Environmental modelling and Web 2.0
- using Connotea to share XML-represented information

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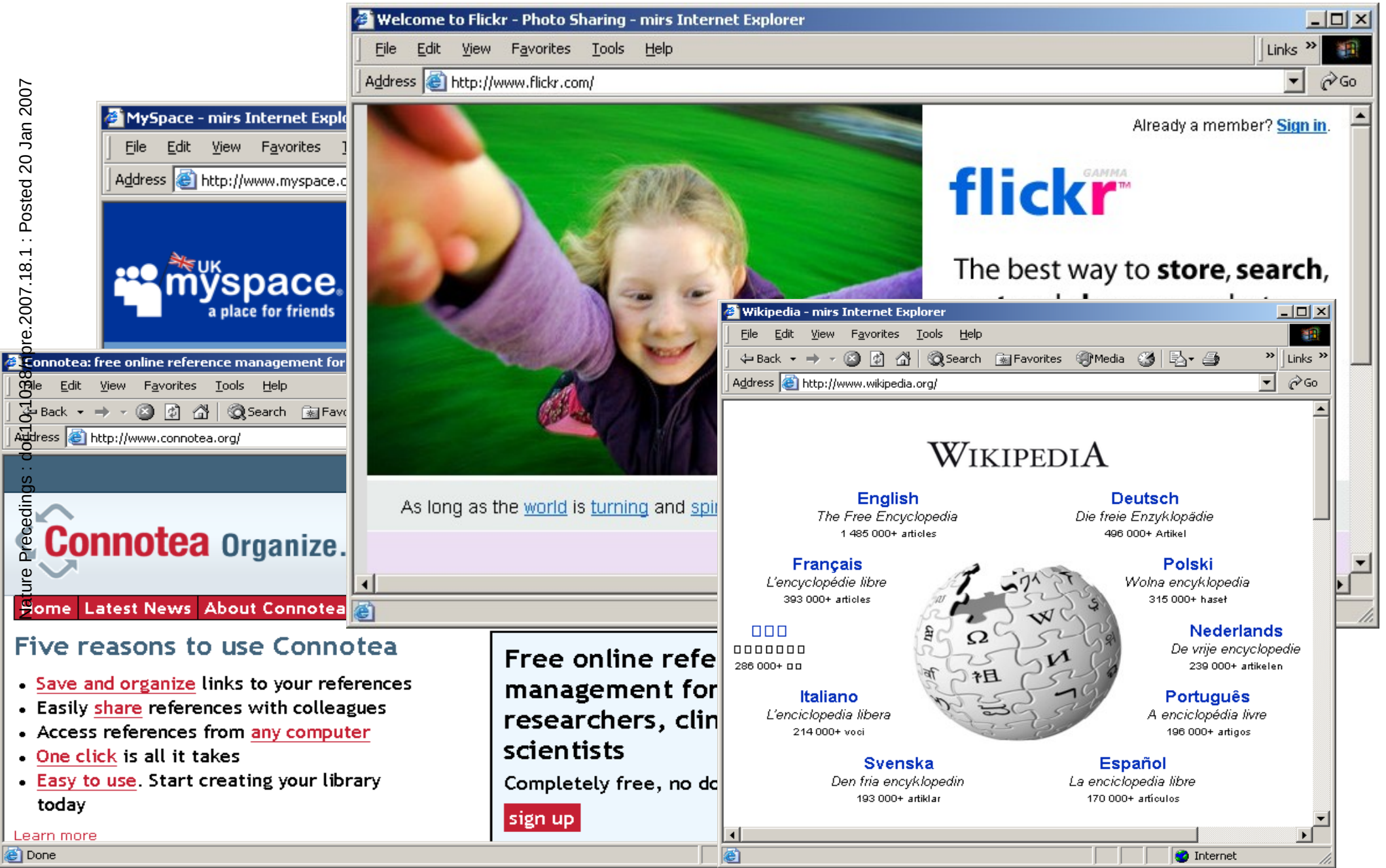
Aims

1. Raise awareness of the value of XML for representing research information

2. Explore how Connotea can be used as a social bookmarking site for XML-represented information

Most Web 2.0 applications are geared towards human-readable content



However, much research information is inherently structured

Obvious examples: database, spreadsheet

But also:

- Biological pathways
- Results of statistical tests
- Mathematics
- Molecular structures
- Logical arguments
- Systems Biology models

and....

- Environmental models

There are huge potental benefits from representing such information in a computer-processable format

Which computer-processable format?

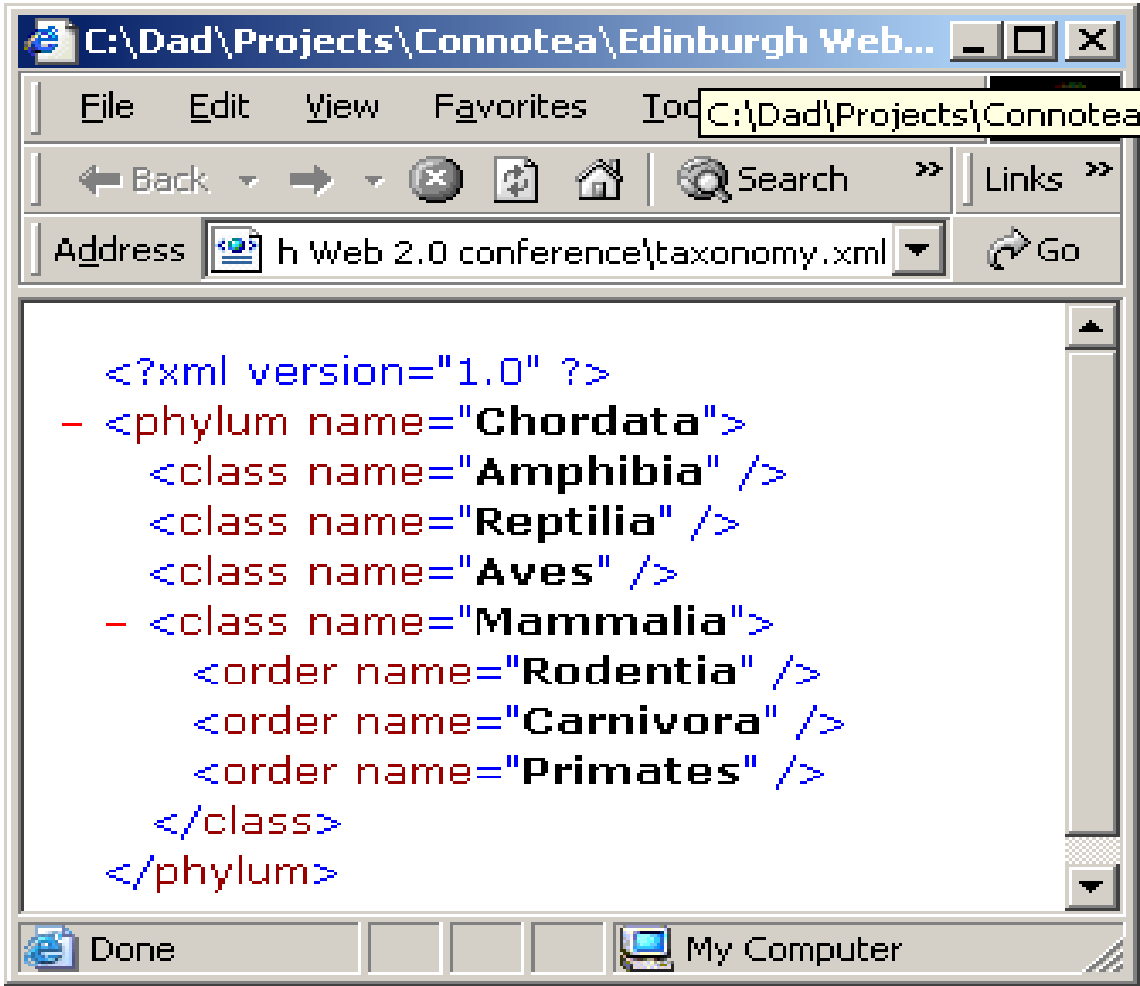
How about XML?

