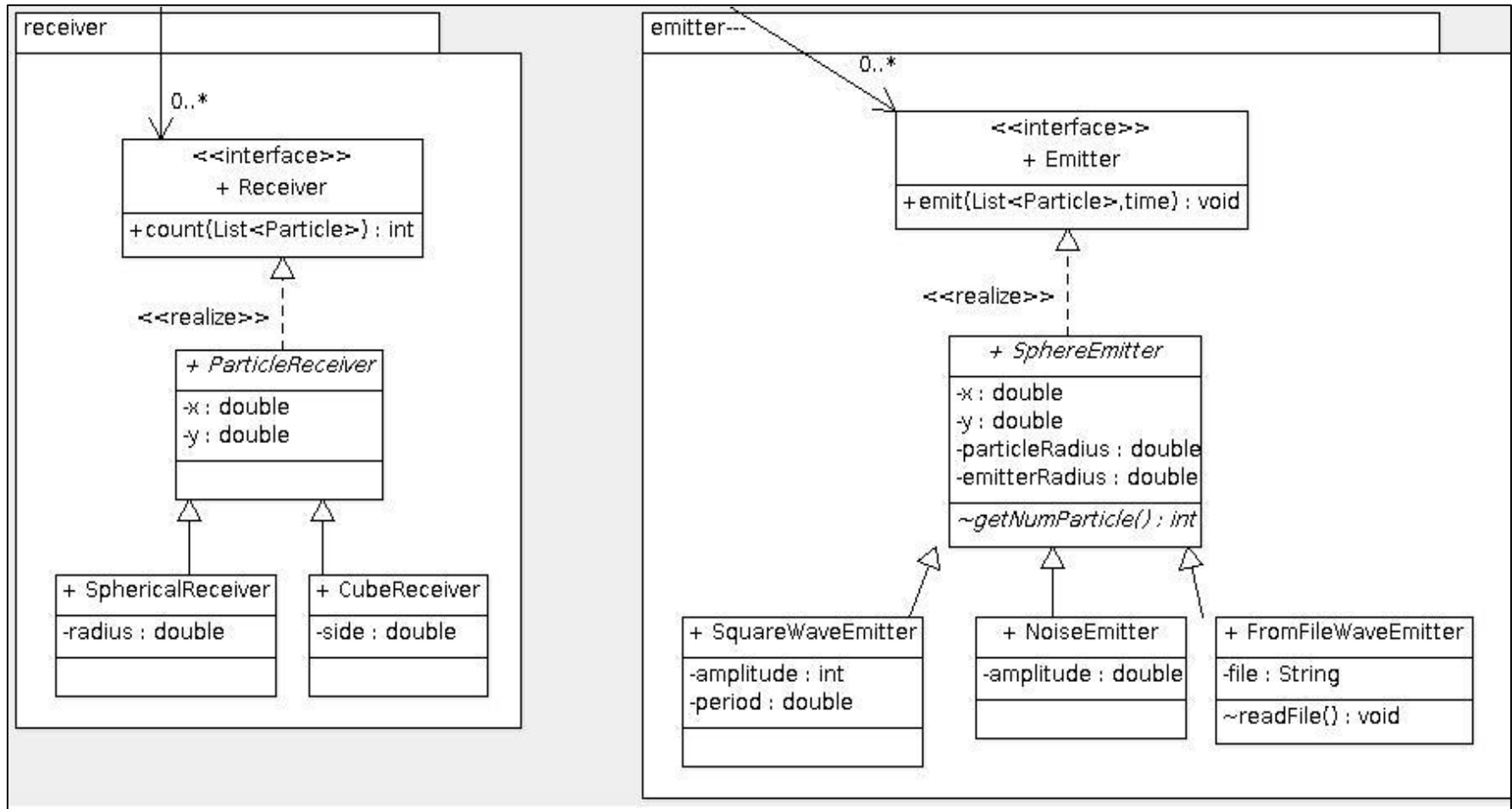
Spiral Development & Rapid Prototyping



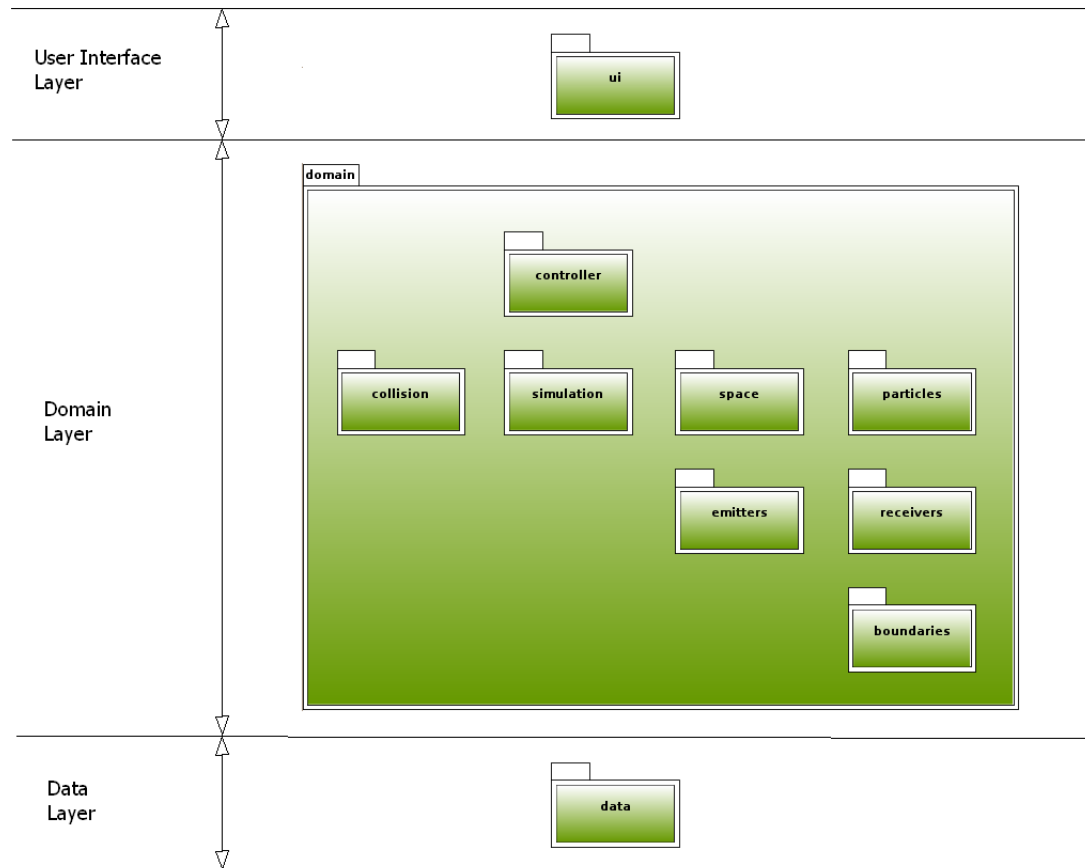
N3Sim – Project Development



Conceptual Model



3-Layer Architecture & Packages Structure



Collision Detection (CD) Algorithm

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

- Sequential Process
 - Each Collision means new Scenario
 - Time Cost = #collisions * $O(n^2)$
