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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.

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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

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- Several technologies have gone into de nano-scale:
  - Chip industry

    Intel's new 3d 22nm architecture
  - Genetics
  - Materials

    Graphene
- Increasing research in nanomachines and nanonetworks

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RESEARCH ARTICLE

Creation of a Bacterial Cell Controlled by a Chemically Synthesized Genome

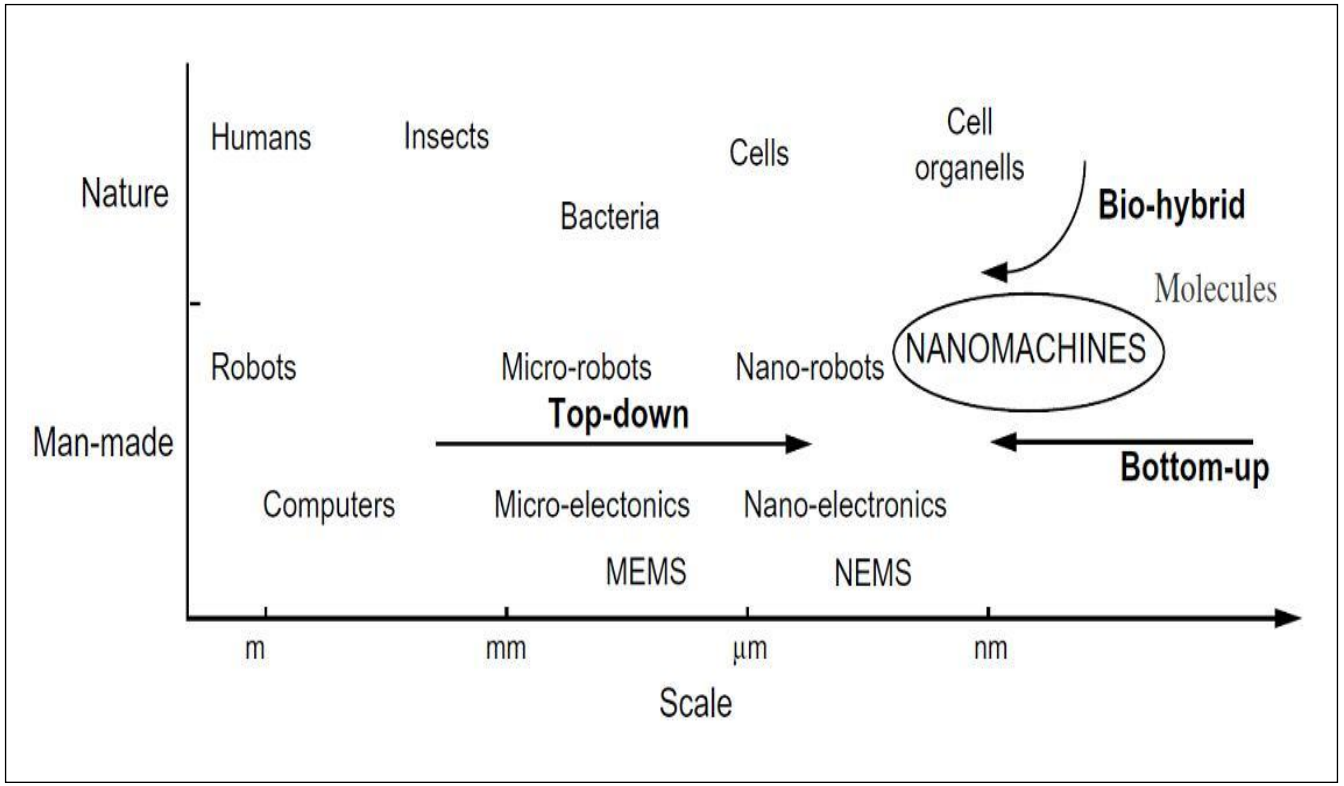
Daniel G. Gibson,[1] John I. Glass,[1] Carole Lartigue,[1] Vladimir N. Noskov,[1] Ray-Yuan Chuang,[1] Mikkel A. Algire,[1] Gwynedd A. Benders,[2] Michael G. Montague,[1] Li Ma,[1] Monzia M. Moodie,[1] Chuck Merryman,[1] Sanjay Vashee,[1] Radha Krishnakumar,[1] Nacyra Assad-Garcia,[1] Cynthia Andrews-Pfannkoch,[1]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

Nanomachines

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 – Molecular Communication

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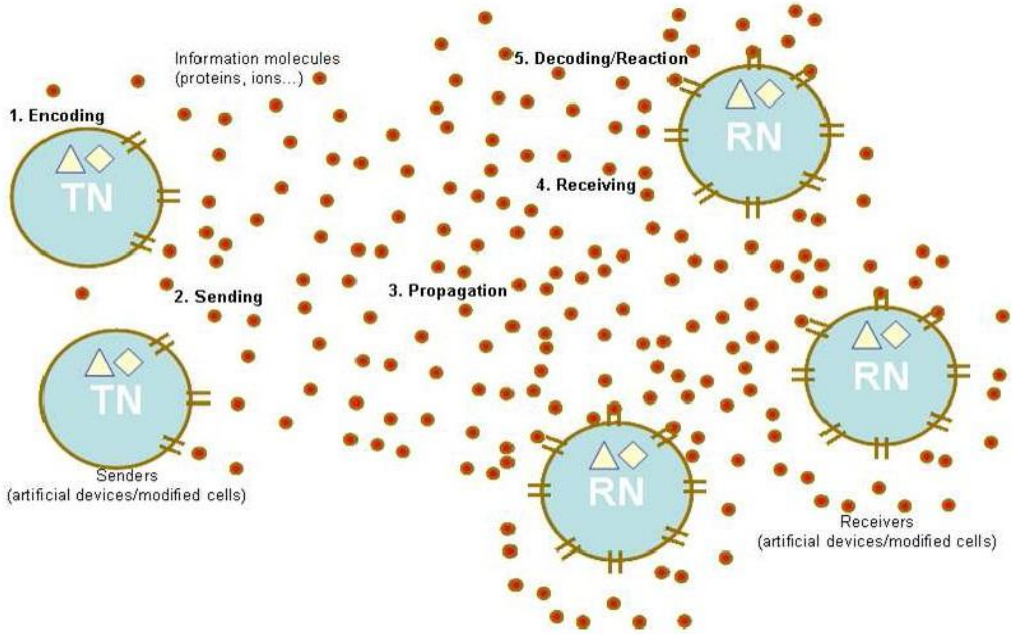
- NanoNetworks, the interconnection of nanomachines
  - will allow nanomachines to execute more complex tasks
  - will expand nanomachines workspace

