

# Object-oriented Programming for Biomodelling

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Université Grenoble Alpes

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# My Previous Research on Formal Models

## Rewriting

## Machines

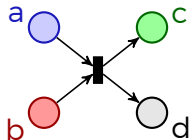
# My Previous Research on Formal Models

## Rewriting Machines

string rewriting

$$A B \rightarrow B a$$

multiset rewriting



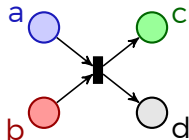
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## Rewriting

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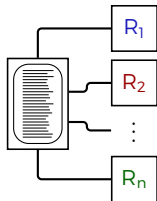
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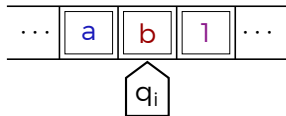


## Machines

Register machines



Turing machines



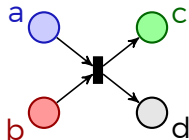
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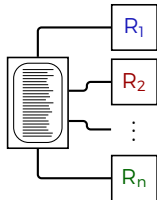
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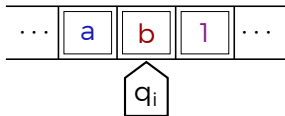


## Machines

Register machines



Turing machines



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Apply to **complex** biological **systems**

# In the Meantime, Much Programming



- ▶ applications in research
- ▶ side projects

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- ▶ side projects

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## Functional programming

Haskell 

- ▶ solvers
- ▶ simulators
- ▶ teaching

## Object-oriented programming

Python  python™

- ▶ category theory module for SymPy 

C++ [no logo :-)]

- ▶ postdoc

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Postdoc: OOP  $\xrightarrow{\text{apply}}$  biomodelling

<https://openclipart.org/>



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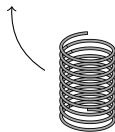
## Modelling framework

- ▶ generic
- ▶ extensible
- ▶ parallel

### Goal:

Develop a **biomechanical** model  
of **microtubules**

- ▶ mass-spring-based



<https://openclipart.org/>

# Outline

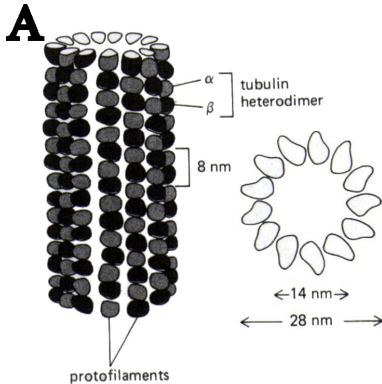
1. Microtubules: Biology and Modelling
2. Grid Registers
3. Grid Register Transformers
4. Real Coordinates

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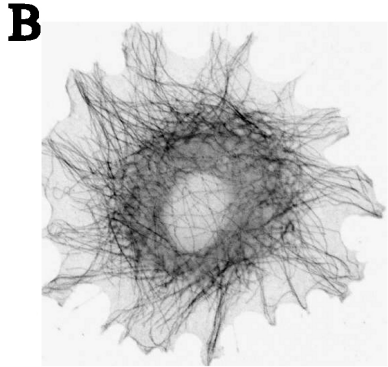
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# Microtubules

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

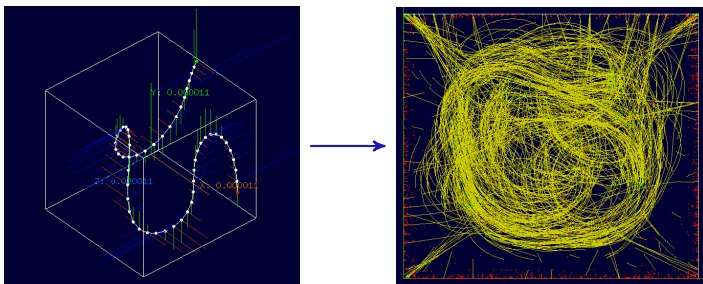


The characteristic **shape** and **size** of a **microtubule**.



**Microtubules** form **dense** structures.

# Microtubules as Mass-spring Systems

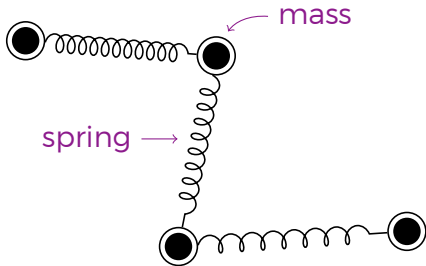


Modelling microtubules as a system of masses connected with springs gives good results.