 - No significant parallelization

- Bottleneck

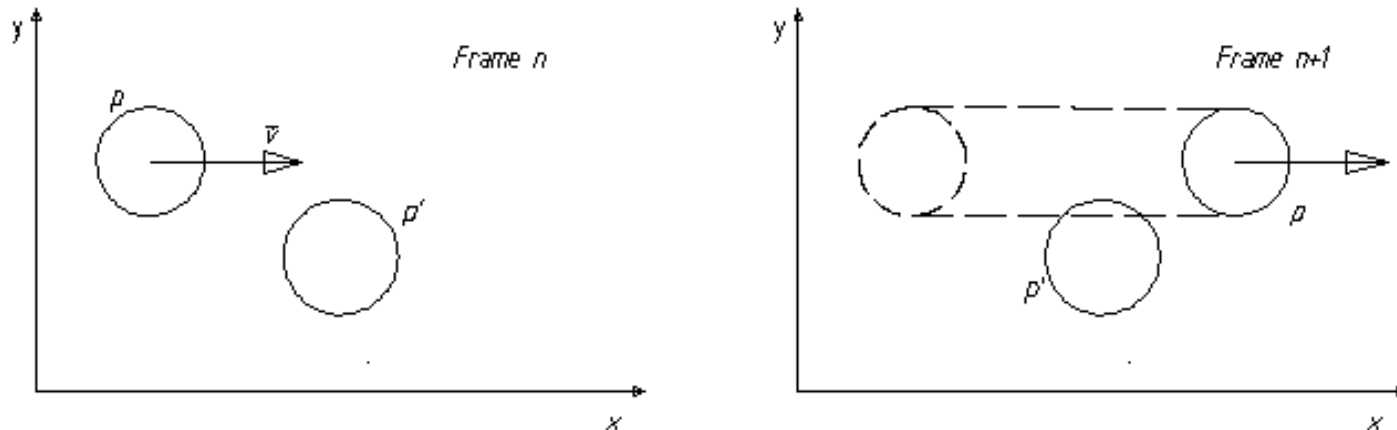
- Well-known problem in graphics, games and simulation software
- Some algorithms take advantage of
 - Spatial locality
 - Temporal locality

Baraff's Algorithm

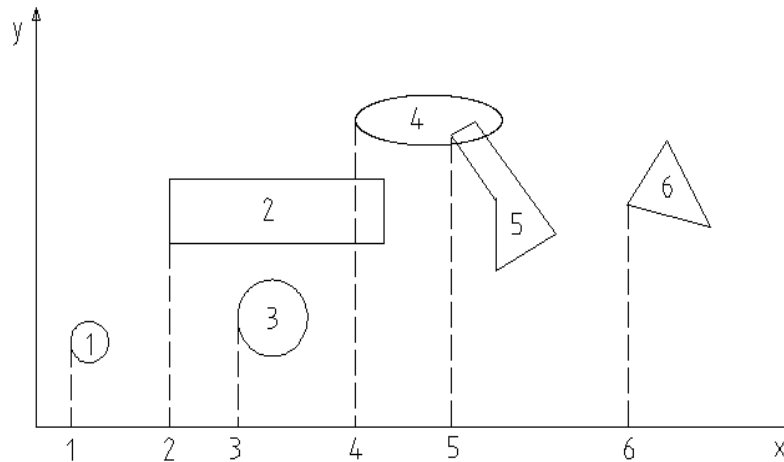
- Proven, efficient, easy to implement
- Spatial & Temporal Locality
- Time Cost
 - First collision $O(n^2)$
 - Next collisions $O(n \log n)$