NanoNetworks – Molecular Communication

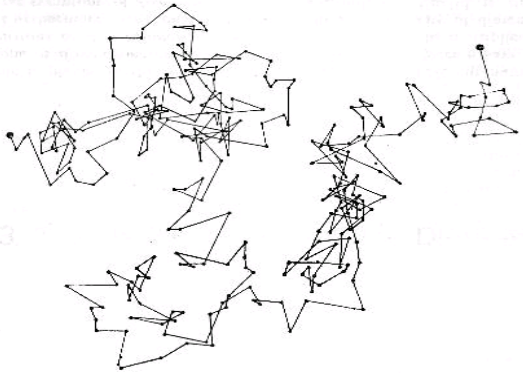
- Molecular communication is a very common process in nature

- Molecular communication emerges as a new communication paradigm



MC – Diffusion

- Brownian Motion : random endless movement of suspended particles in a fluid



- Fick's Laws (1855) $$J = -D\frac{\partial \emptyset}{\partial x}$$
- 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

Collective diffusion

- 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

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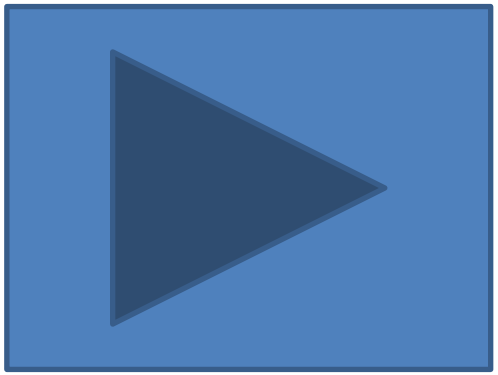
N3Sim - Demo



N3Sim - Goals

Build a simulator that :

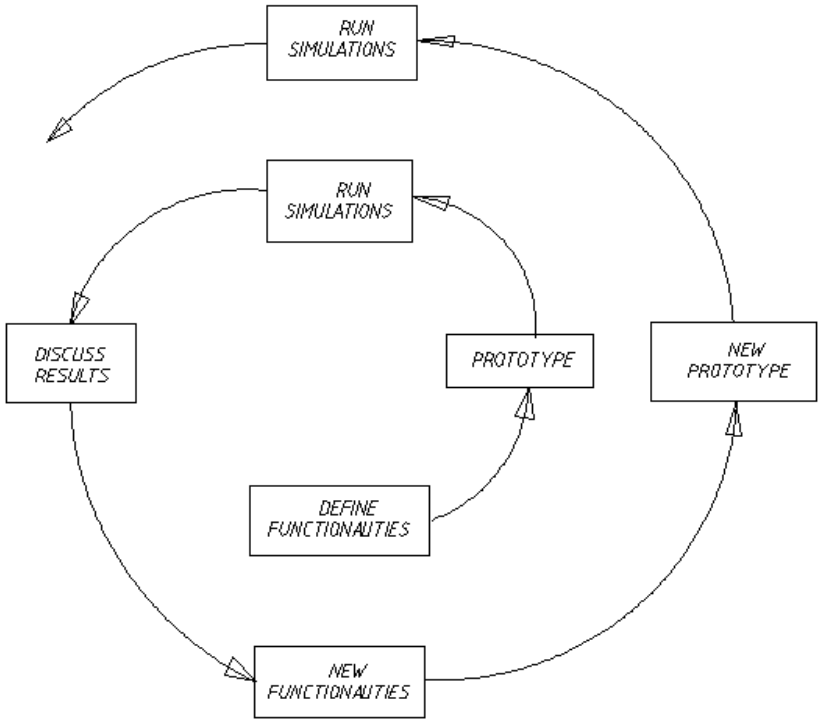
- Allows study of the physical layer:
  - Signal modulation
  - Communication mechanisms
  - Main communication channel metrics
- Implements collective diffusion (Brownian motion + Collisions)
- Is extensible. Future versions may include:
  - Receiver and emitter modules
  - More components of collective diffusion
  - …

N3Sim – Requeriments

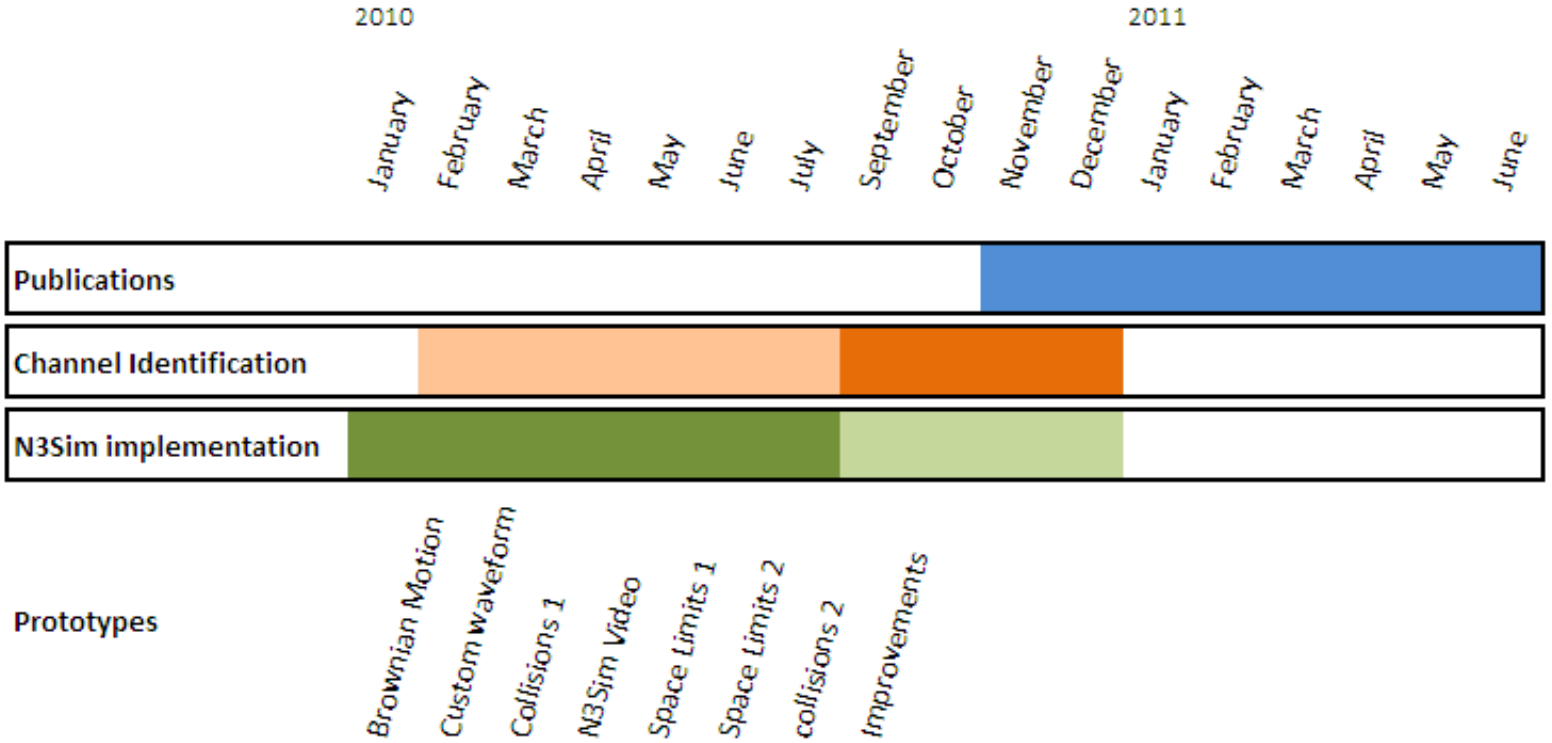
- Functional Requeriments
  - Multiple Emitters and Receivers
  - Custom emission waveform
  - Collective Diffusion (Brownian Motion & Collisions)
  - Initial background concentration
- Non-functional Requirements
  - Reliability
  - Extensibility
  - Modifiability
  - Usability