- Widely used
- Many tools available
- Has expressive power required
- Suitable for web publishing

Nature Precedings : doi:10.1038/npre.2007.18.1 : Posted 20 Jan 2007

```
?xml version="1.0" ?>

phylum name="Chordata">
  <class name="Amphibia"/>
  <class name="Reptilia"/>
  <class name="Aves"/>
  <class name="Mammalia">
    <order name="Rodentia"/>
    <order name="Carnivora"/>
    <order name="Primates"/>
  </class>
/phylum>
```



There are probably hundreds of XML-based “ markup languages” in use in academia

AML	Astronomical Markup Language
Archelogos	Representation of philosophical arguments
CML	Chemical Markup Language
EMDL	Emergency Data Exchange Language
HEML	Historical Event Markup and Linking
MathML	Mathematical Markup Language
NeuroML	Neuroscience Markup Language
XDELTA	XML Format for Taxonomic Information
SBML	Systems Biology Markup Language
MAML	MicroArray Markup Language
MatML	Materials Property Data Markup Language
NLSML	Natural Language Semantics Markup Language
ThML	Theological Markup Language

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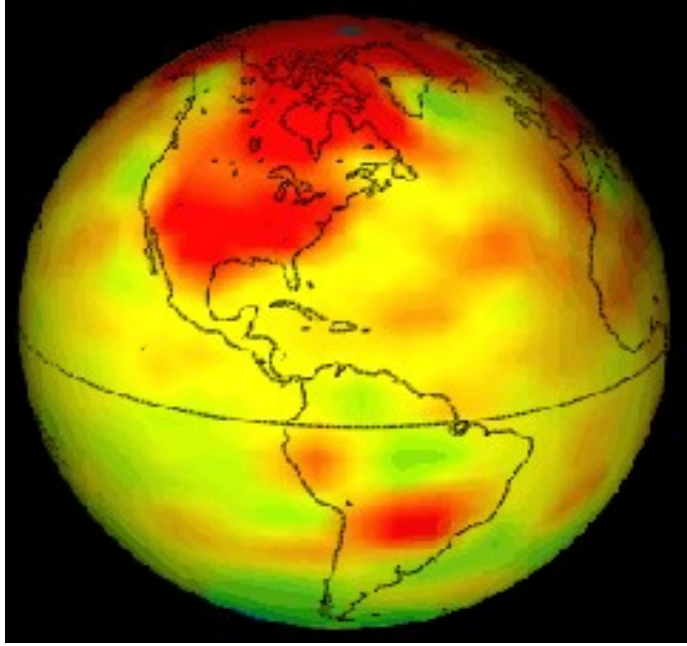
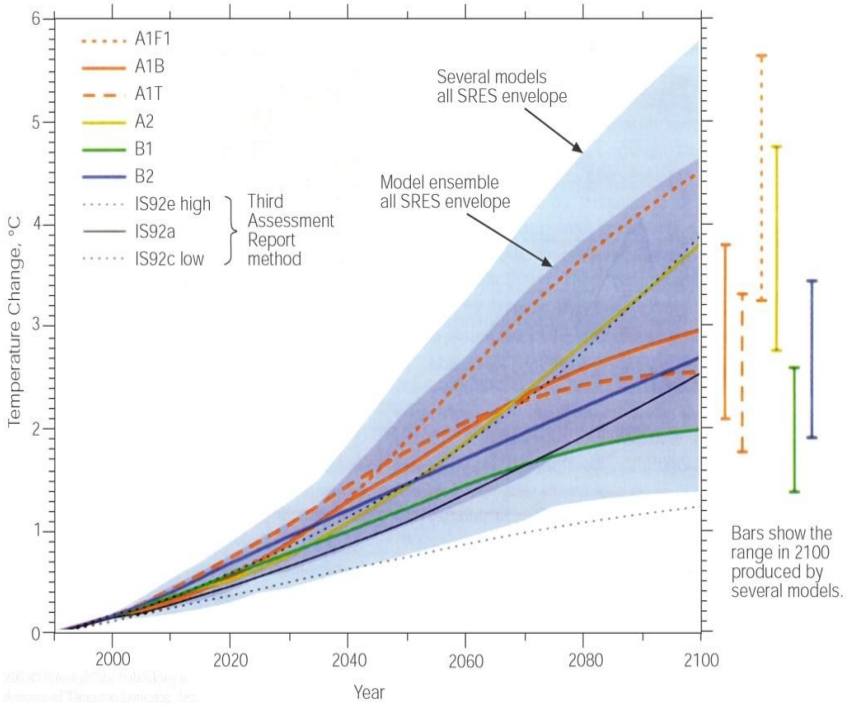
Environmental modelling



