sybila

Comprehensive Modelling Platform

Annotation in modelling of complex systems

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Model

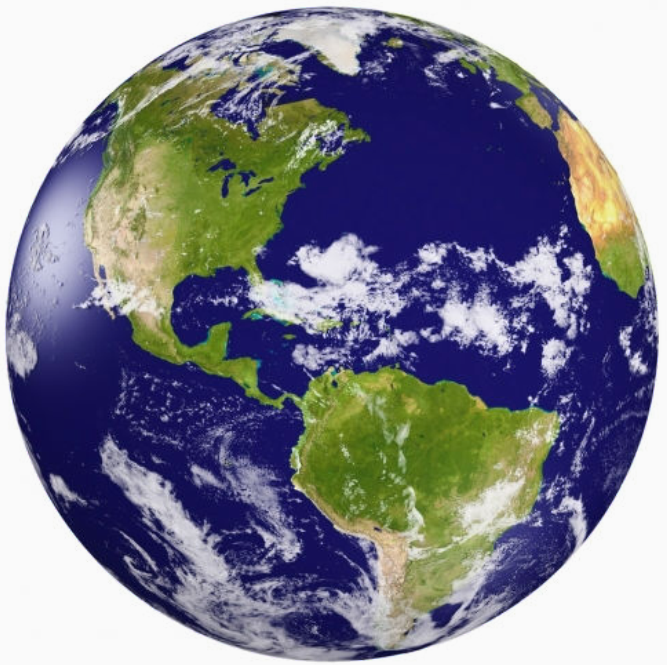
Model: simplified representation of the real system.

E.g. physical miniature, mathematical formula, computer program...

> **"All models are wrong. Some models are useful."**
>
> *George Box*

The real system is always more detailed than the model. Less details make reasoning about the model much simpler. It allows us to predict the behaviour of the system or control it. Saves **time** and **resources**.

Model – globe



Model – globe

- Measure the distance from Brno to Prague? Not really.

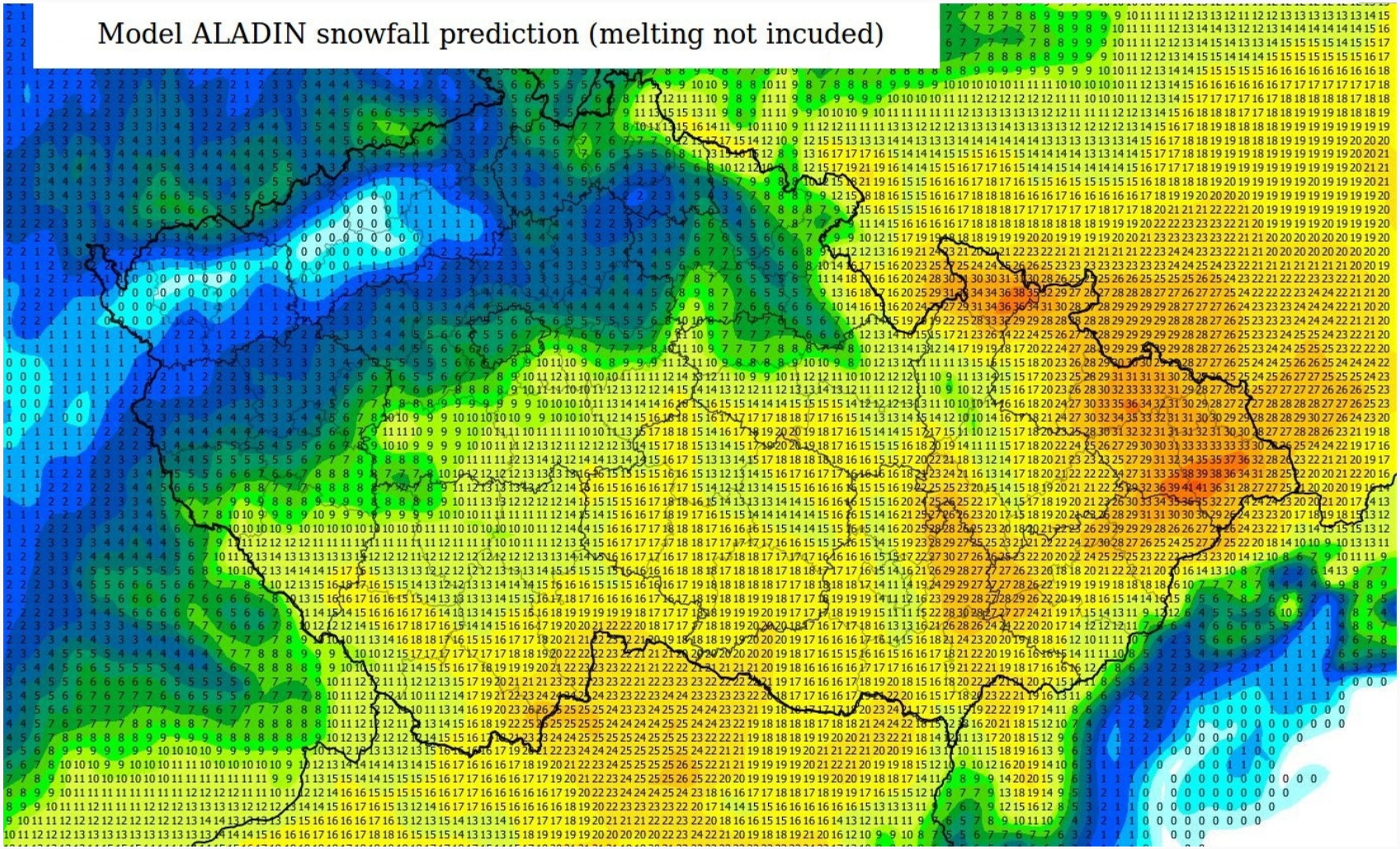
  $\Rightarrow$ **Globe is not detailed enough!**

- Determine the neighbouring countries with Algeria? Yes.

