SIMEBAC - *in-vivo* bacteria simulation

Eric Fourmentin-Guilbert Fourmentin-Guilbert Scientific Foundation



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Fourmentin-Guilbert Scientific Foundation

Objective : "To catalyse and promote basic reseach in biology"

The main themes:

- Support initiatives to improve our knowledge in life sciences
- Help the broadcast of high quality information about biological processes



Why a simulation project?

Three observations:

- Data deluge
- Constant increase in processing power
- A lack of synthesis tools
- A computer simulation:
 - Based on the topology of the components
 - Validated and enriched by experiments
 - Interdisciplinary



SIMEBAC project

Initial phase:

- Topologic simulation of a specific function (operon lactose transcription)
- Longer term:
 - Introduction of dynamic features
 - Integration of several functions
 - Integration of additional abstraction layers



Framework

Global structure

Cube of 100x100 nm

Resolution of 1 nm 10⁶ nm³ or 10⁶ points





Sliding cube of 20x20x25 nm

Resolution of 1 A 10⁴ nm³ or 10⁷ points



Project structure

6 research groups:

- Computer Modelling
- Transcription function
- Bacterial cytoplasm (surrounding of the transcription function)
- Instrumentation MNR electronic microscopy
- Water in the cell
- Energetic of molecular interactions in enclosed areas



E. Coli International Alliance (IECA)

Several projects are part of IECA:

- Cybercell (Institute of Biomolecular Design)
- E-Cell (Institute for Advanced Biosciences Keio University)
- Silicon Cell (Biocentrum Amsterdam),....



Minicube representation