Baraff's Algorithm

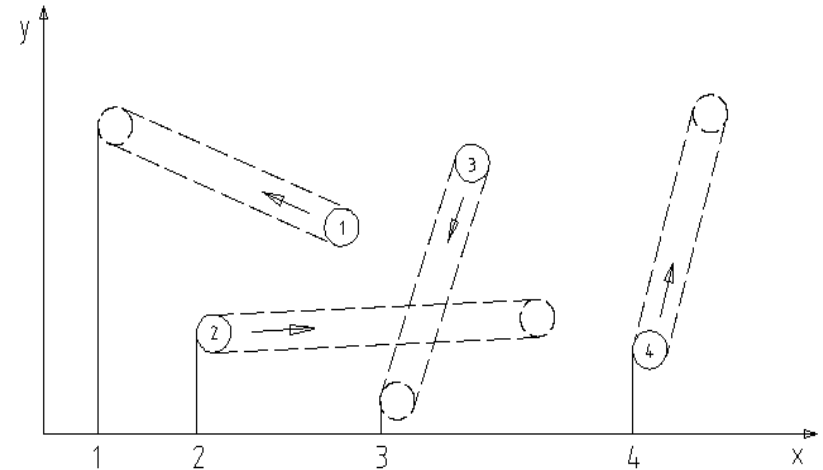
- **A *posteriori* algorithm**
 - May lose collisions



Baraff's (*a posteriori*)



N3Sim (*a priori*)



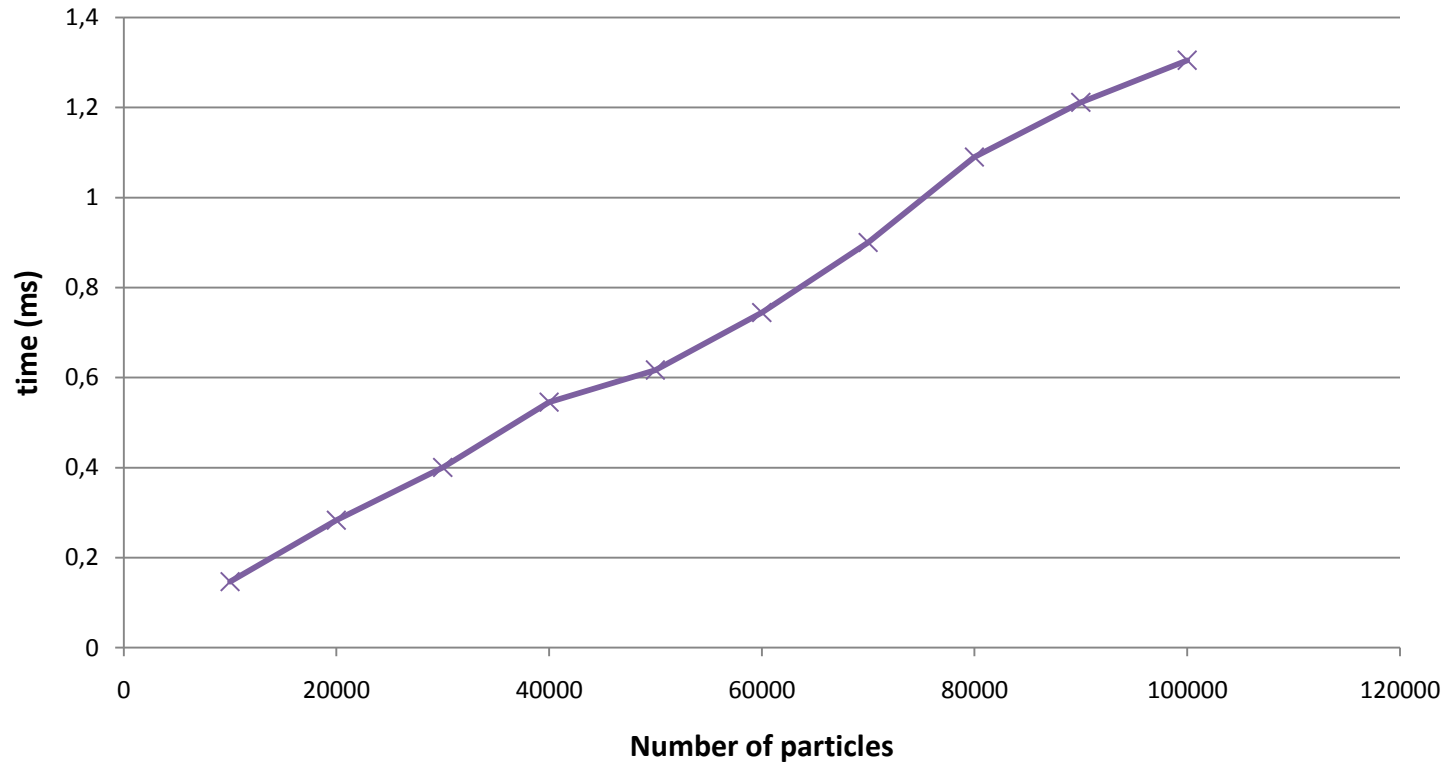
CD – N3Sim CD Algorithm



Stage	Operation	Time Cost
1	Pre-processing	
1a	Sort Sphere List	$O(n \log n)$
1b	Create collisions queue	$O(n^2 \log n)$
2	Processing	
2	While collisions queue is not empty	nc iterations
2a	Obtain first collision	$O(1)$
2b	Solve collision	$O(1)$
2c	Sort Sphere List	$O(n)$
2d	Delete invalid collisions	$O(1)$
2e	Find new collisions	$O(n \log n)$