  $\Rightarrow$ **Globe is useful!**

  (Marocco, Tunisia, Libya, Niger, Mali, Mauritania, Western Sahara)

Model – weather

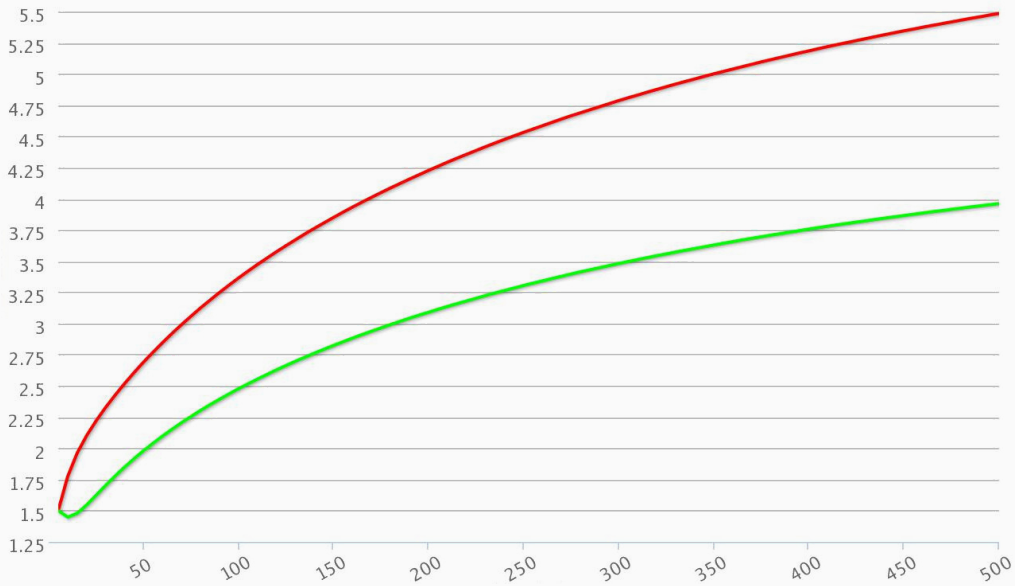


(snowfall forecast using model ALADIN)