N3Sim – Project Development

Spiral Development & Rapid Prototyping

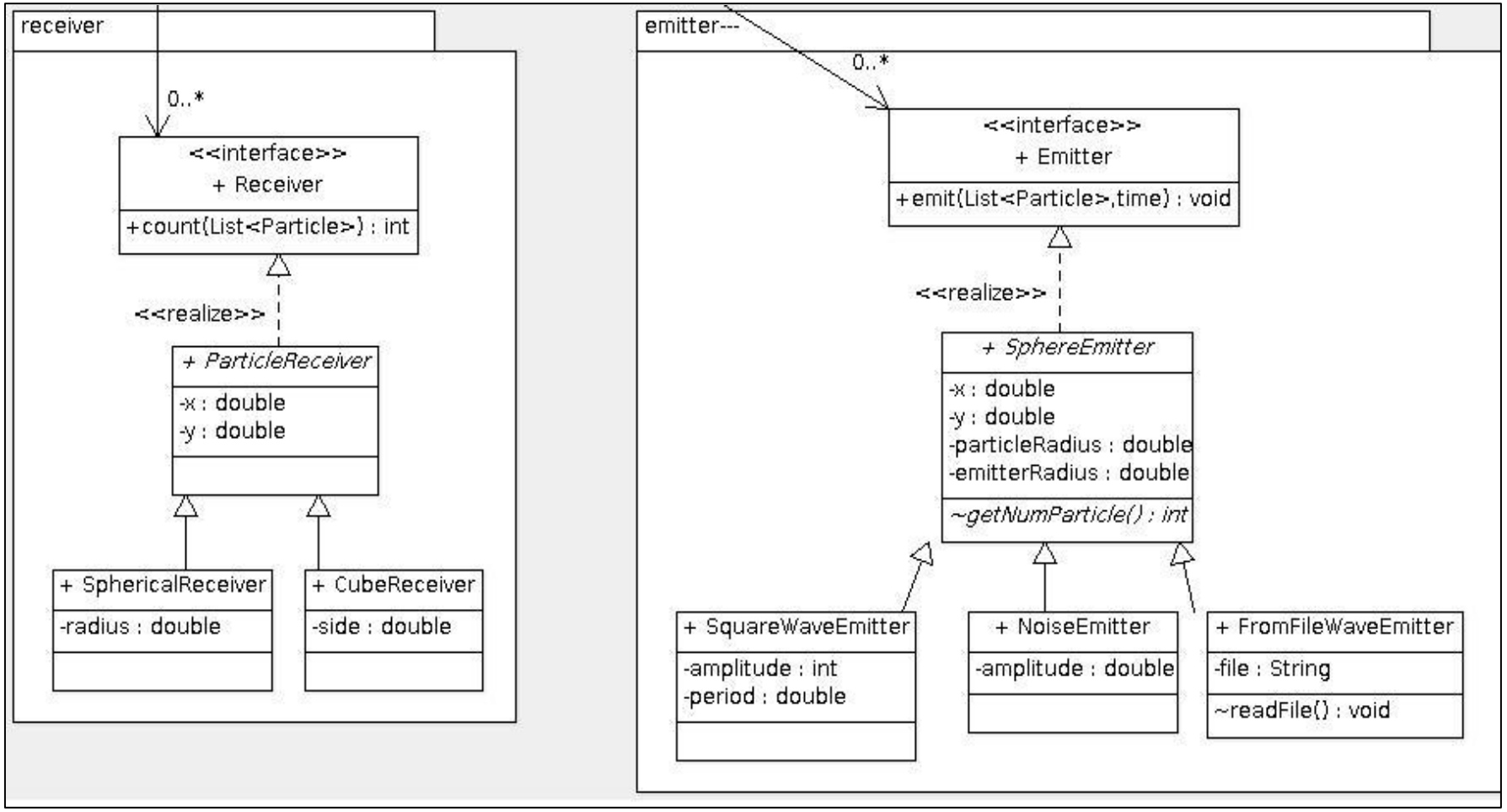


N3Sim – Project Development



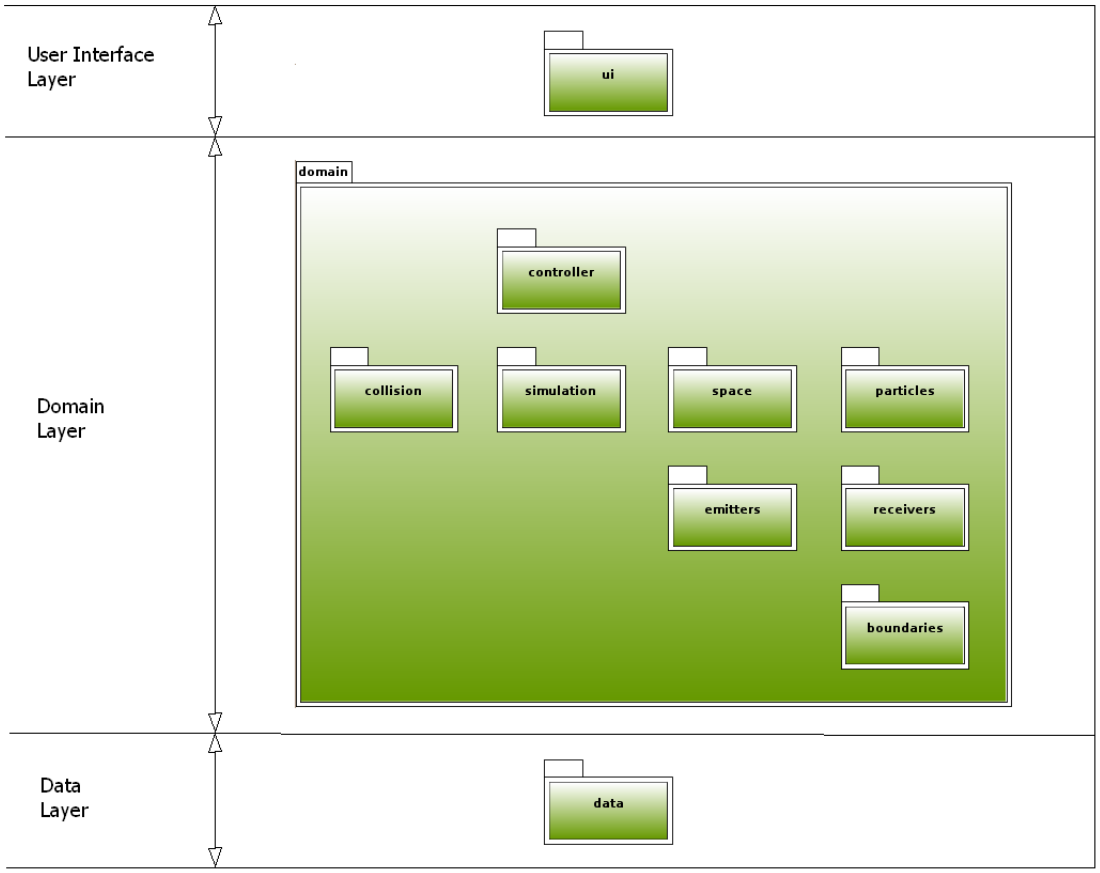
N3Sim – Design & Implementation

Conceptual Model



N3Sim – Design & Implementation

3-Layer Architecture & Packages Structure



Collision Detection (CD) Algorithm

CD – Problem Statement

- N-body problem
  - Time Cost = $O(n^2)$
- Sequential Process
  - Each Collision means new Scenario
  - Time Cost = #collisions *$O(n^2)$
  - No significative parallelization
- Bottleneck