Hugely important

- climate change
- biodiversity
- resource management
- pollution
- land-use change

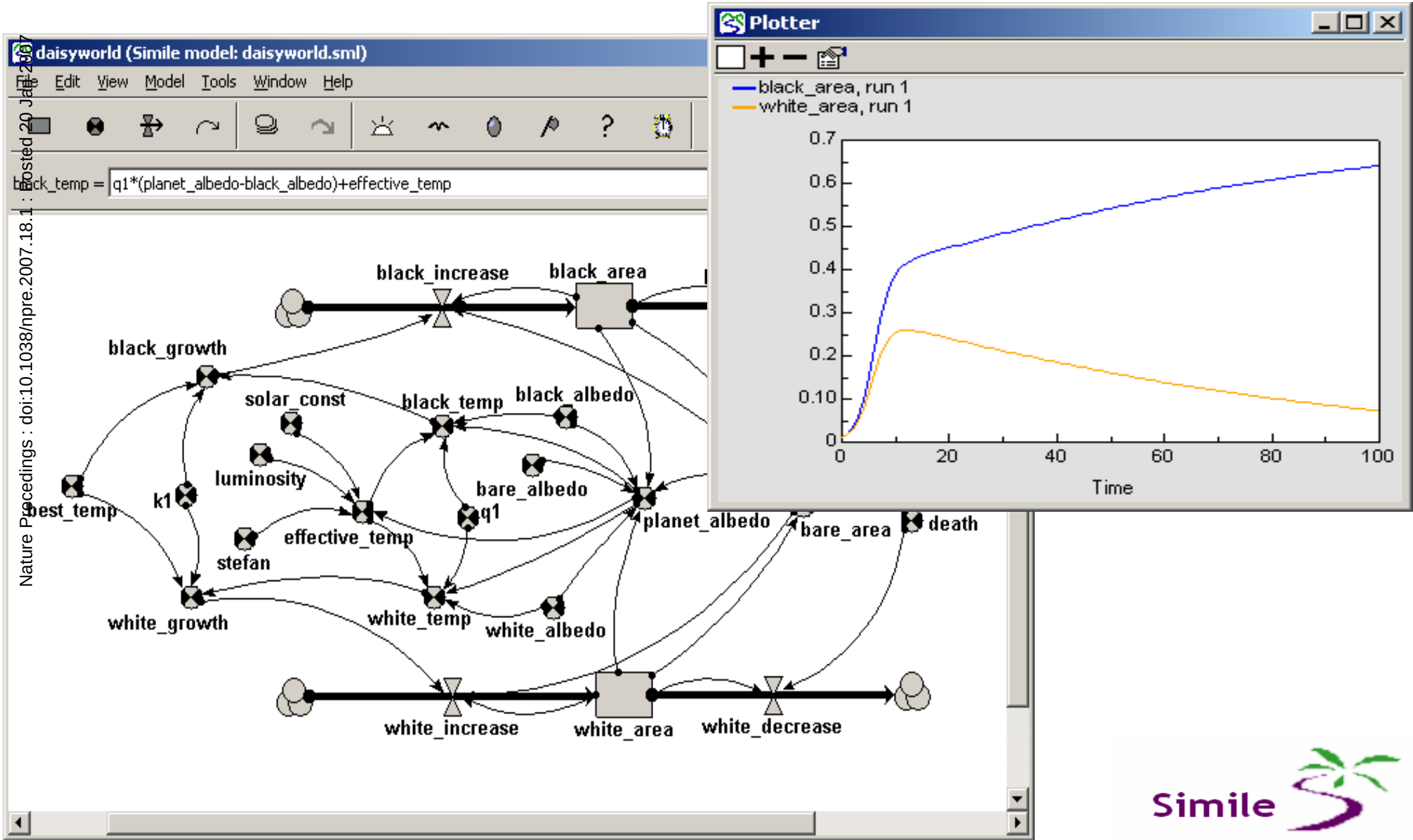


Current practice

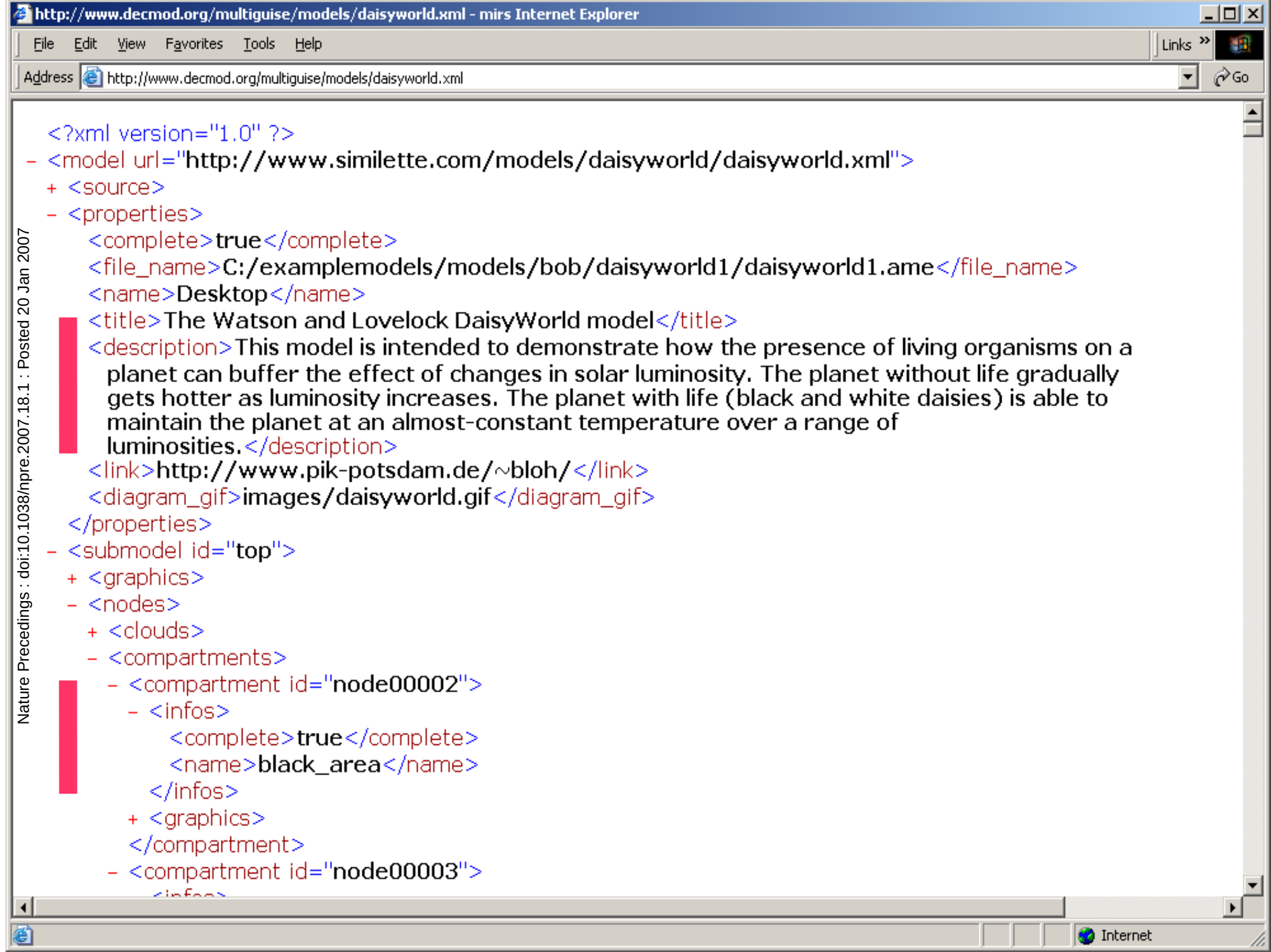
- Models are implemented as computer programs
- This is fraught with problems:
  - costly
  - hard to maintain
  - lack of transparency
  - lack of re-usability
  - poor shelf life