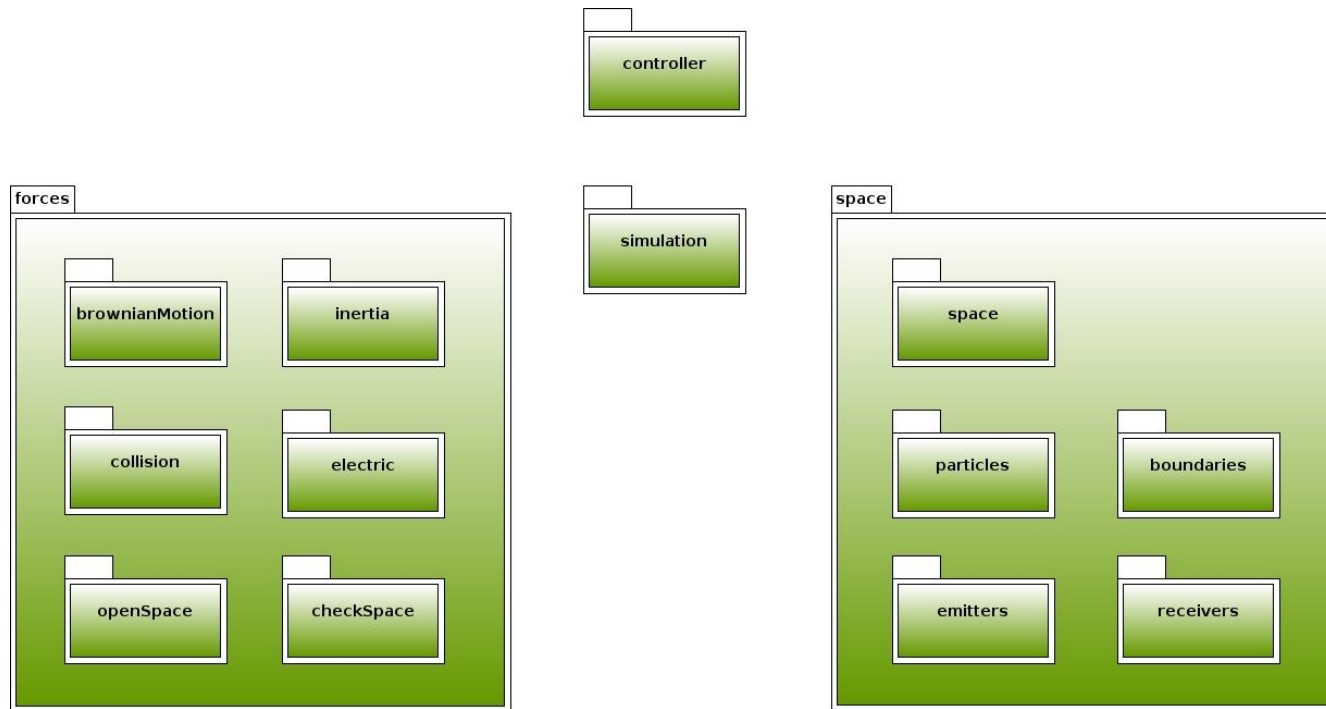
● Cost (time) = $nc * O(n \log n)$

Time cost per collision



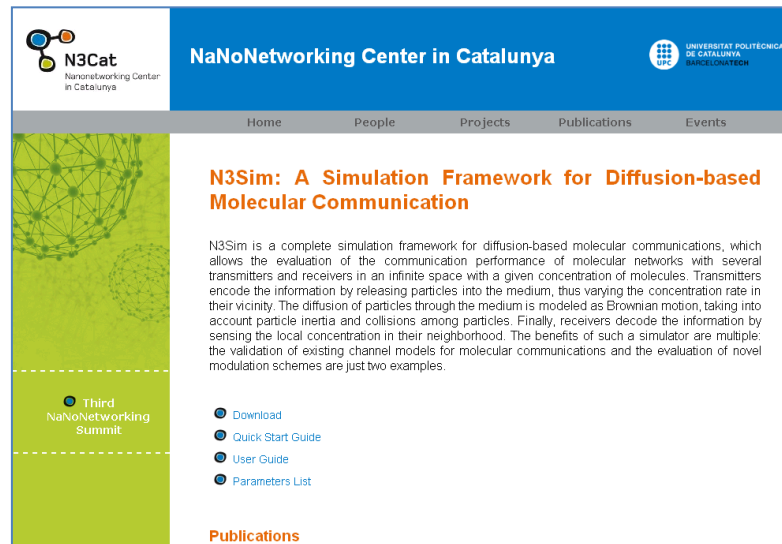
Future Work

Future Work



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



The screenshot shows the website for the NaNoNetworking Center in Catalunya. The header includes the N3Cat logo, the center's name, and the UPC logo. A navigation menu contains links for Home, People, Projects, Publications, and Events. The main content area features a green sidebar with a network diagram and a 'Third NaNoNetworking Summit' announcement. The main text introduces N3Sim as a simulation framework for diffusion-based molecular communications, detailing its capabilities and benefits. A list of links for Download, Quick Start Guide, User Guide, and Parameters List is provided, along with a 'Publications' section.