CD – Problem Statement

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

CD – State of the Art

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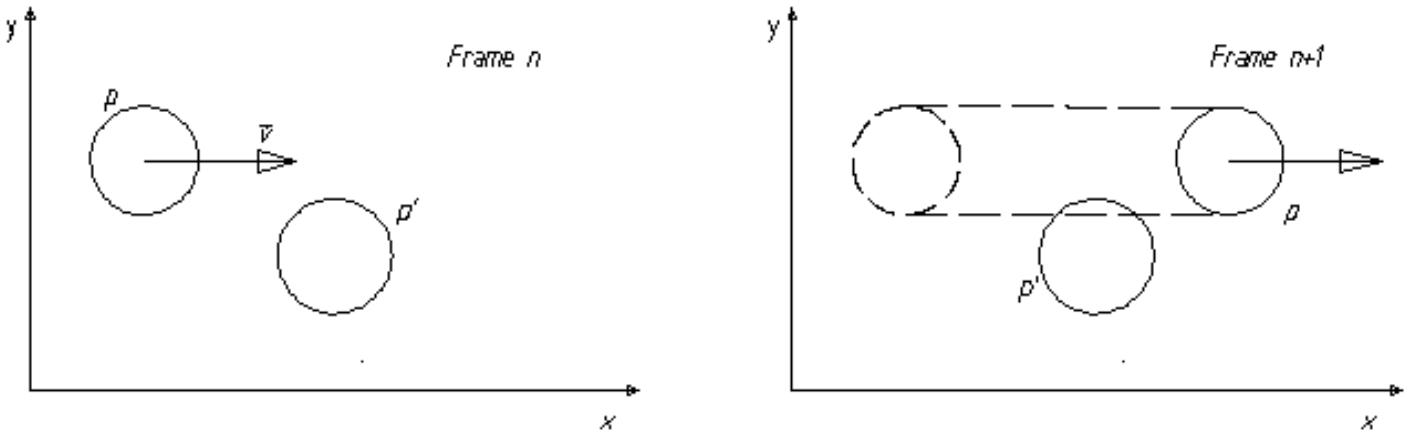
Baraff's Algorithm

- Proven, efficient, easy to implement
- Spatial & Temporal Locality
- Time Cost
  - First collision O(n2)
  - Next collisions O(nlogn)

CD – State of the Art

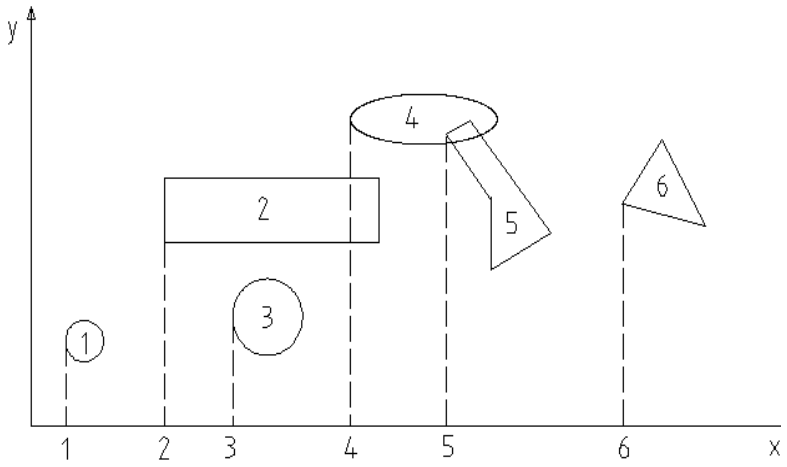
Baraff's Algorithm

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

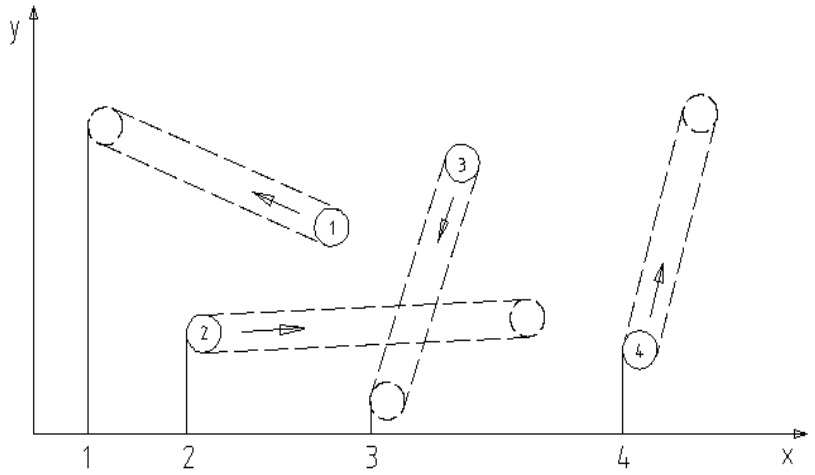


CD – Implementation

- Baraff's (*a posteriori*)