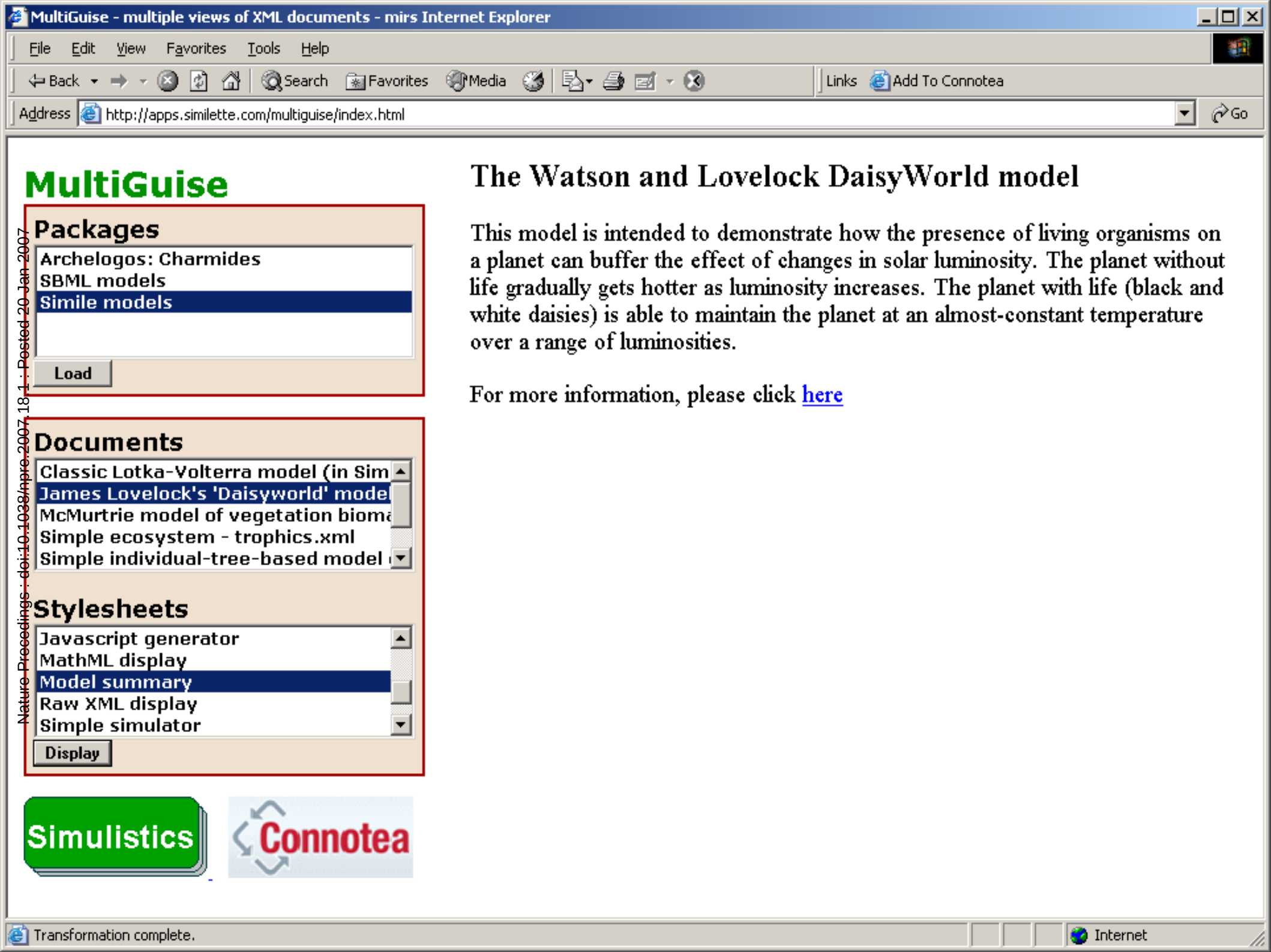
The answer:

Separate the **representation** of the model from
the program used to simulate its behaviour



Simile





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Packages

Archelogos: Charmides
SBML models
Simile models

Load

Documents

Classic Lotka-Volterra model (in Sim
James Lovelock's 'Daisyworld' model
McMurtrie model of vegetation bioma
Simple ecosystem - trophics.xml
Simple individual-tree-based model

Stylesheets

Model summary
Raw XML display
Simple simulator
Summary statistics
SVG model diagram