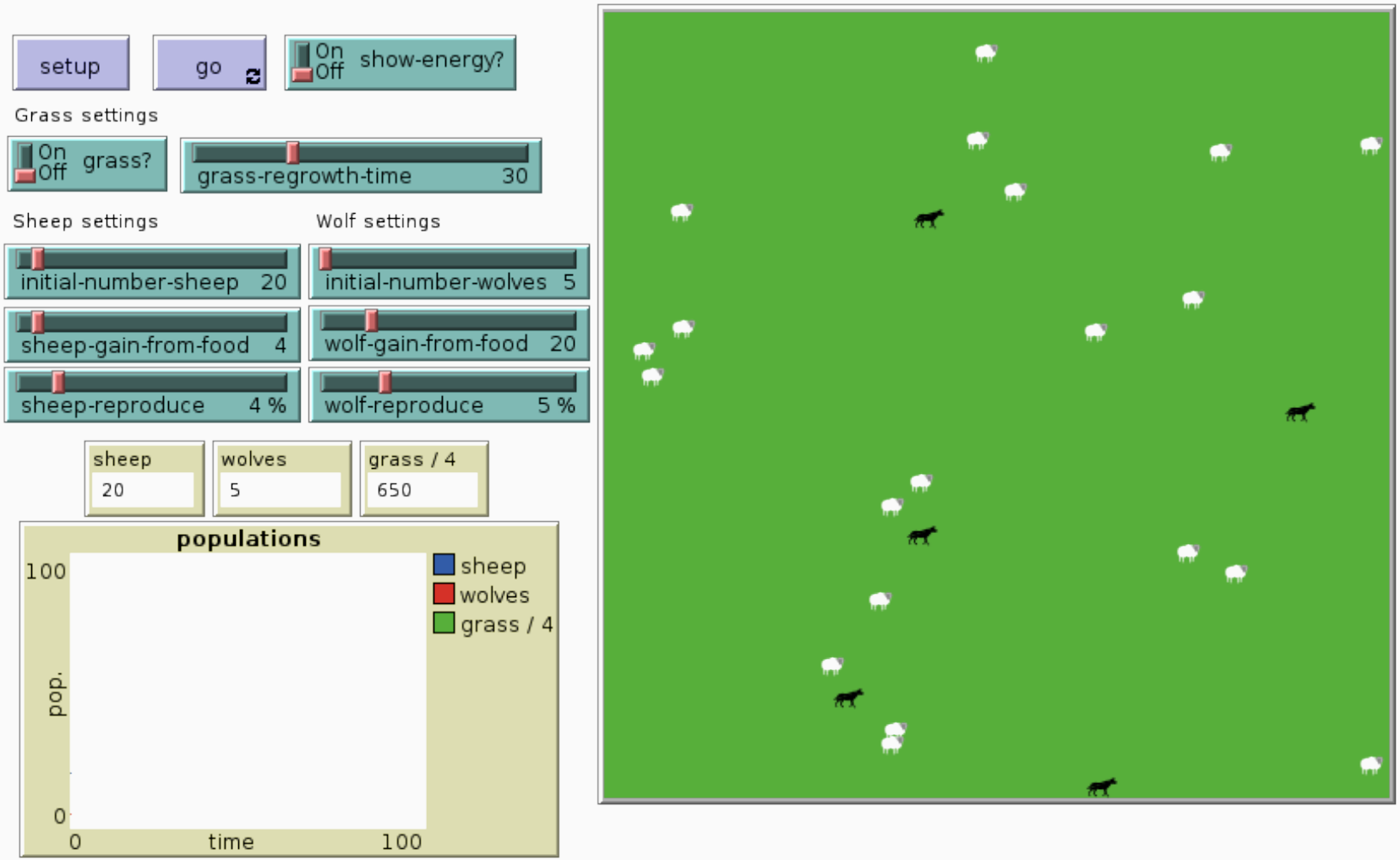
Model – Ordinary differential equations

$$\frac{dx}{dt} = A\frac{x}{t} + By$$

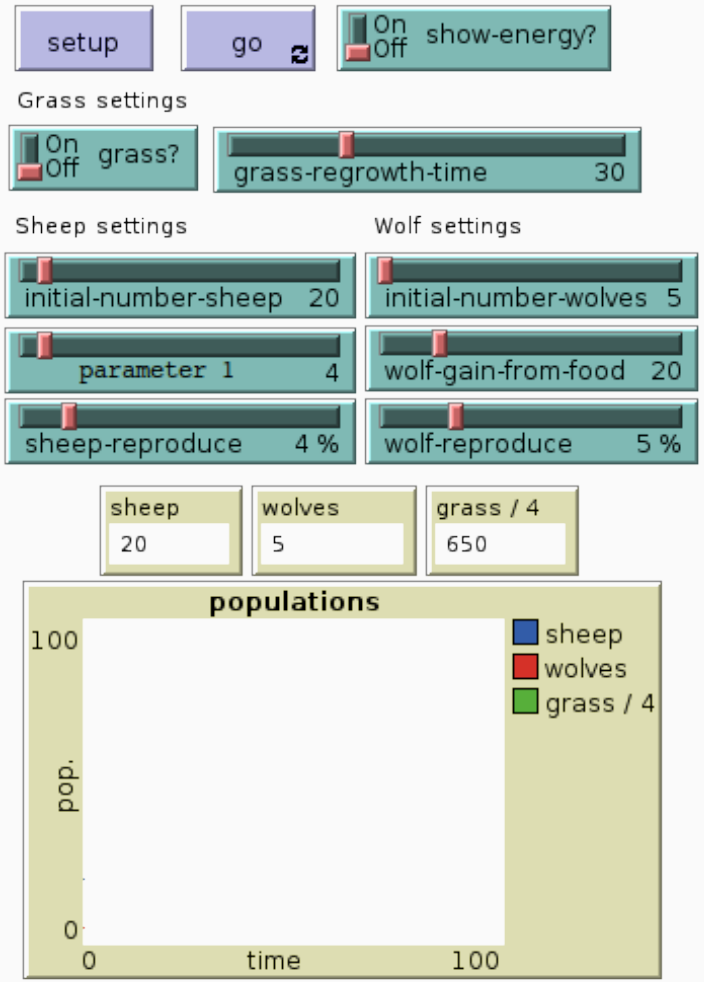
$$\frac{dy}{dt} = C\frac{x}{t^2} - Dy$$

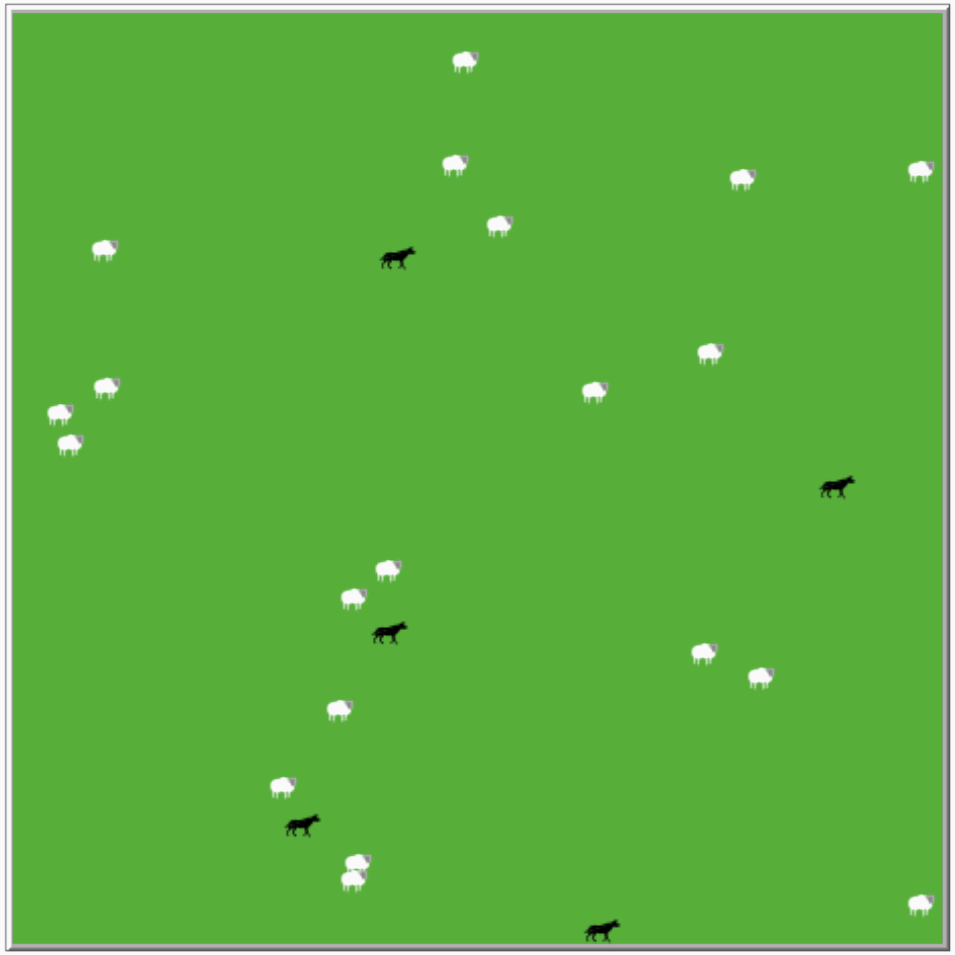