- N3Sim (*a priori*)



CD – N3Sim CD Algorithm

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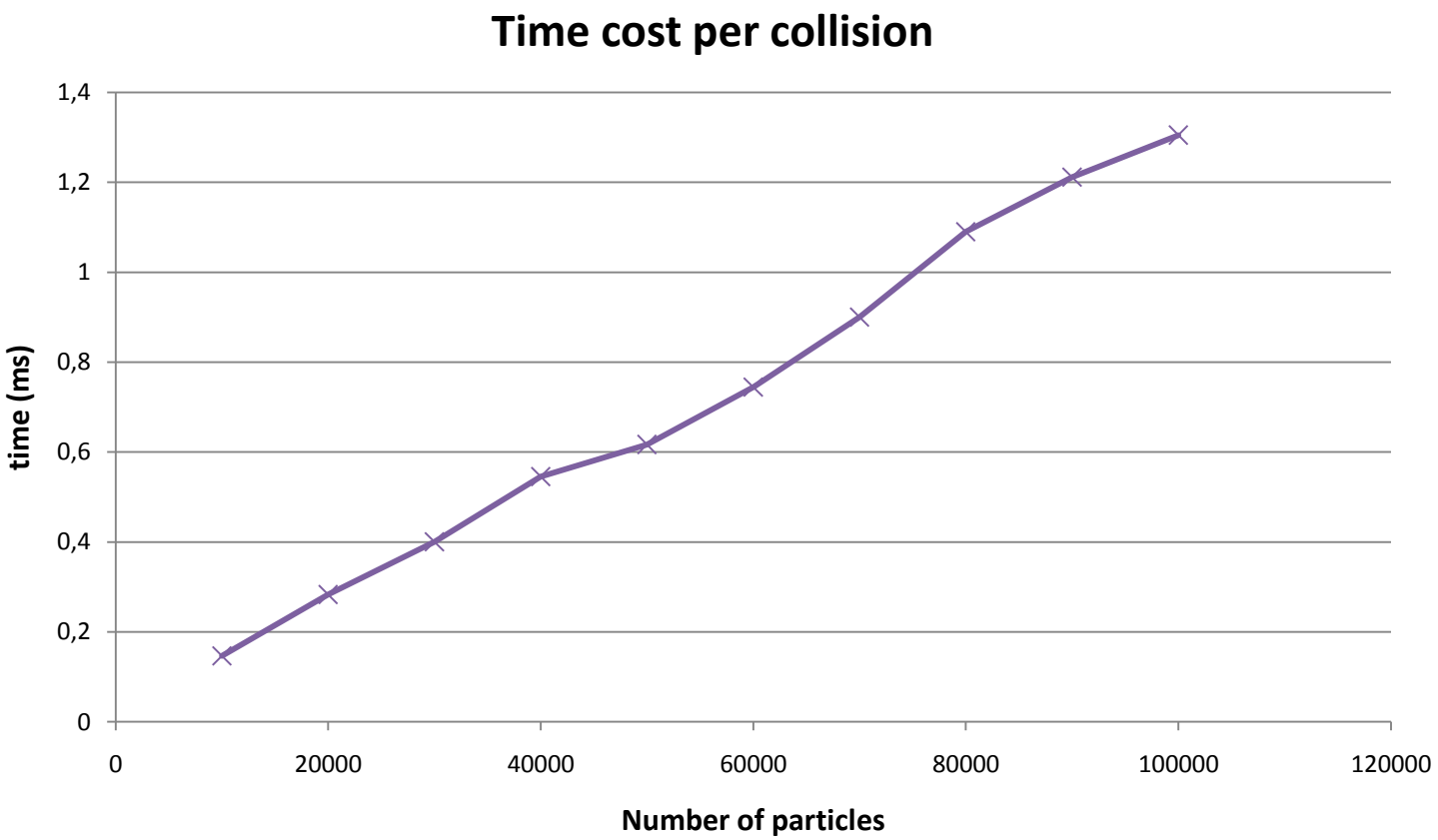
Stage	Operation	Time Cost
1	**Pre-processing**	
1a	Sort Sphere List	O(nlogn)
1b	Create collisions queue	$O(n^2 logn)$
2	**Processing**	
2	While collisions queue is not empty	nc iterations
2a	Obtain first collision	O(1)
2b	Solve collision	O(1)
2c	Sort Sphere List	O(n)
2d	Delete invalid collisions	O(1)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