Display

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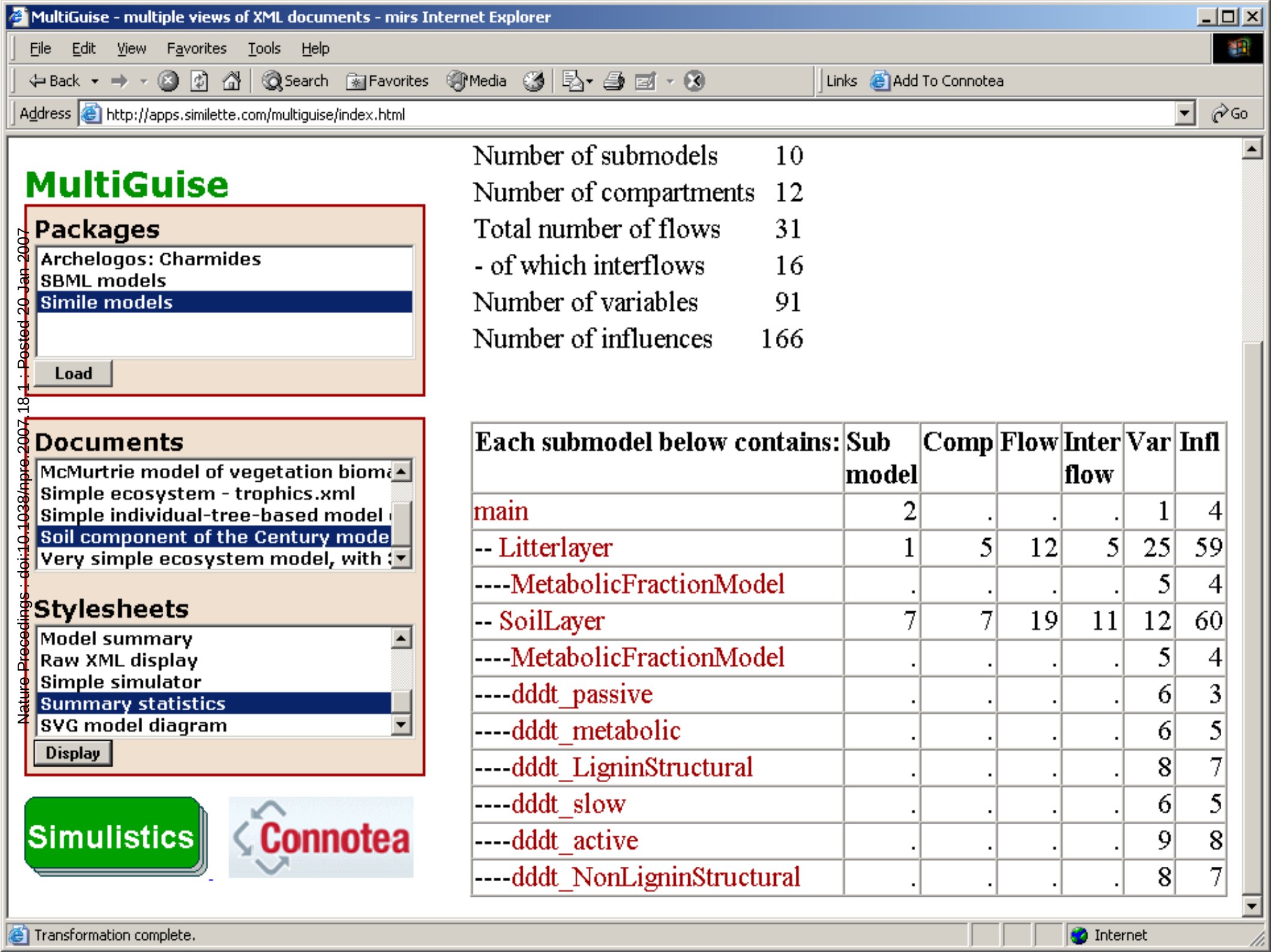
The Watson and Lovelock DaisyWorld model: Summary stats

Whole model:

Number of compartments	2
Total number of flows	4
Number of variables	17
Number of influences	36

Each submodel below contains:	Sub model	Comp	Flow	Inter flow	Var	Infl
main	.	2	4	.	17	36



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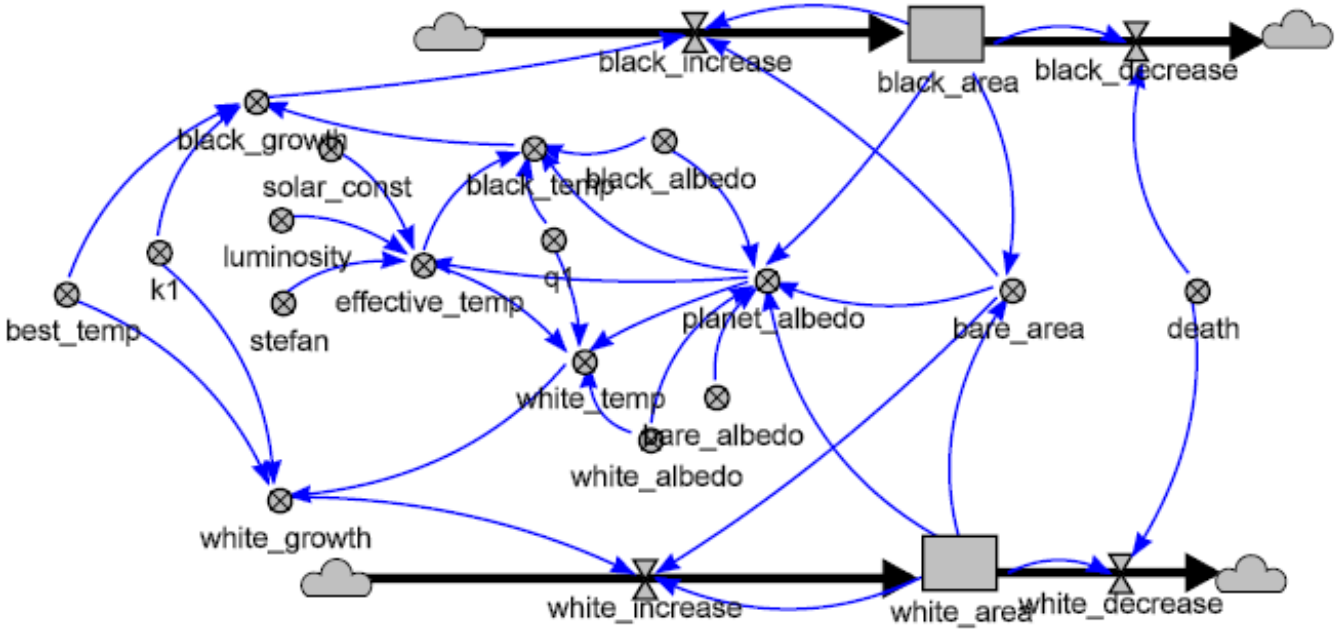