- Llatser, I., Pascual, I., Garralda, N., Cabellos-Aparicio, A., Pierobon, M., Alarcón, E. and Solé-Pareta, J., "***N3Sim: A Simulation Framework for Diffusion-based Molecular Communication***," IEEE TC on Simulation, No. 8, pp. 3-4, March 2011.
- Llatser, I., Pascual, I., Garralda, N., Cabellos-Aparicio, A., Pierobon, M., Alarcón, E. and Solé-Pareta, J., "***Exploring the Physical Channel of Diffusion-based Molecular Communication by Simulation***", submitted for publication, March 2011.
- Llatser, I., Alarcón, E., Pierobon, M., "***Diffusion-based Channel Characterization in Molecular Nanonetworks***", in Proc. of the 1st IEEE International Workshop on Molecular and Nano Scale Communication (MoNaCom), held in conjunction with IEEE INFOCOM, April 2011.
- Garralda, N., Llatser, I., Cabellos-Aparicio, A., Pierobon, M., "***Simulation-based Evaluation of the Diffusion-based Physical Channel in Molecular Nanonetworks***", in Proc. of the 1st IEEE International Workshop on Molecular and Nano Scale Communication (MoNaCom), held in conjunction with IEEE INFOCOM, April 2011.

Conclusions – Channel Identification

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

Metric	EM channel	Molecular channel
Pulse delay	$\Theta(r)$	$\Theta(r^2)$
Pulse amplitude	$\Theta(1/r^2)$	$\Theta(1/r^3)$
Pulse width	$\Theta(1)$	$\Theta(r^2)$

Llatser, I., Alarcón, E., Pierobon, M., *“Diffusion-based Channel Characterization in Molecular Nanonetworks”*, in Proc. of the 1st IEEE International Workshop on Molecular and Nano Scale Communication (MoNaCom), held in conjunction with IEEE INFOCOM, April 2011.

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Thank you!

N3Sim: Simulator for diffusion-based molecular communications in nanonetworks

QUESTIONS ?

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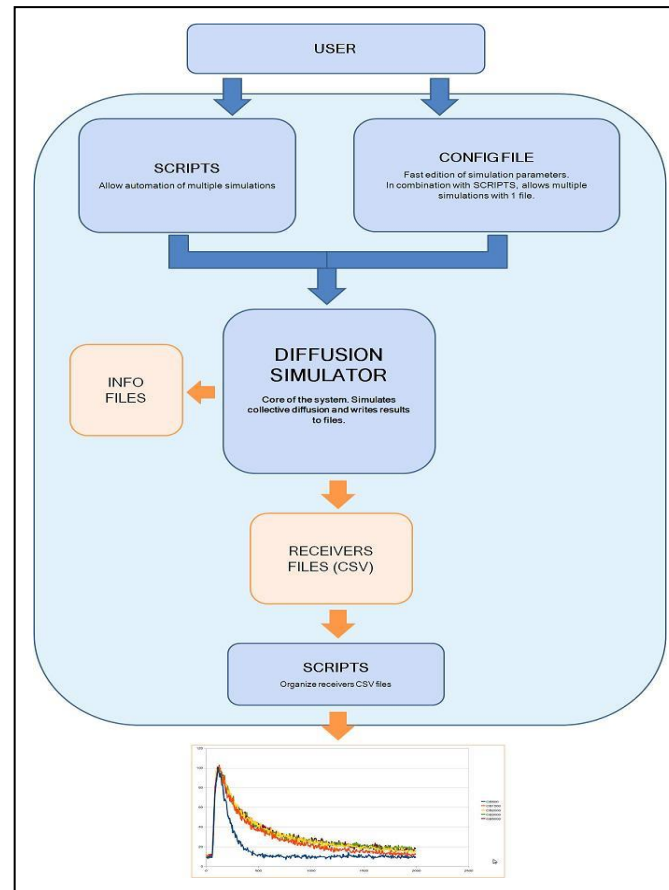
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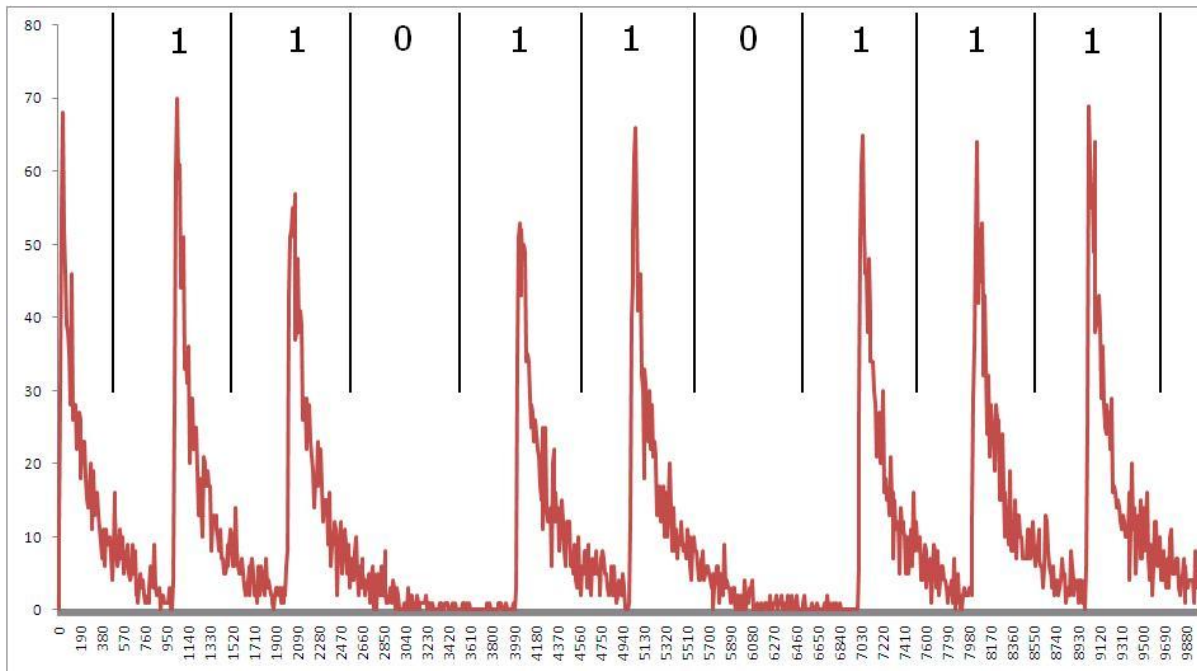
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- Mostly educational simulators for Brownian Motion
 - Do not include emitters/receivers
 - Do not include collective diffusion
- NanoNS (June 2010) : module for NS2
 - Does not include collective diffusion
- Universita di Perugia “A simulation tool for nanoscale biological communication systems”