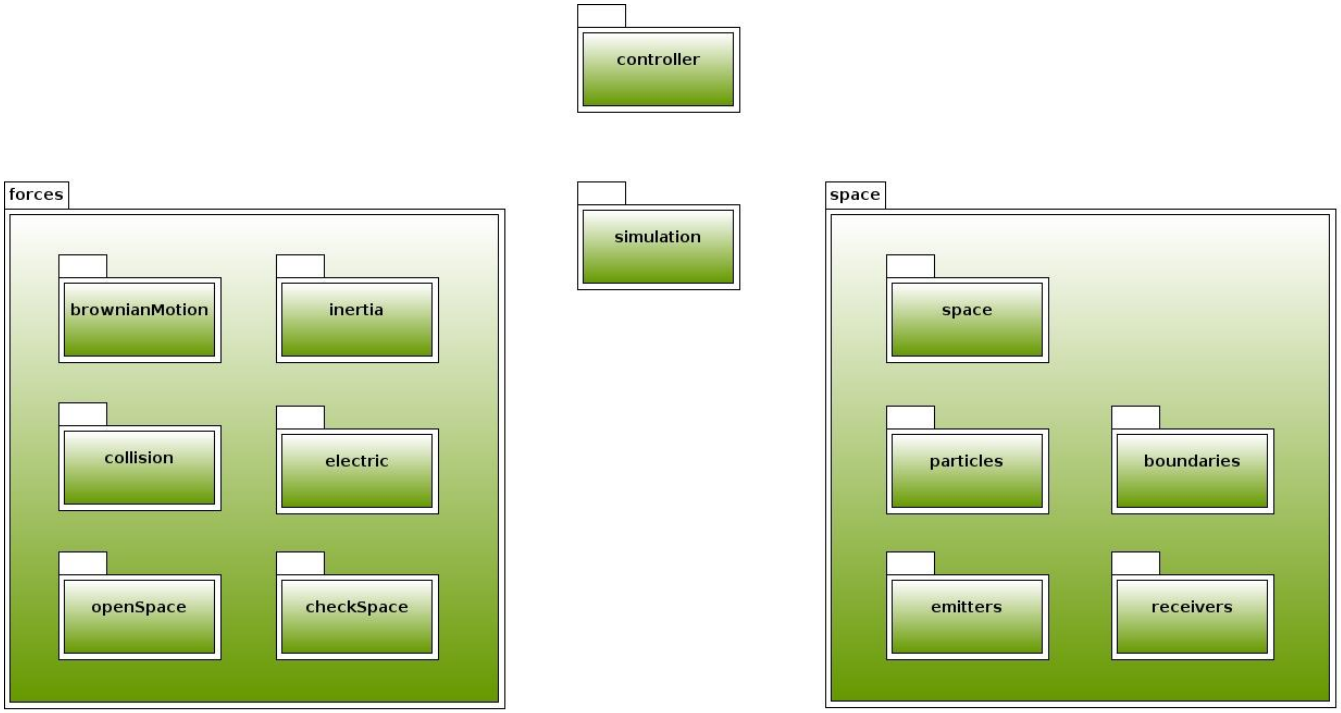
CD – N3Sim CD Algorithm

- Cost (time) = nc * O(nlogn)



Future Work

Future Work

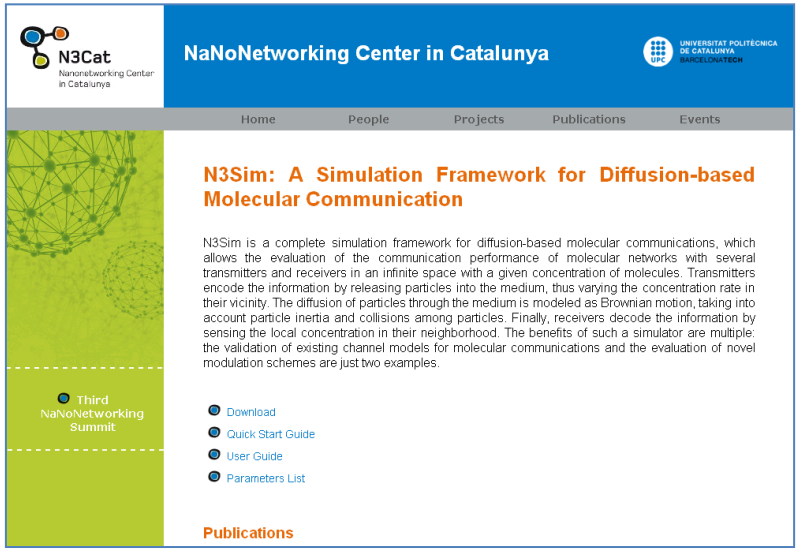

controller
forces
simulation
space
brownianMotion
inertia
collision
electric
openSpace
checkSpace
space
particles
boundaries
emitters
receivers

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

- 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	$\Theta(1)$	$\Theta(r^2)$

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Thank you!

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QUESTIONS ?

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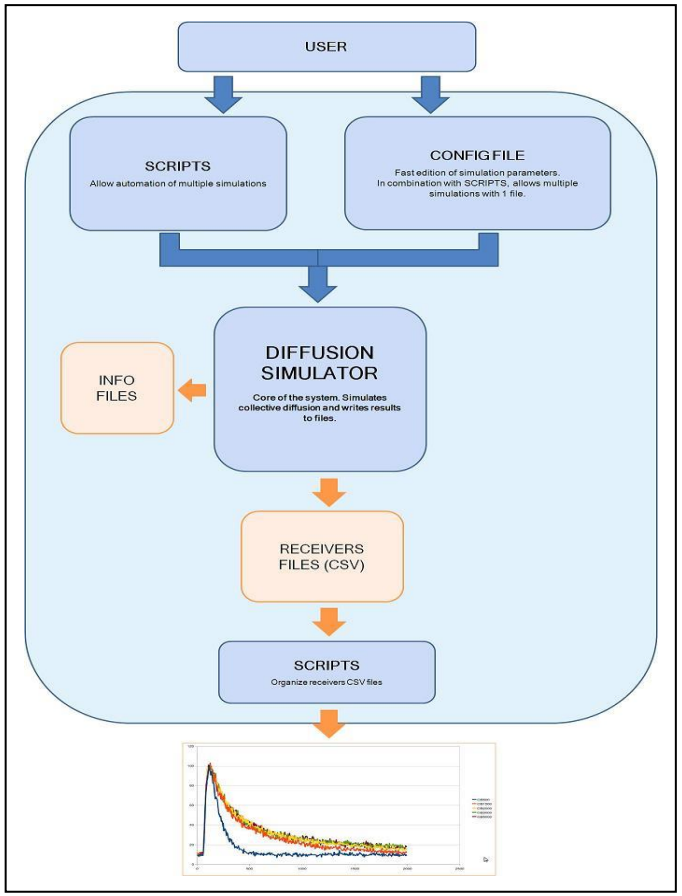
N3Sim – State of the Art

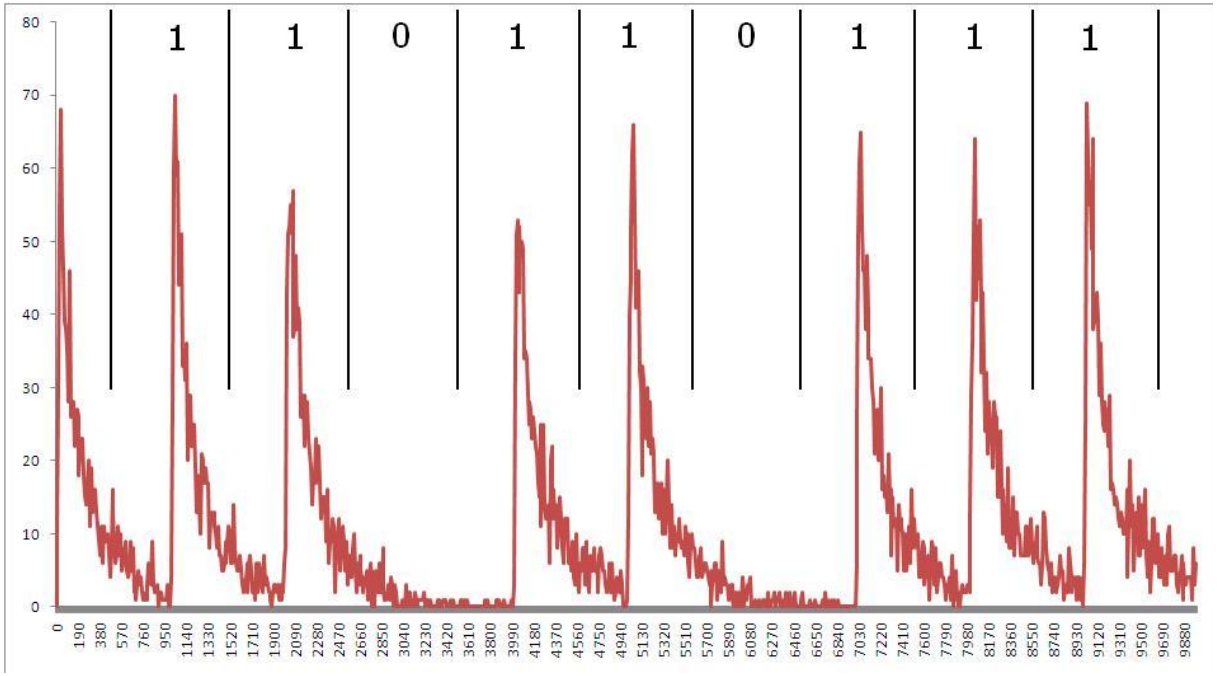
- Mostly educational simulators for Brownian Motion
  - Do not include emitters/receivers
  - Do not include collective diffusion
- NanoNS (June 2010) : module for NS2
  - Does not include collective diffusion
- Universita di Perugia “A simulation tool for nanoscale biological communication systems”