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Stylesheets

Fortran generator for BFG framework
Graphical simulator
Javascript generator
MathML display
Model summary

Display

Simulistics

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Equations for Predator-prey model with single-character variables

$$P = 100$$

$$Q = 1$$

$$r = 0.1$$

$$K = 10000$$

$$E = \frac{aP}{1 + (aP)h}$$

$$a = 0.1$$

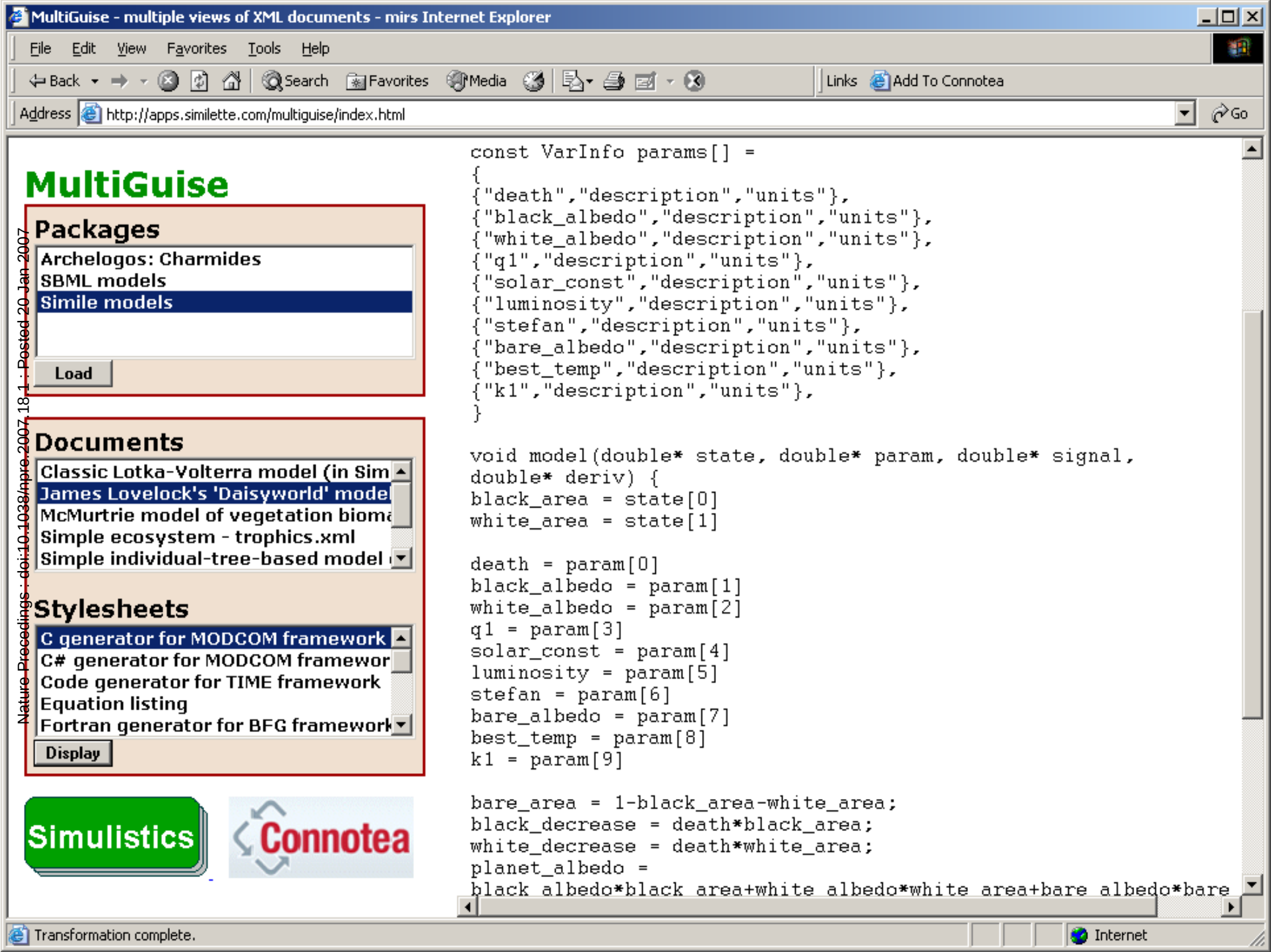
$$h = 10$$

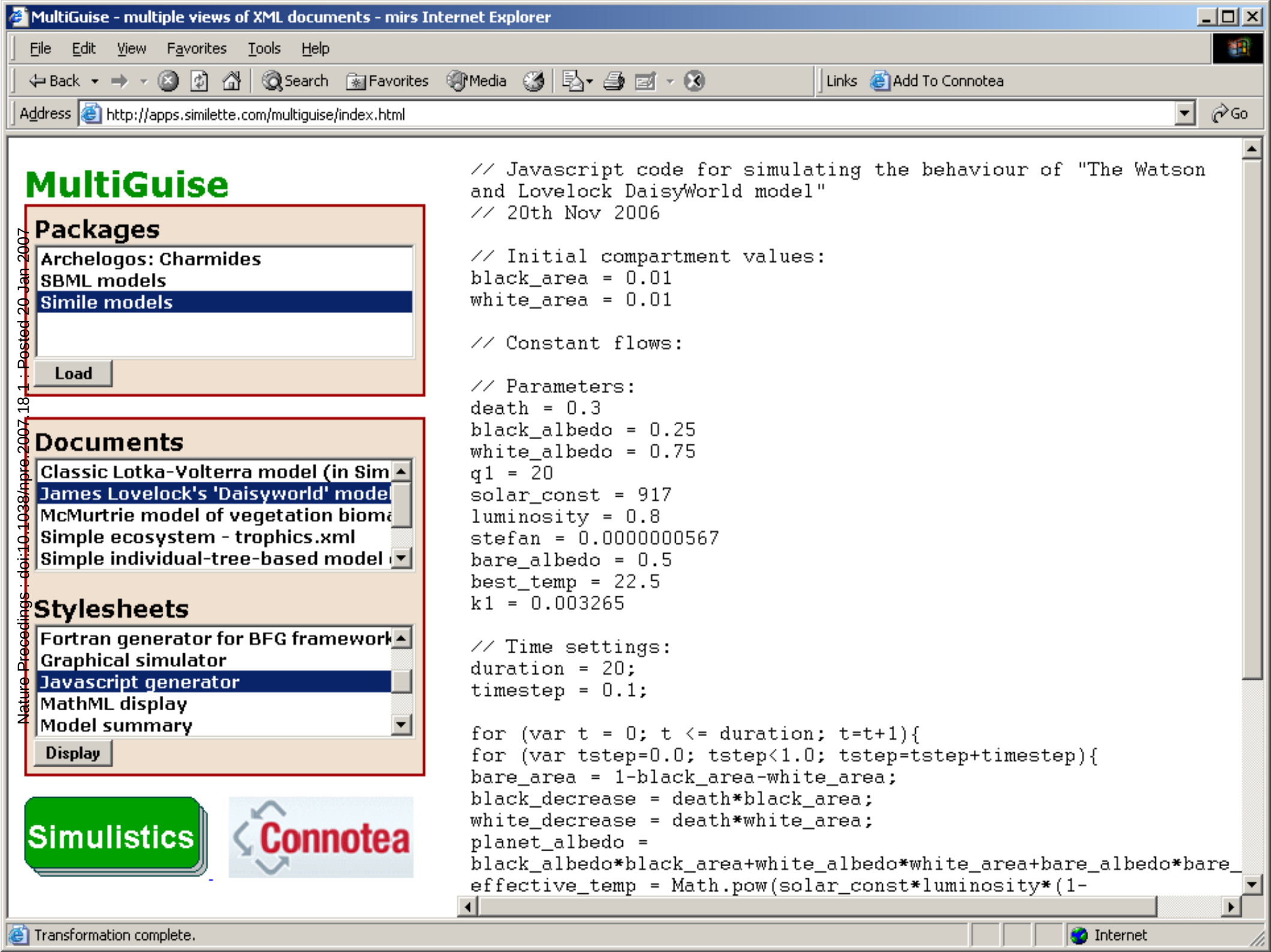
$$c = 0.2$$

$$m = 0.01$$

$$R = (rP)\left(1 - \frac{P}{K}\right)$$

$$C = EQ$$





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Transforms

- Graphical simulator
- Javascript generator (on similette.co
- Model summary (on similette.com)
- Model summary statistics (on similet
- Simile-XML transform: displays the n

Display

Initial compartment values