Predator-prey model



Predator-prey model





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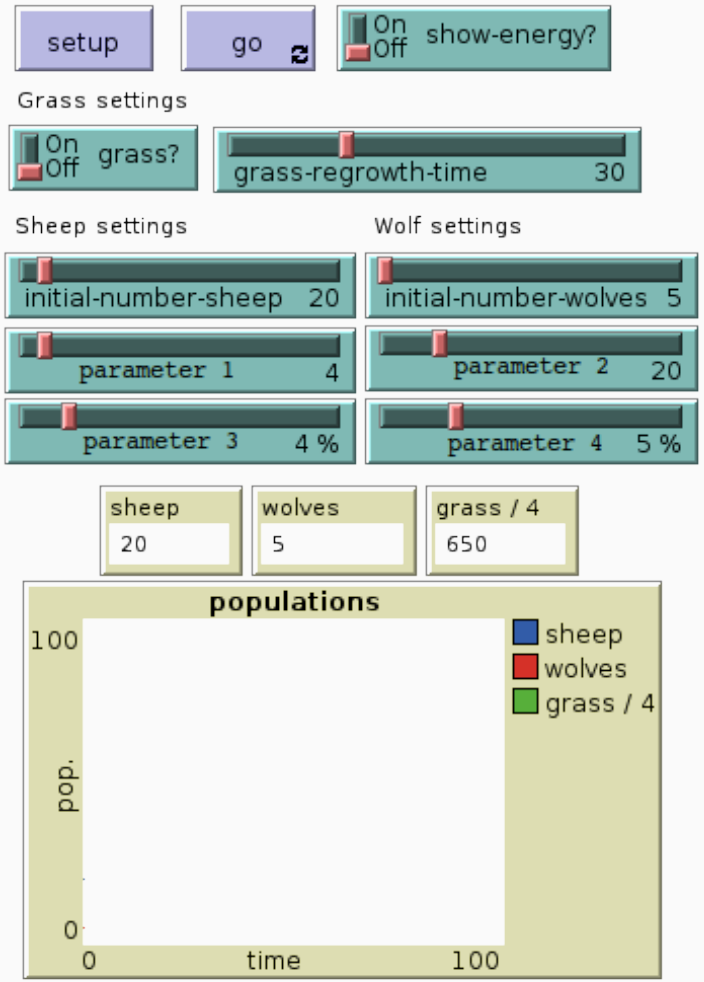
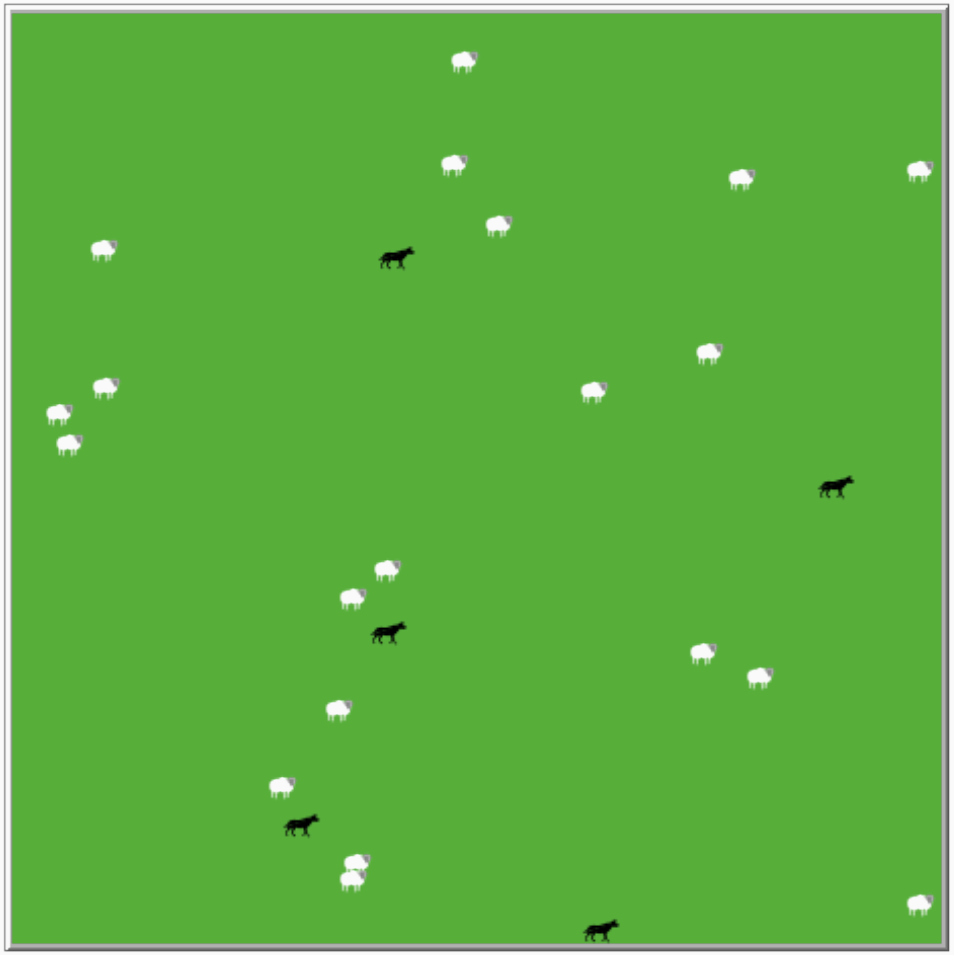
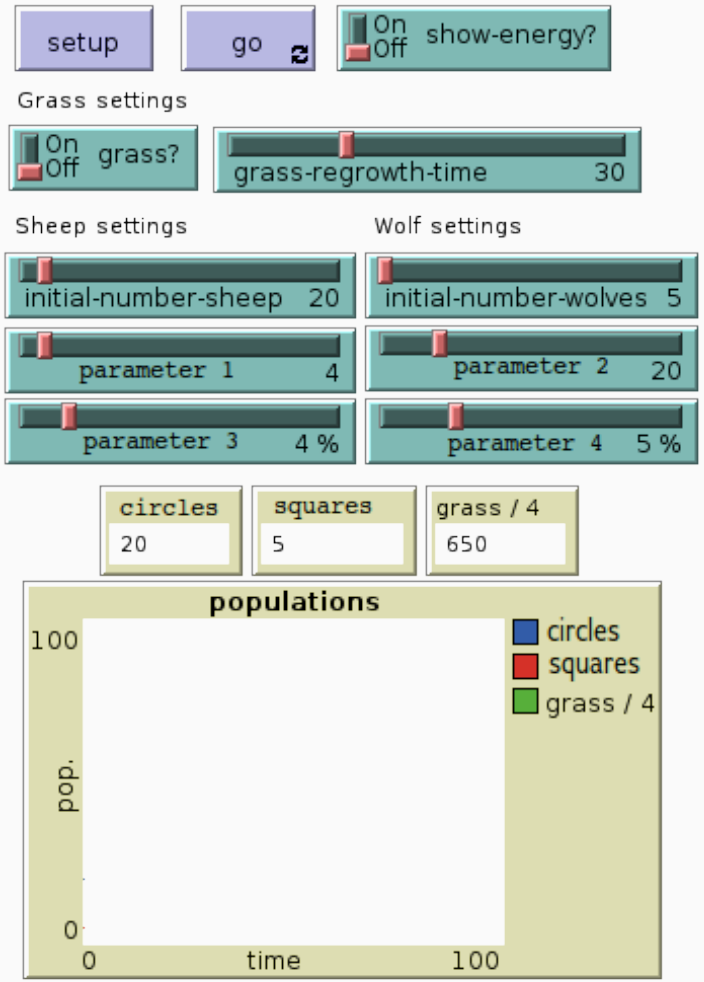
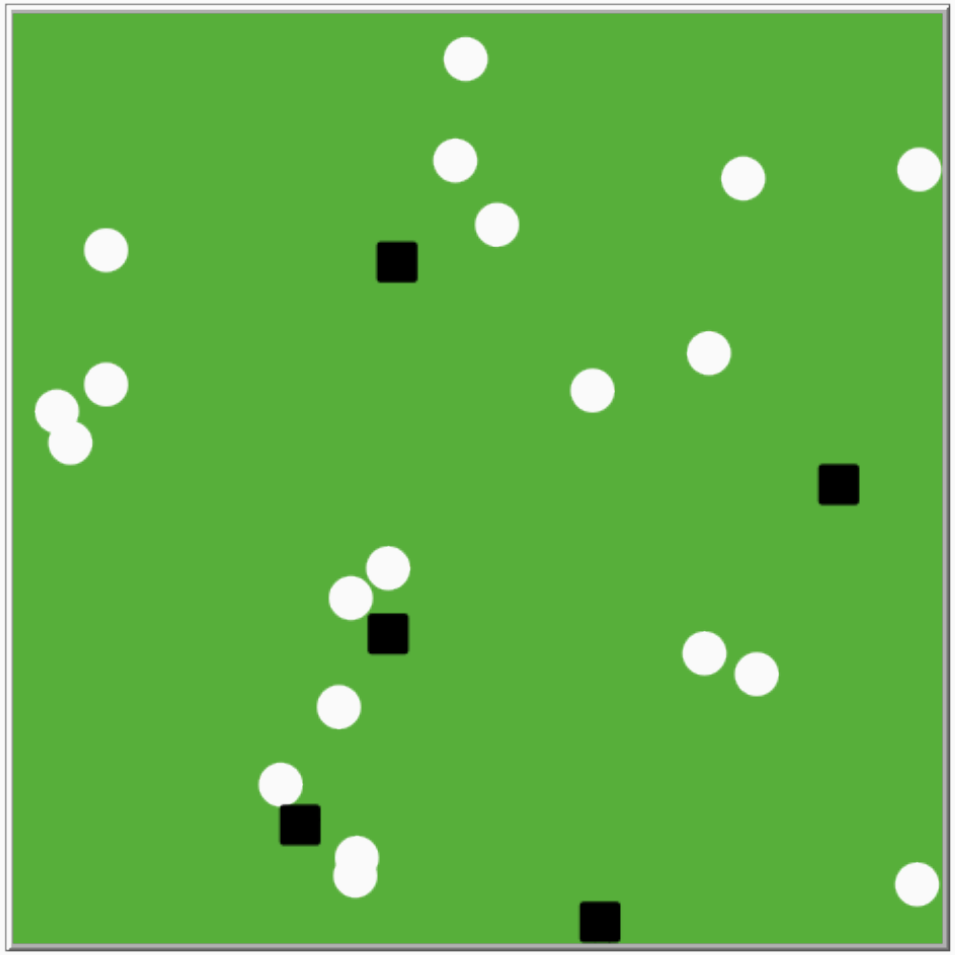