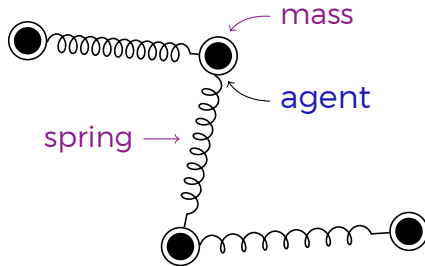
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# What We Want: Masses and Springs

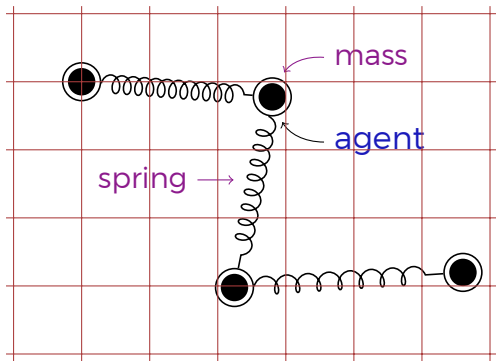


# What We Want: Masses and Springs





# What We Want: Masses and Springs



Discretise on a grid

- ▶ to simulate the diffusion of reactants

# What We Want: Grid Registers of Agents

agent = payload + cursor

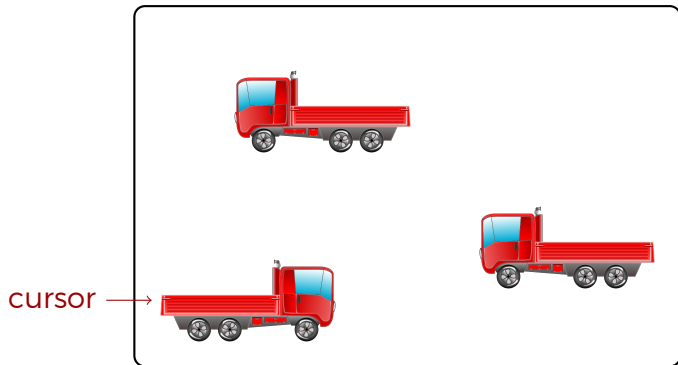
The **cursor**s handle (abstract away) the **mouvement**.

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Register (grid of cursors)



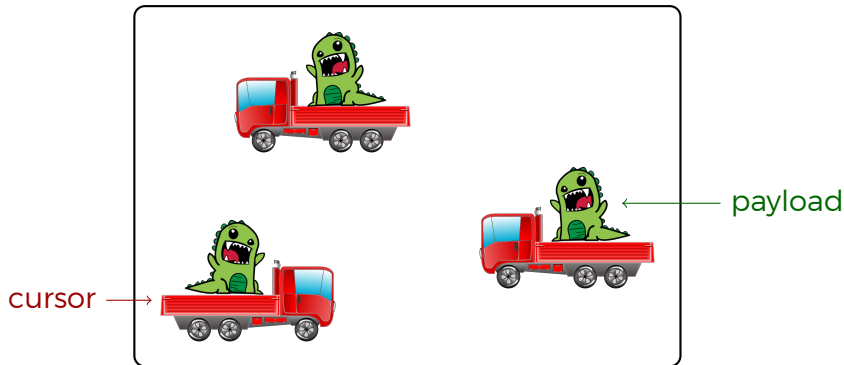
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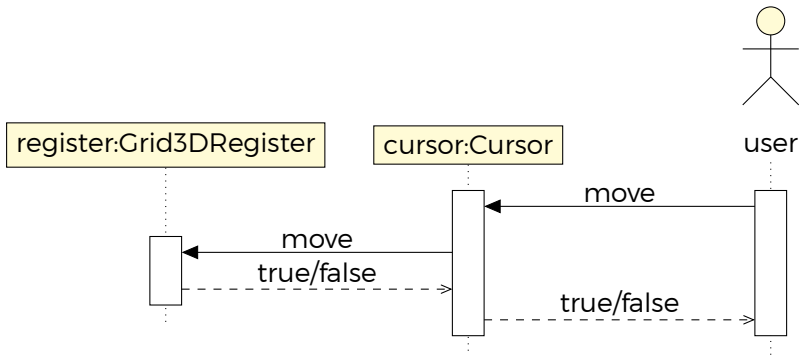
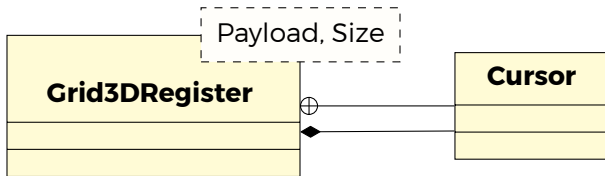
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Register (grid of cursors)



<https://openclipart.org/>

# Grid Registers of Cursors: Implementation



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

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# Grid Register Transformers



# Grid Register Transformers

- ▶ a kind of a register
- ▶ **changes** the way the **cursors** move
- ▶ **superposition** of behaviour
  - ▶ transformers can be superposed