black_area	0.01	0.01
white_area	0.01	0.01

Parameter values

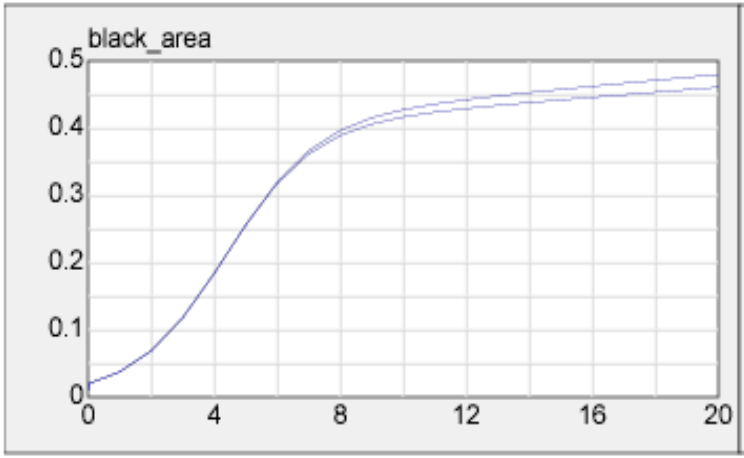
death	0.3	0.3
black_albedo	0.25	0.25
white_albedo	0.75	0.85
q1	20	20
solar_const	917	917
luminosity	0.8	0.8
stefan	0.000000	0.000000
bare_albedo	0.5	0.5
best_temp	22.5	22.5
k1	0.003265	0.003265

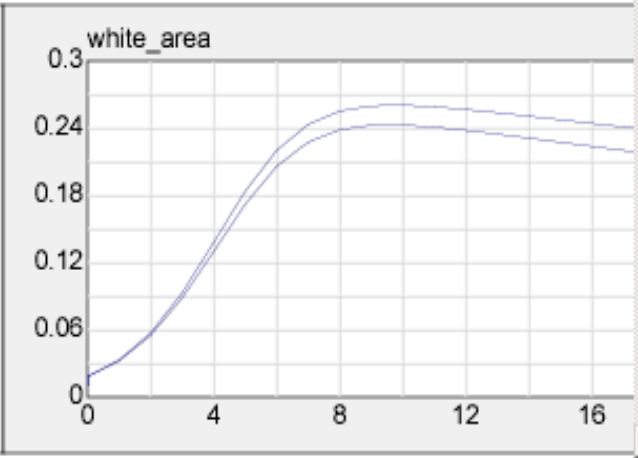
Run control

Time step	0.1
Run duration	20
Display interval	1

Run

Run: 1 2





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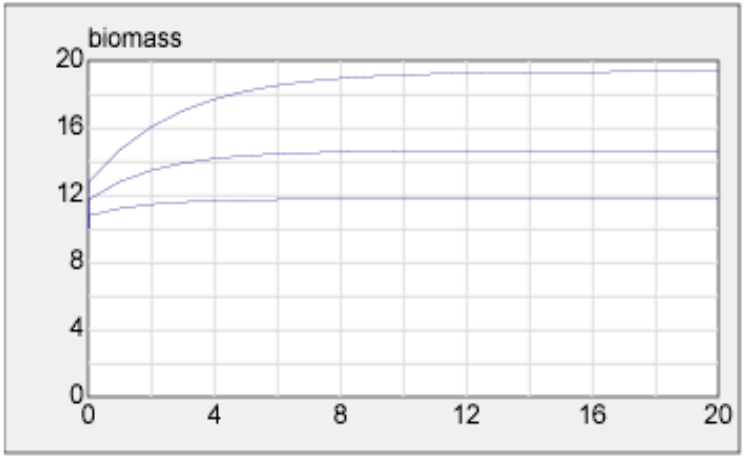
Display

Initial compartment values			Parameter values			Run control	
biomass	10	10	kloss	0.25	0.45	Time step	0.1
			SLA	3.5	3.5	Run duration	20
			k	0.6	0.6	Display interval	1
			r	0.5	0.5		
			Pmax	50	50	Run	
			leaf_fraction	0.2	0.2		
			efficiency	0.6	0.6		

Run: 1 2 3



Transformation complete. Internet

What's this got to do with Web 2.0?