Predator-prey model





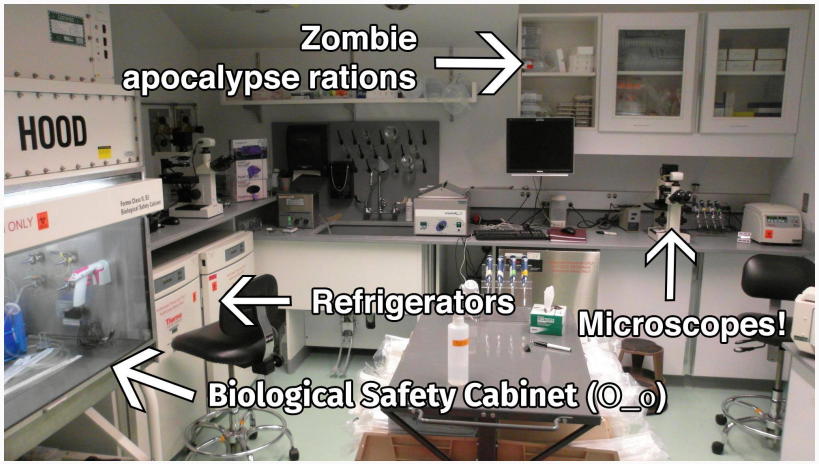
Annotation

Additional description of the {model} which allows us completely understand the system.

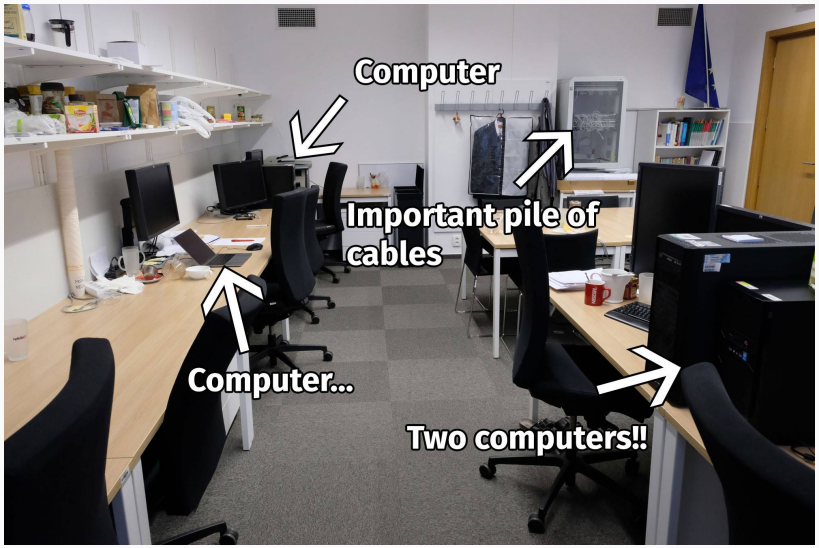
Biologically relevant issues:

- we can simulate the model – now what?
  - what is biological meaning of the results?
- we have time-series from an experiment – is it confident?
  - what were the conditions?
  - can we repeat the experiment?
- we have a particular value – is it correct?
  - how was it measured?
  - is it organism specific?
- etc.