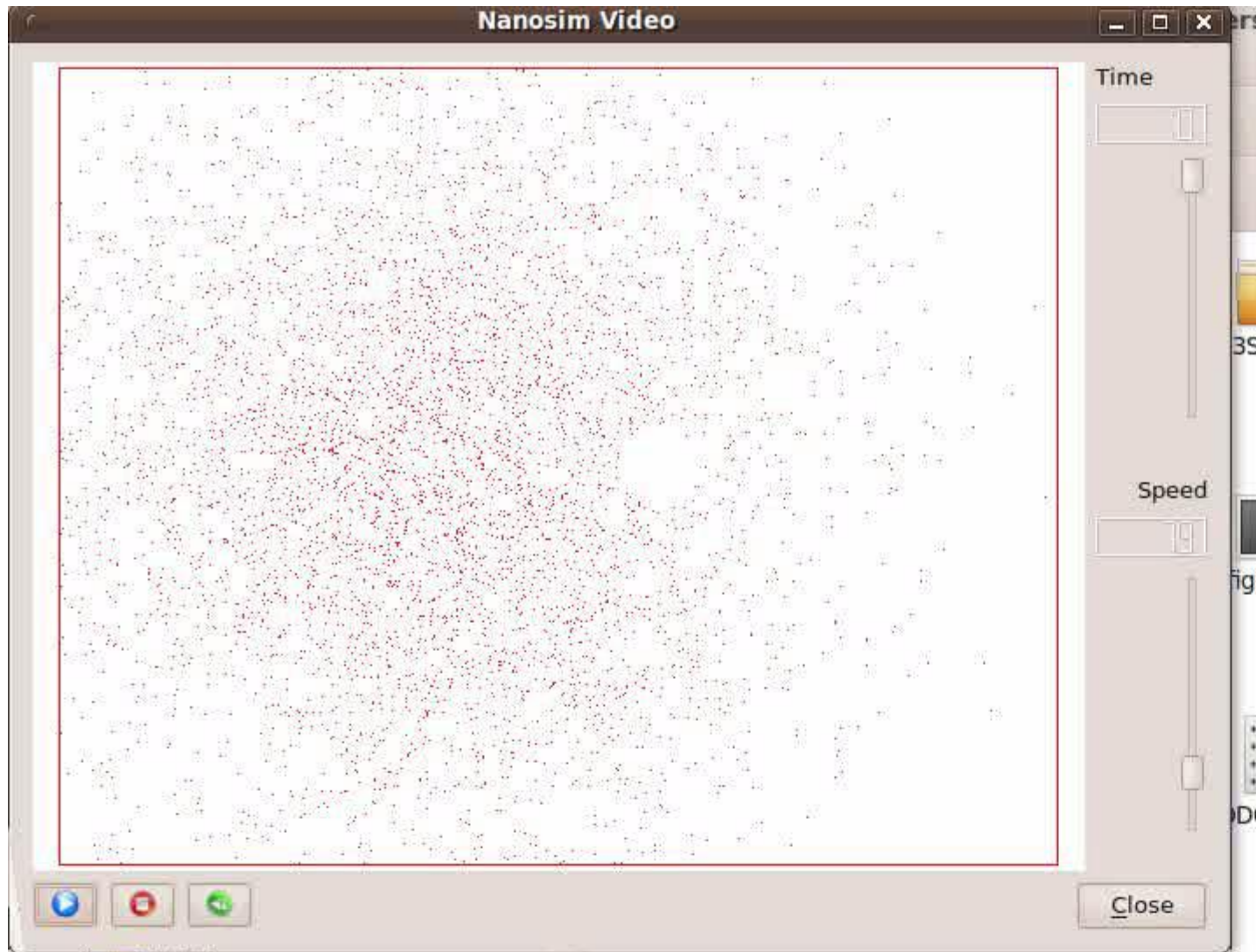
Block Diagram



MC - Receiver



Molecular Communication – N3SimVideo

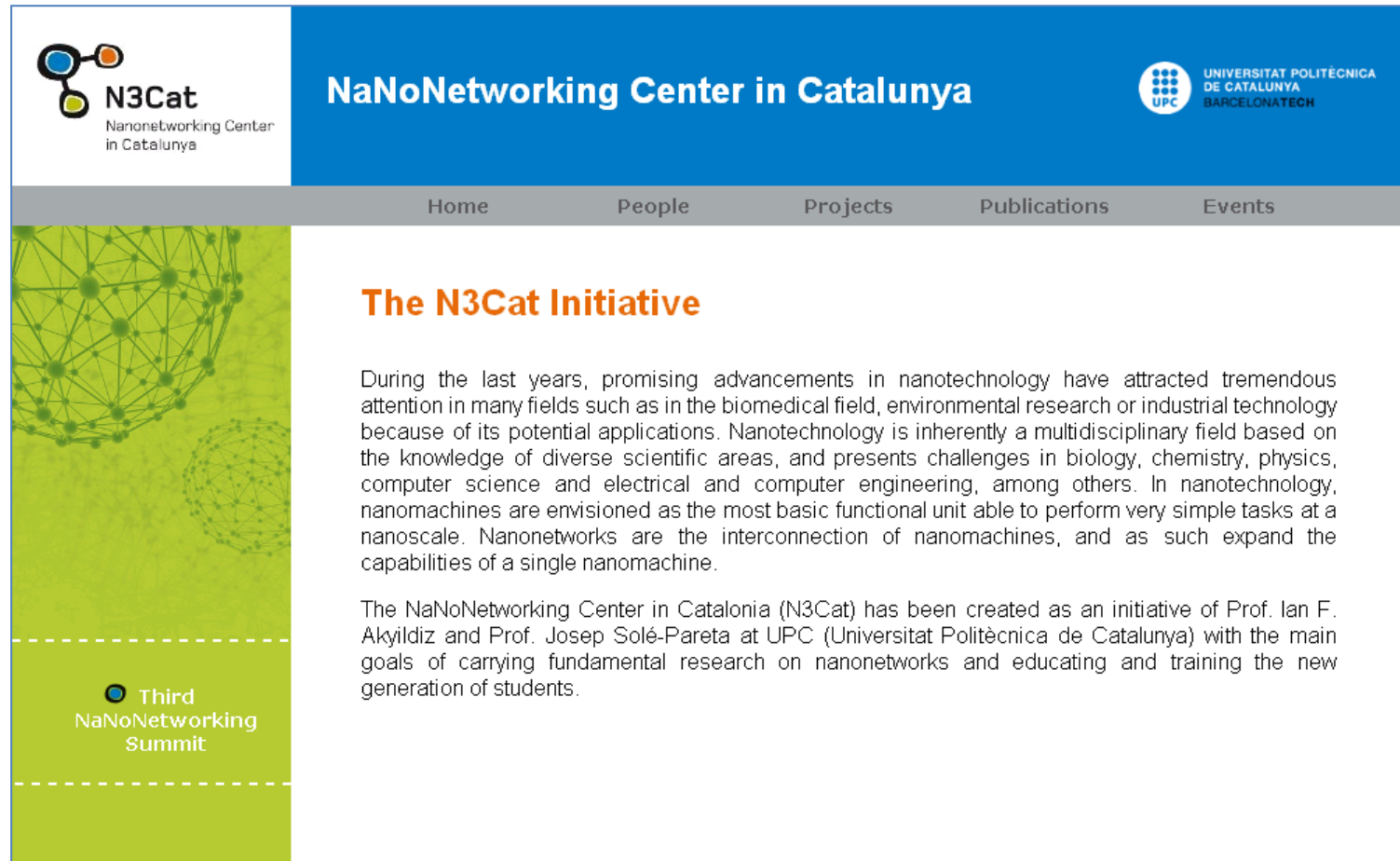


- ▼ Papers
- ▶ Tests
- ▶ TestTemp

N3Cat – N3Sim Project

www.n3cat.upc.edu

Fundamental Research on Nanonetworks



The screenshot shows the N3Cat website homepage. The header is blue with the N3Cat logo on the left and the UPC logo on the right. The main content area is white with a green sidebar on the left. The sidebar contains a large green graphic of a network and a section titled 'Third NaNoNetworking Summit'. The main content area features a navigation bar with links for Home, People, Projects, Publications, and Events. The main heading is 'The N3Cat Initiative' in orange. Below it is a paragraph of text describing the initiative and its goals.

