Agent-based framework to simulate metabolic processes

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Outline

Biological context

Agent based systems

Object Oriented design for multi-agent systems

Mitochondrial metabolism application

New developments

Metabolic processes principles

- Metabolism is a set of biochemical reactions involving molecules: **enzymes** and **metabolites**.
- A reaction occurs when molecules are close enough.
- Rules of **biochemistry** or **physics** are applied to compute molecules transformations, when two molecules collide.

Metabolism modeling

- To understand how biological systems work, results of observations are put into **mathematical models**.
- The main goal is to follow *“how”* molecules interact in ***normal*** or ***pathological*** situations.
- Classical tools are **differential equations**.

Metabolism modeling

- To understand how biological systems work, results of observations are put into **mathematical models**.
- The main goal is to follow *"how"* molecules interact in ***normal*** or ***pathological*** situations.
- Classical tools are **differential equations**.
- **Limitations**:
  - only **average behavior** is computed,
  - no way to take into account molecule **localization**,
  - really difficult to do for a **large set of reactions**.

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- The goal is to observe **emergence** of structures, auto-organization between molecules.
- Multi-agent systems allow to design and to compute a whole set of correlated functions, difficult to observe in vivo or in vitro.
- One of the main interests of multi-agent systems is to give an in **silico laboratory** to build biological experiments.

Agent based simulations

- A **multi-agent system** can be viewed as set of objects - the agents - which have the capability to interact following local rules.
- For molecular biology, we use **reactive agents**, situated in **3D space** .
- Simulations are driven by a **life cycle** which defines the sequence of operations:
  - **perception**: fing neighbouring,
  - **decision**: try to do something to do,
  - **action**: move, fire a reaction ...

Object oriented design

- **`BioAgent`** with position, common biological attributes and a life cycle.
- Two subclasses :
  - **`Catalyser`**: interaction rules and list of specific partners.
  - **`ReactiveUnit`**: brownian movement.
- **Environment** is just global attributes.
- **Simulation engine** manages the time steps and the grid dimensions.
- Graphic needs to have **`gridAgents`** with graphical characteristics.

Mitochondrial metabolism application

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- MitoScoP project:
  - **Capitalizing** knowledge about mitochondria.
  - **Analysis** of metabolism network structure.
  - **Simulations** of several parts of mitochondrial metabolism: TCA cycle with differential equations, Qcycle and membranes with multi-agent systems.

Redox Applications

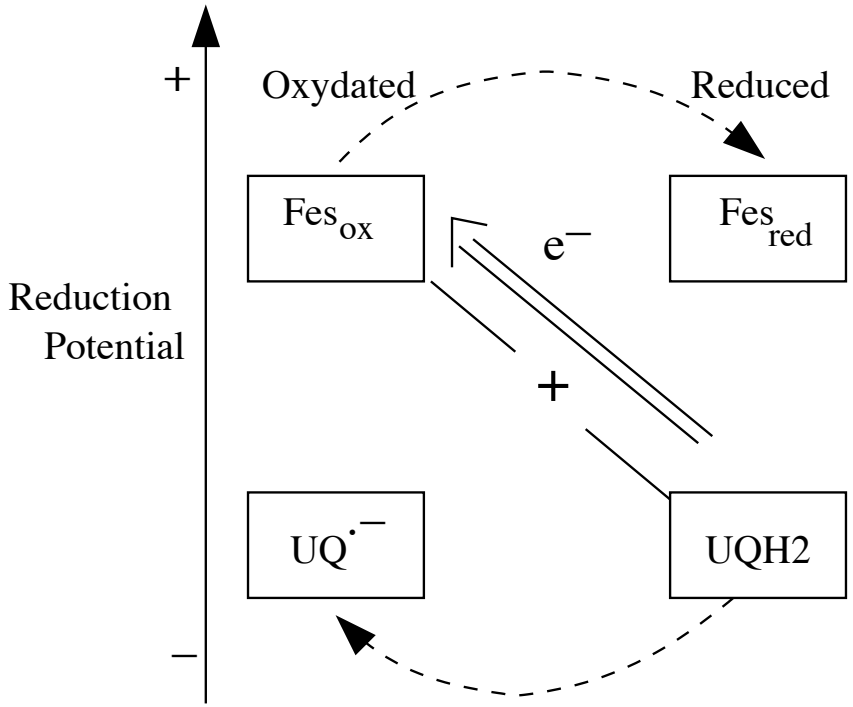

Figure: electron exchange between two molecules

Questions about using Lisp

- `Catalyser` can be defined as a superclass for several types of enzymes - `dynamical generation of classes` from data files.
- `Interactions` with users is essential during simulations: repairing of abnormal cases or at the opposite inclusion of perturbations.

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- **`Catalyser`** can be defined as a superclass for several types of enzymes - **`dynamical generation of classes`** from data files.
- **`Interactions`** with users is essential during simulations: repairing of abnormal cases or at the opposite inclusion of perturbations.
- **`Memory management`** and number of agents - molecules.
- **`No parser`**.
- **`Small code`**!!!

Perspectives

- 3D graphic library: McClim and OpenGL
- How to present results: graph,diagrams, selection of entities.

Perspectives

- 3D graphic library: McClim and OpenGL
- How to present results: graph,diagrams, selection of entities.
- Addition of more biochemical reactions.
- Simulations of membranes structuration.