Systems Biology Laboratory



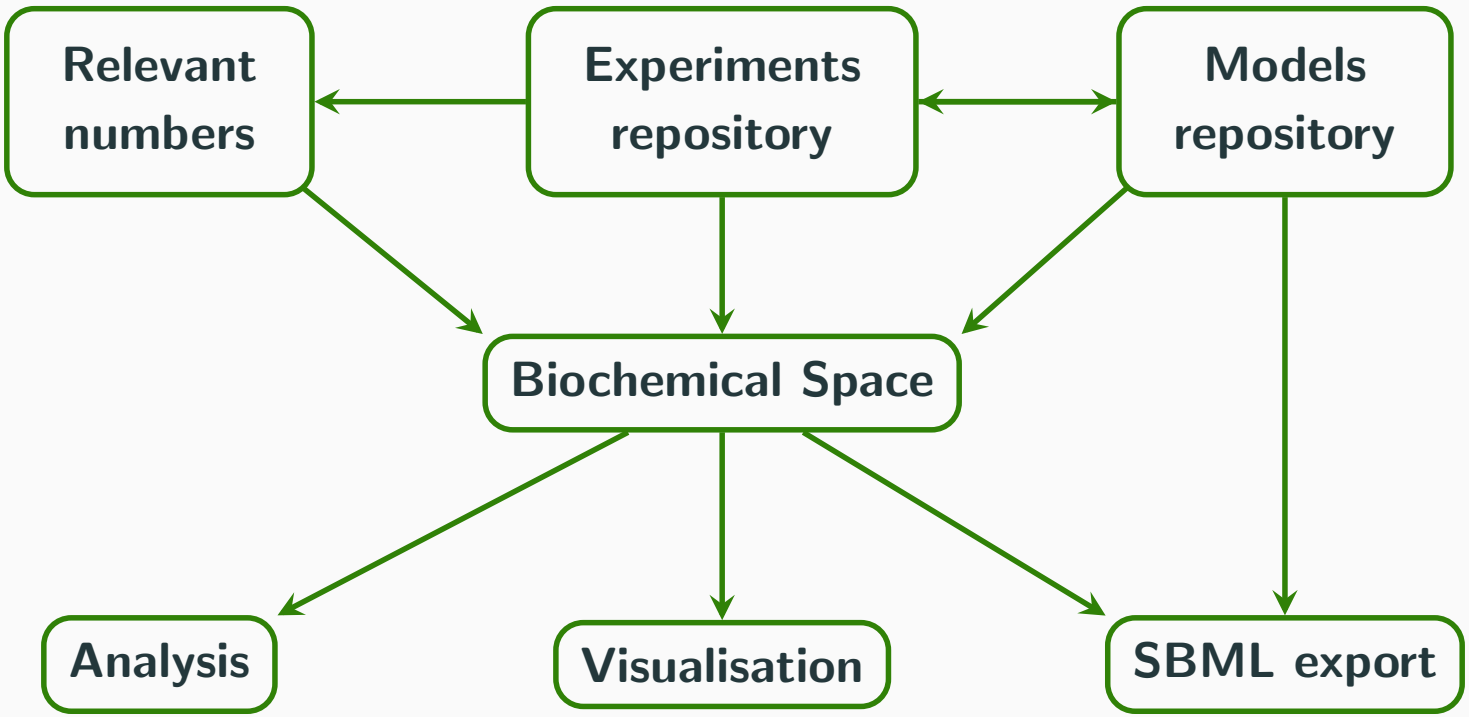
Expectation



Reality

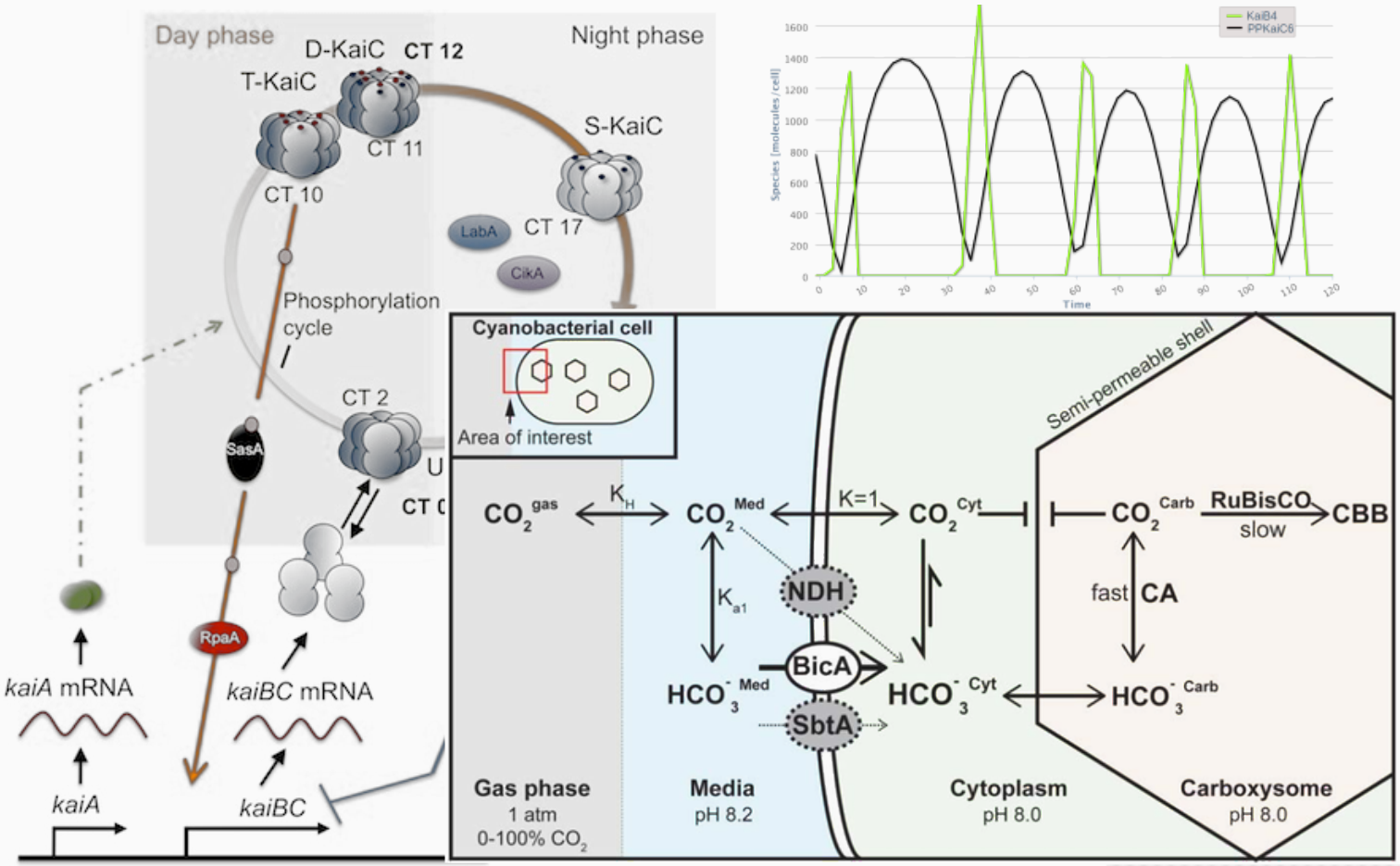
Comprehensive Modelling Platform

Web-based framework for integration of biological knowledge with computational models and wet-lab experiments.