## Transformer

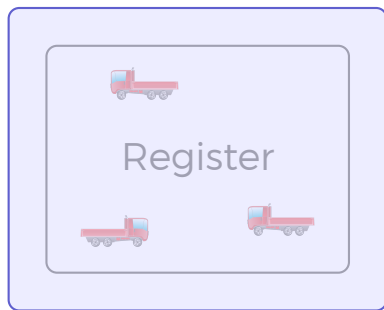




# Grid Register Transformers

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## Transformer



wink-wink Haskell and monad transformers ;-)

<https://openclipart.org/>

# Grid Register Transformers: Examples

Obstacles  

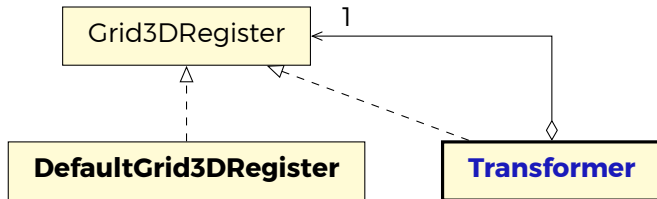
Adaptors 

[demo]

- ▶ connect **several** registers
- ▶ connect a register **to itself**

# Grid Register Transformers: Implementation

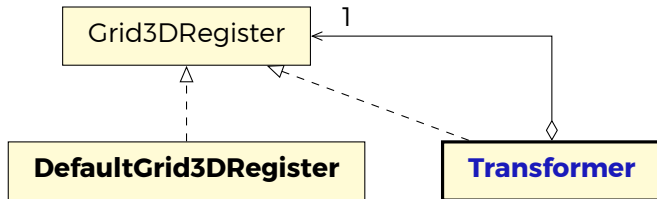
Explode Grid3DRegister:



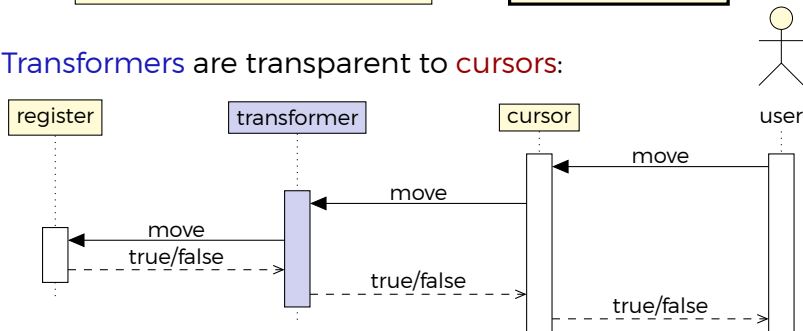
<https://perso.ensta-paristech.fr/~kielbasi/tikzuml/>

# Grid Register Transformers: Implementation

Explode Grid3DRegister:



Transformers are transparent to **cursor**s:

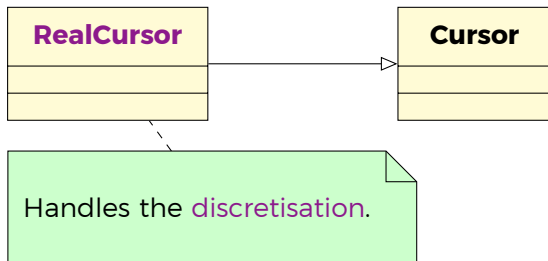


<https://perso.ensta-paristech.fr/~kielbasi/tikzum1/>

# Outline

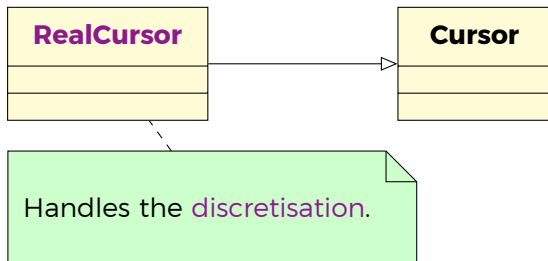
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# Cursors with Real Coordinates



Real coordinates  $\xrightarrow{\text{influence}}$  grid coordinates

# Cursors with Real Coordinates



Real coordinates  $\xrightarrow{\text{influence}}$  grid coordinates

~~grid coordinates  $\xrightarrow{\text{influence}}$  Real coordinates~~

- ▶ unnecessary dependence
- ▶ difficult to maintain

# Real Coordinates + Transformers = ?





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Cast is your friend.



- ▶ only at cursor creation
- ▶ everything works with casts

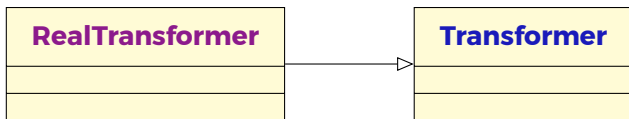
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<https://openclipart.org/>

# Conclusions and Open Questions

▶ OOP  $\xrightarrow{\text{apply}}$  biomodelling

▶ agent = payload + cursor



▶ **Transformer** for compositional behaviour

?

**Transformer**

+

**RealCursor**