N3Sim – Design & Implementation

Block Diagram



MC - Receiver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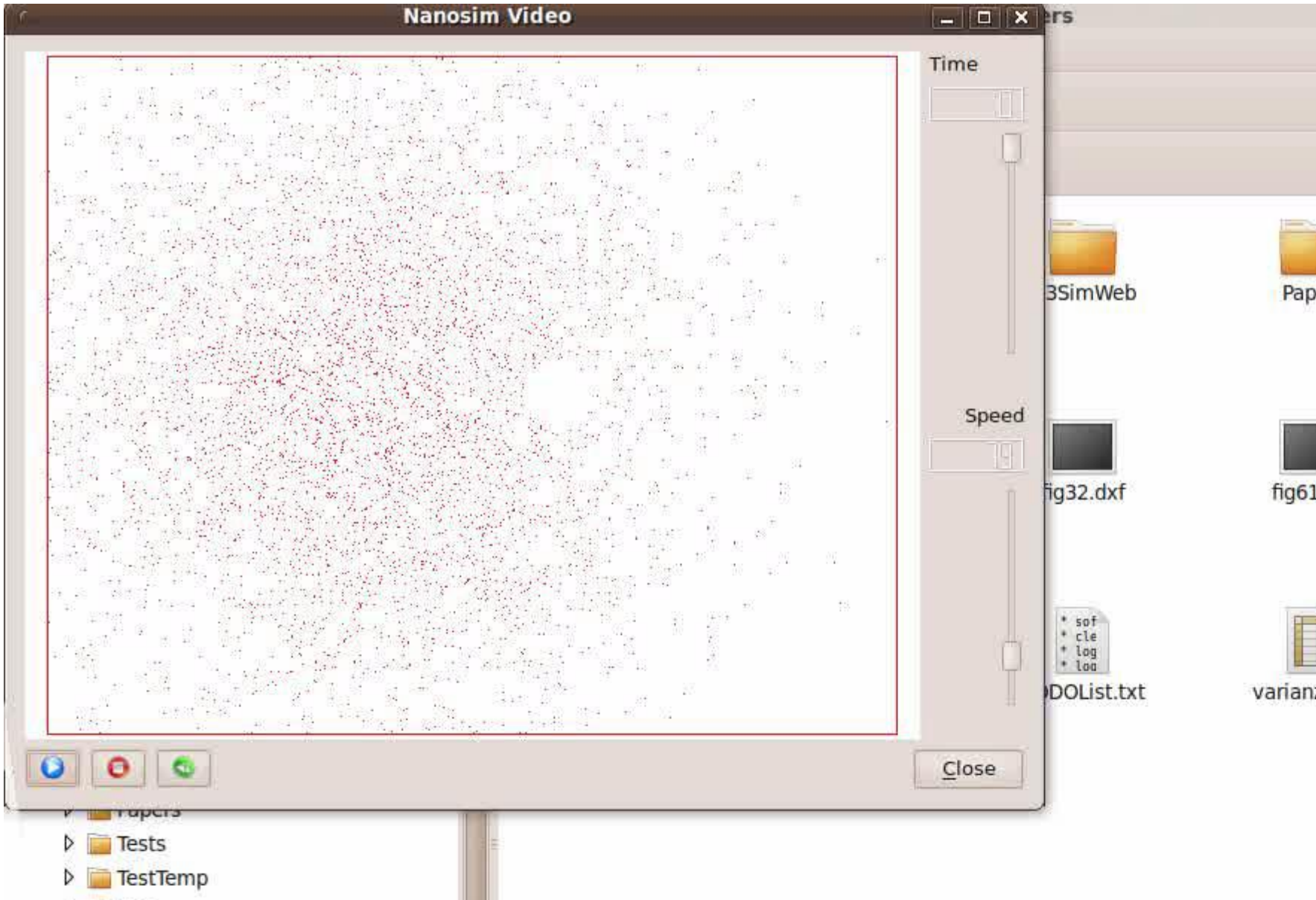
Molecular Communication – N3SimVideo