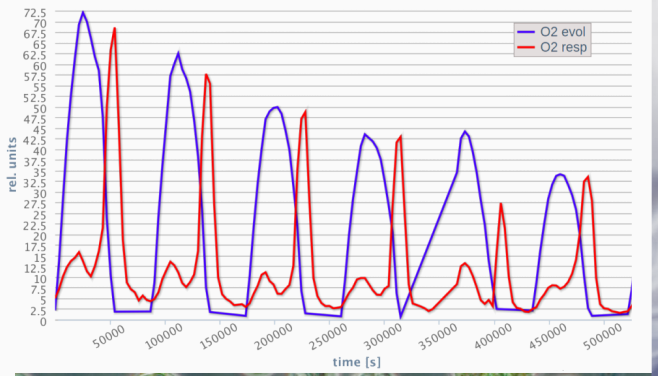
Model repository

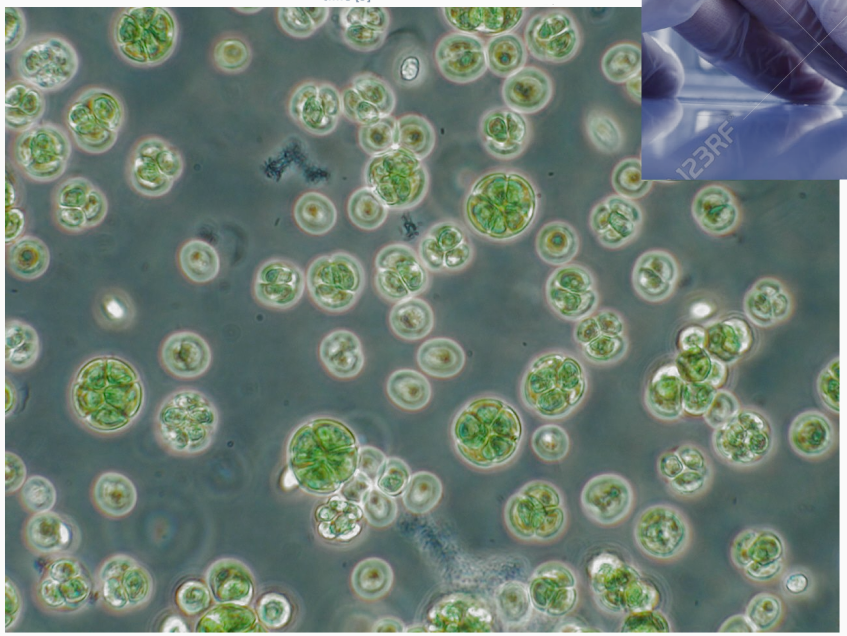
- collection of implemented models
- online simulation with custom parameter settings