N3Cat
Nanonetworking Center
in Catalunya

NaNoNetworking Center in Catalunya

UNIVERSITAT POLITÈCNICA
DE CATALUNYA
UPC BARCELONATECH

Home People Projects Publications Events

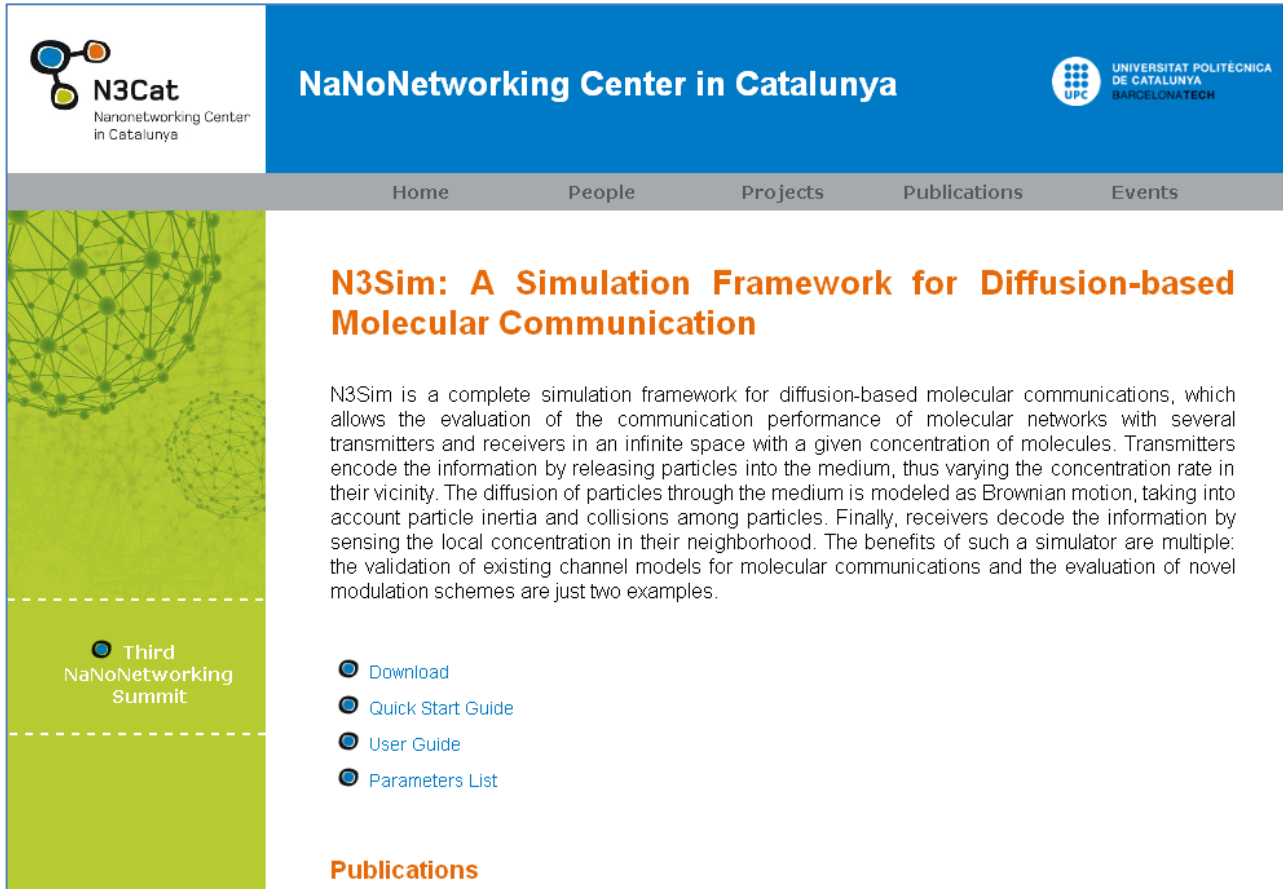
The N3Cat Initiative

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 Solé-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.

● Third
NaNoNetworking
Summit


Simulator, user guides, publications and source code available at
www.n3cat.upc.edu/n3sim



The screenshot shows the N3Cat website homepage. The header features the N3Cat logo and name on the left, the text 'NaNoNetworking Center in Catalunya' in the center, and the UPC logo and name on the right. A navigation bar below the header contains links for Home, People, Projects, Publications, and Events. The main content area has a green background with a network diagram. The title 'N3Sim: A Simulation Framework for Diffusion-based Molecular Communication' is displayed in orange. Below the title is a paragraph describing the simulator. A list of links (Download, Quick Start Guide, User Guide, Parameters List) is provided. A 'Publications' section is also visible at the bottom. A sidebar on the left mentions the 'Third NaNoNetworking Summit'.

 **N3Cat**
Nanonetworking Center
in Catalunya

NaNoNetworking Center in Catalunya

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Home People Projects Publications Events

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.

- [Download](#)
- [Quick Start Guide](#)
- [User Guide](#)
- [Parameters List](#)

Publications

Third
NaNoNetworking
Summit

Aknowledgements

N3Sim has been developed by:

- Iñaki Pascual
- Nora Garralda
- Ignacio Llatser
- Albert Cabellos-Aparicio
- Eduard Alarcón
- Massimiliano Pierobon

N3Sim Video – Demo

