Object-oriented Programming for Biomodelling

Sergiu Ivanov
sergiu.ivanov@univ-grenoble-alpes.fr

Université Grenoble Alpes

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My Previous Research on Formal Models

Rewriting

Machines
My Previous Research on Formal Models

Rewriting

string rewriting

A B → B a

multiset rewriting

- a
- b
- c
- d

Register machines

Turing machines

Apply to complex biological systems
My Previous Research on Formal Models

Rewriting

string rewriting
A B → B a

multiset rewriting

Machines

Register machines

Turing machines

\[
\begin{array}{c}
R_1 \\
R_2 \\
\vdots \\
R_n \\
\end{array}
\]

\[
\begin{array}{c}
\cdots \ a \ b \ 1 \ \cdots \\
\end{array}
\]

\[
q_i
\]
My Previous Research on Formal Models

Rewriting

string rewriting
A B → B a

multiset rewriting

Machines

Register machines
R1
R2
...
Rn

Turing machines
...
q1
a b 1

Apply to complex biological systems
In the Meantime, Much Programming

- applications in research
- side projects
In the Meantime, Much Programming

- applications in research
- side projects

Functional programming

- Haskell
  - solvers
  - simulators
  - teaching

Object-oriented programming

- Python
  - category theory module for SymPy
  - postdoc

C++ [no logo :-(]
In the Meantime, Much Programming

- applications in research
- side projects

Functional programming

- Haskell
  - solvers
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Object-oriented programming

- Python
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Postdoc: OOP apply biomodelling

https://openclipart.org/
Postdoc: OOP \(\text{apply}\) biomodelling

Modelling framework

- generic
- extensible
- parallel

Goal:

Develop a biomechanical model of microtubules
- mass-spring-based

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Outline

1. Microtubules: Biology and Modelling
2. Grid Registers
3. Grid Register Transformers
4. Real Coordinates
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Microtubules

- tubular polymers of tubuline
- support the shape of the cell
- support the cellular transport

A

The characteristic shape and size of a microtubule.

B

Microtubules form dense structures.
Microtubules as Mass-spring Systems

Modelling microtubules as a system of masses connected with springs gives good results.
Outline

1. Microtubules: Biology and Modelling
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4. Real Coordinates
What We Want: Masses and Springs
What We Want: Masses and Springs

![Diagram of masses and springs connected by springs]
What We Want: Masses and Springs

Discretise on a grid

- to simulate the diffusion of reactants
What We Want: Grid Registers of Agents

\[ \text{agent} = \text{payload} + \text{cursor} \]

The **cursors** handle (abstract away) the **mouvement**.
What We Want: Grid Registers of Agents

\[ \text{agent} = \text{payload} + \text{cursor} \]

The \textit{cursors} handle (abstract away) the \textit{mouvement}.

Register (grid of cursors)

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What We Want: Grid Registers of Agents

\[ \text{agent} = \text{payload} + \text{cursor} \]

The \textit{cursors} handle (abstract away) the \textit{mouvement}.

Register (grid of cursors)

https://openclipart.org/
Grid Registers of Cursors: Implementation

```
Grid3DRegister

Payload, Size

Cursor

register: Grid3DRegister

cursor: Cursor

move true/false

move true/false

https://perso.ensta-paristech.fr/~kielbasi/tikzuml/
```
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1. Microtubules: Biology and Modelling
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Grid Register Transformers

Register

Changes the way the cursors move

Superposition of behaviour

Transformers can be superposed

Haskell and monad transformers

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Grid Register Transformers

- a kind of a register
- changes the way the cursors move
- superposition of behaviour
  - transformers can be superposed
Grid Register Transformers

- a kind of a register
- changes the way the cursors move
- superposition of behaviour
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wink-wink Haskell and monad transformers ;-)
Grid Register Transformers: Examples

Obstacles

Adaptors

- connect several registers
- connect a register to itself

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Grid Register Transformers: Implementation

Explode Grid3DRegister:

```
Grid3DRegister

DefaultGrid3DRegister

Transformer
```

https://perso.ensta-paristech.fr/~kielbasi/tikzuml/
Grid Register Transformers: Implementation

Explode Grid3DRegister:

Transformers are transparent to cursors:

https://perso.ensta-paristech.fr/~kielbasi/tikzuml/
Outline

1. Microtubules: Biology and Modelling
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4. Real Coordinates
Cursors with Real Coordinates

RealCursor

Handle the discretisation.

Cursor

Real coordinates influence grid coordinates

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Cursors with Real Coordinates

RealCursor

Cursor

Handles the discretisation.

Real coordinates influence grid coordinates

- unnecessary dependence
- difficult to maintain

https://perso.ensta-paristech.fr/~kielbasi/tikzuml/
Real Coordinates + Transformers = ?

Transformer ◀ «don't know» ◁ RealCursor

Real Coordinates $+$ Transformers $=$ ?

**Transformer**

- - - «don't know» - - →

**RealCursor**

Cast is you friend. 🍌

- only at cursor creation
- everything works with casts

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Real Coordinates + Transformers = ?

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Conclusions and Open Questions

- OOP \textit{apply} biomodelling

- \textit{agent} = \textit{payload} + \textit{cursor}

- \textbf{Transformer} for compositional behaviour

- ? \textbf{Transformer} + \textbf{RealCursor}