Experiments repository

- storage of time-series data from wet-lab experiments

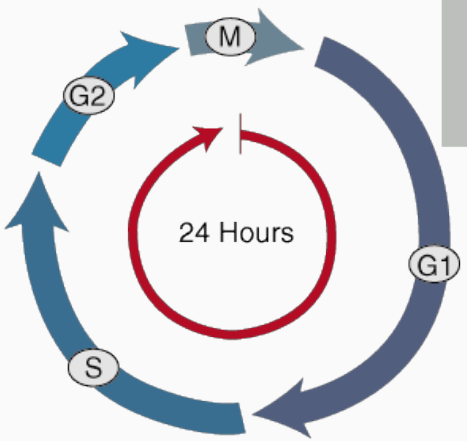


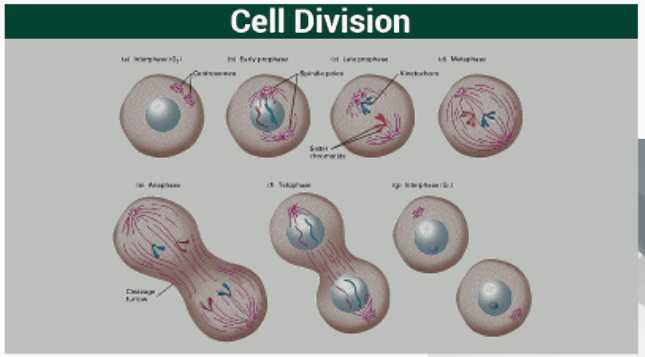


Relevant numbers

- important measured data about biological systems

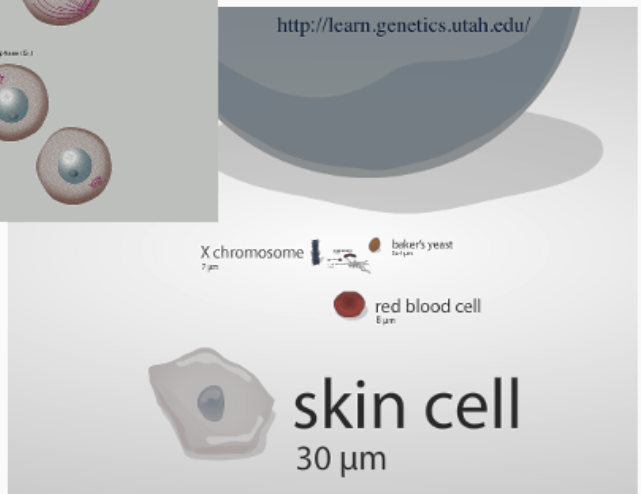
Cell cycle duration





Cell division duration

Cell diameter



Biochemical Space

Biochemical Space (BCS) is a semi-formal knowledge-base providing

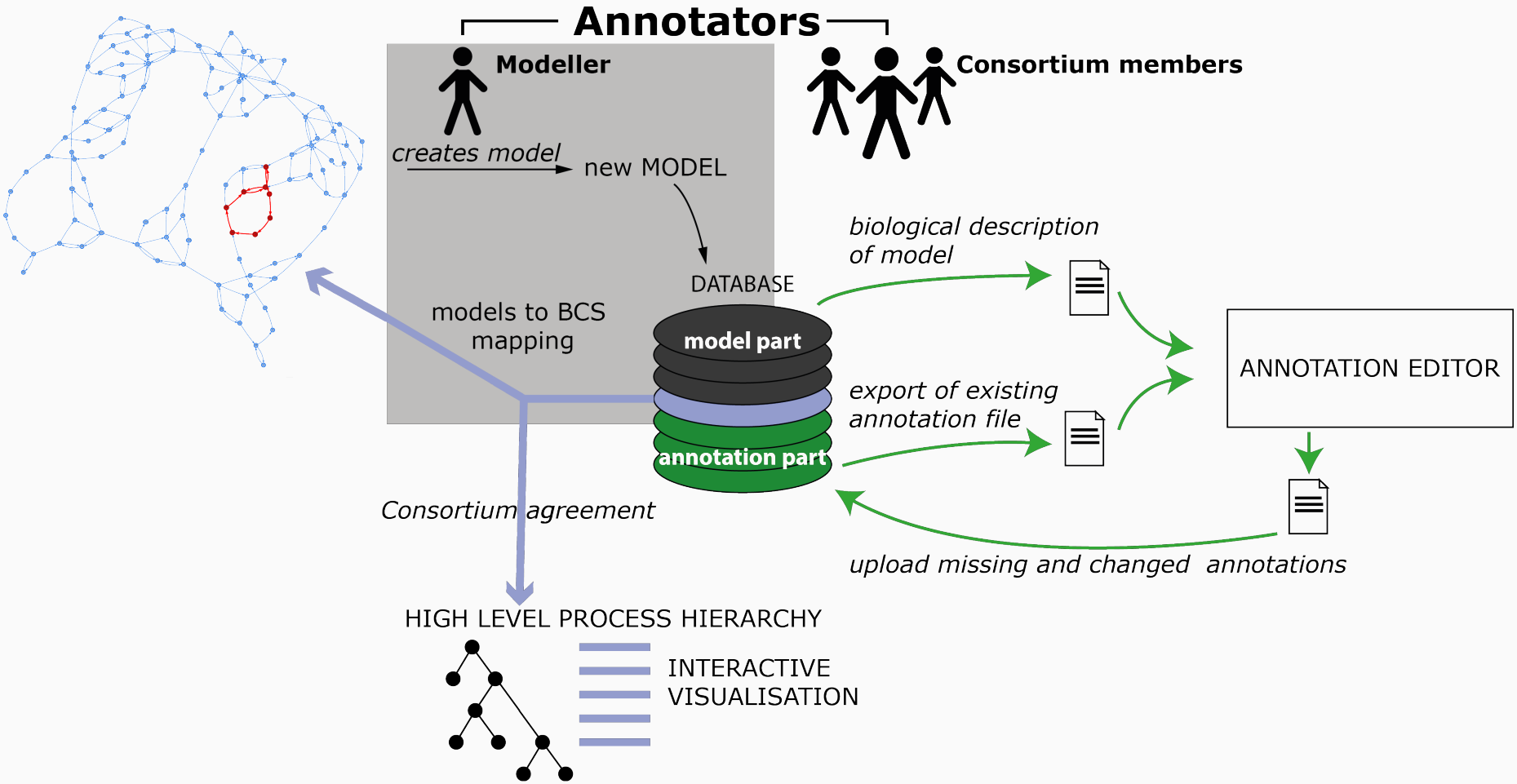
- description,
- annotation,
- public sharing

of domain-specific biological systems.

Formal description of biology preserving relevant **annotation** details.

~~Solves~~ Avoids data re-use problem.

How it works


Annotators
Modeller
Consortium members
creates model
new MODEL
DATABASE
models to BCS mapping
model part
annotation part
biological description of model
export of existing annotation file
ANNOTATION EDITOR
upload missing and changed annotations
Consortium agreement
HIGH LEVEL PROCESS HIERARCHY
INTERACTIVE VISUALISATION

How it works

- models
  - relating variables and reactions to BCS (parameters)
  - not necessary 1:1 mapping
  - BCS might be extended (never compressed!)
- experiments
  - relating of variables to BCS
  - particular conditions and equipment
- numbers
  - relating to an attribute and organism/process
  - source (an experiment / B1ONUMB3R5 /...)

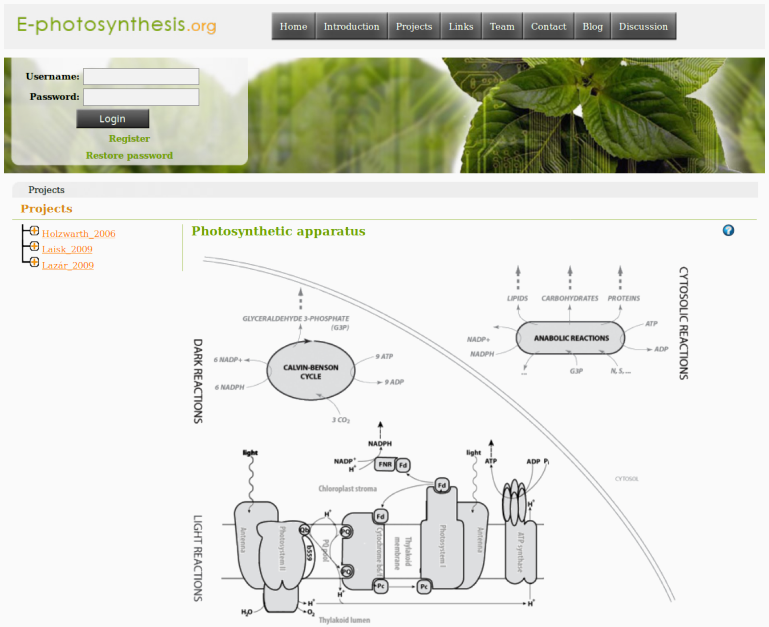
Advantages

- gives biological meaning back to the model
  - individual annotation for entities/reactions easily accessible
  - implemented model available online
- BCS for given domain is evolving
  - by each new model, BCS is improved
- helps to reveal differences between models
  - and also what they have in common
- connection between models and experiments (numbers)

Applicability

- range of organisms and processes
- not limited by biology

- `e-photosynthesis.org`



- `e-cyanobacterium.org`