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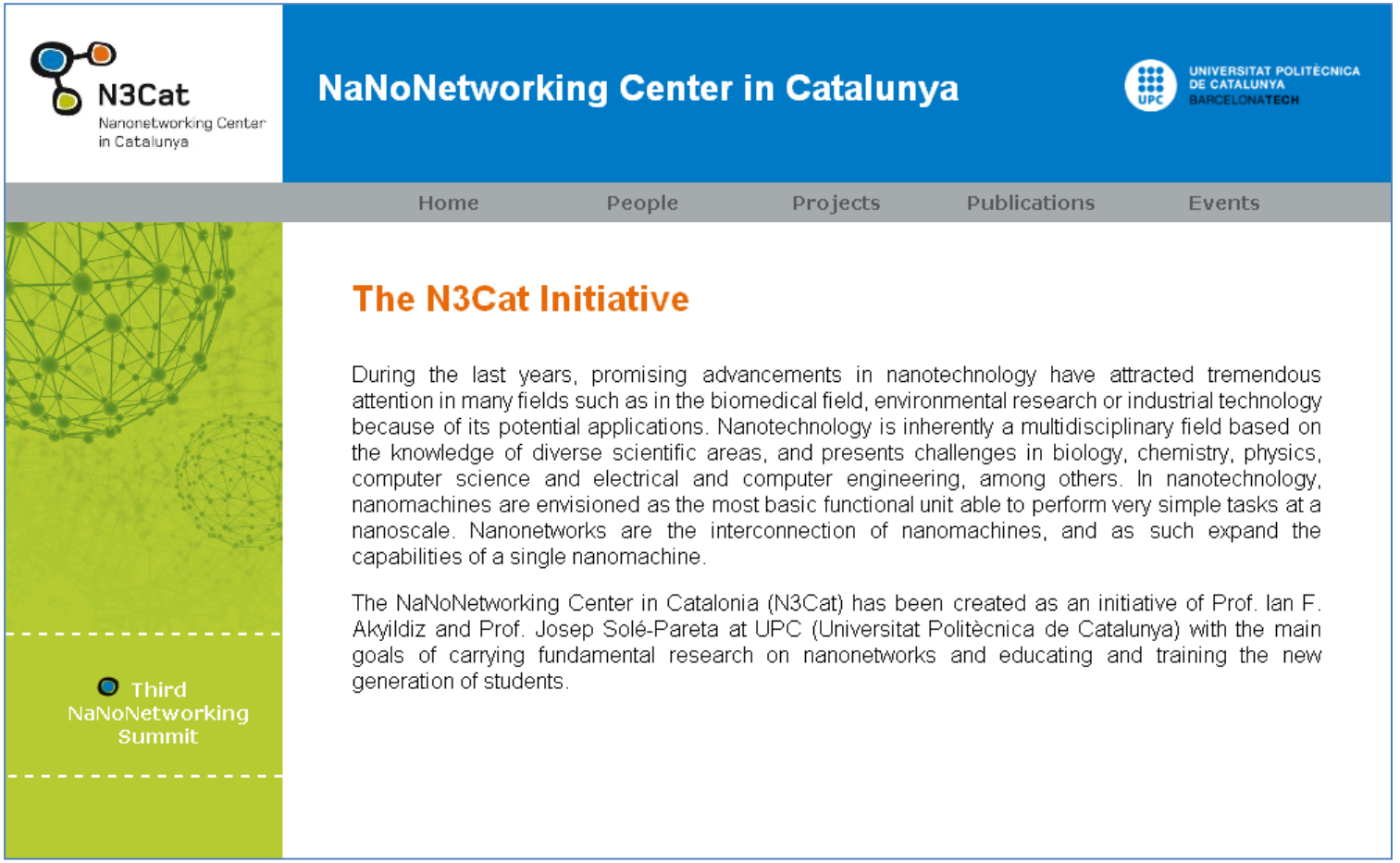
Fundamental Research on Nanonetworks



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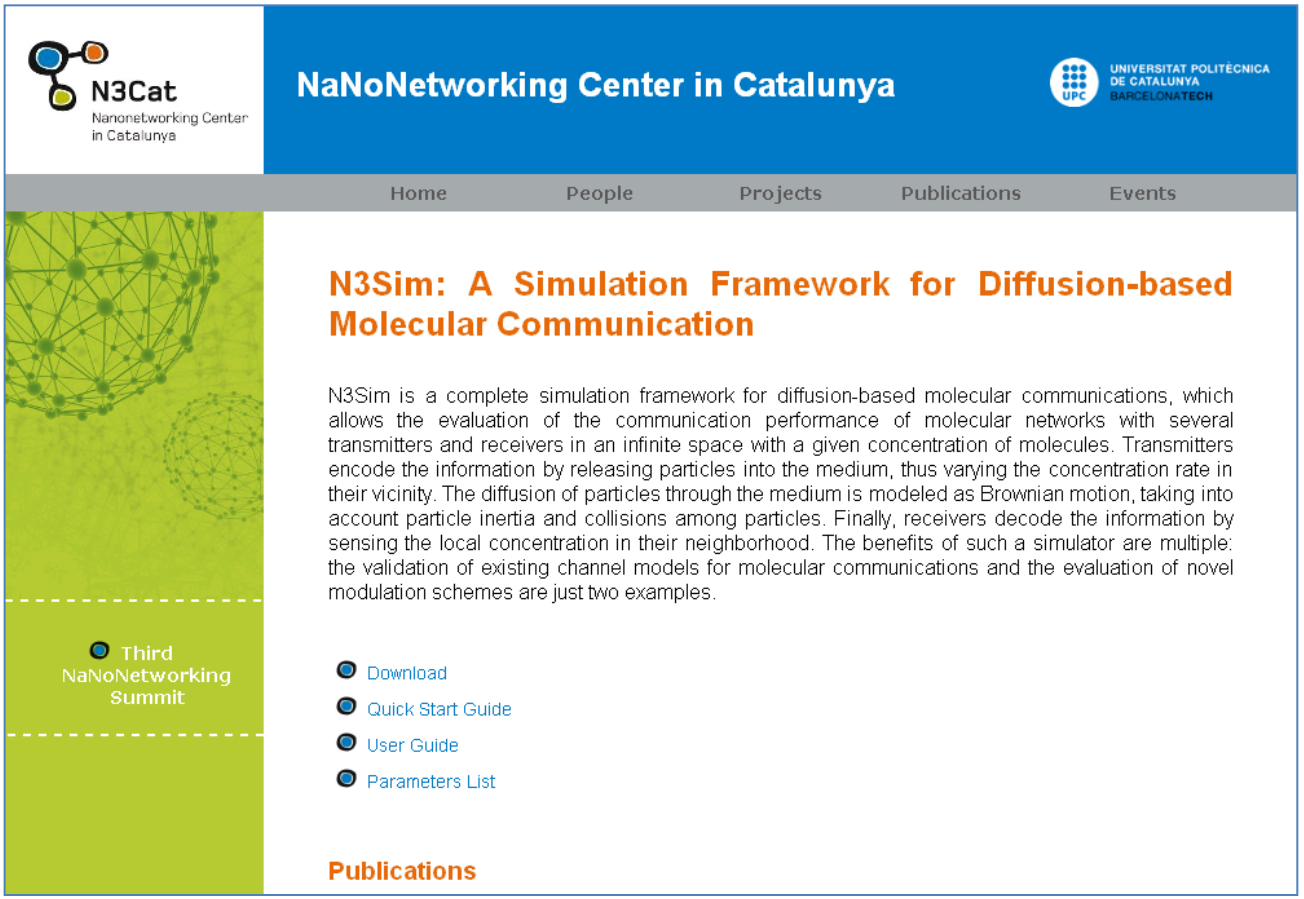

N3Sim Project

Aknowledgements

N3Sim has been developed by:

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

N3Sim Video – Demo