Connotea is used to bookmark:

- the XML files containing the models;
- the stylesheets for displaying the models.

These files (i.e. the models, and the stylesheets for displaying them) can be anywhere on the Web.

Thus...

- MultiGuise starts off empty.
- It only starts to contain models and stylesheets when people bookmark them in Connotea.

ANYBODY can bookmark a model or a stylesheet, their own or somebody else's.

All they have to do is to include a specified tag when they tag it.

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Declarative modelling (edit)

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archelogos-styleshee- t

biomass

cdc2

cdc2 kinase

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Number of bookmarks per page: 10 | 25 | 50 | 100

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Simple ecosystem: 3 trophic layers

www.similette.com

Posted by robertm to Simile-XML on Tue Nov 14 2006 at 15:27 UTC | info

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Lotka-Volterra predator-prey model

www.decmod.org

Posted by robertm with 1 comment to Simile model predator-prey model xml Simile Simile-XML on Tue May 30 2006 at 22:40 UTC | info

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James Lovelock's 'Daisyworld' model

www.decmod.org

Toolbox ?

Add a bookmark

Create a new group

Create a tag note

Rename a tag

Import from local file

Export my library

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C# generator for MODCOM framework

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MultiGuise

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Archelogos: Charmides
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Simile models

Load

Documents

Cdc2 and cyclin interactions
Mitotic oscillator: cyclin and cdc2 kinas
Mitotic oscillator: cyclin and cdc2 kinas
Nicotinic acetylcholine receptor kinetic
Nicotinic EPSP in a Torpedo electric org

Stylesheets

SBML display of constituents
SBML display of constituents (table)
SBML summary

Display

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Goldbeter1991_MinMitOscil_ExplInact

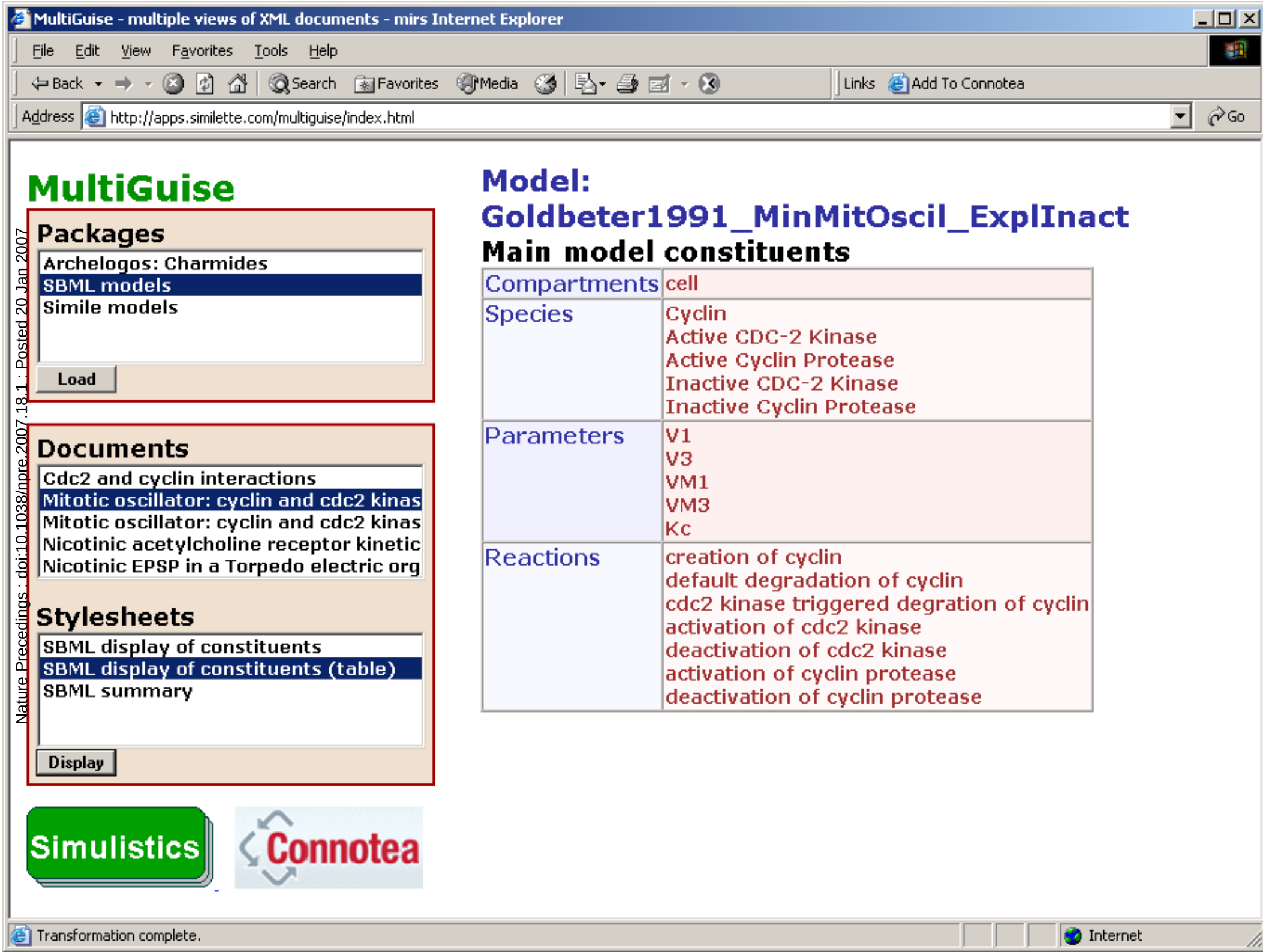
A Simple Mitotic Oscillator

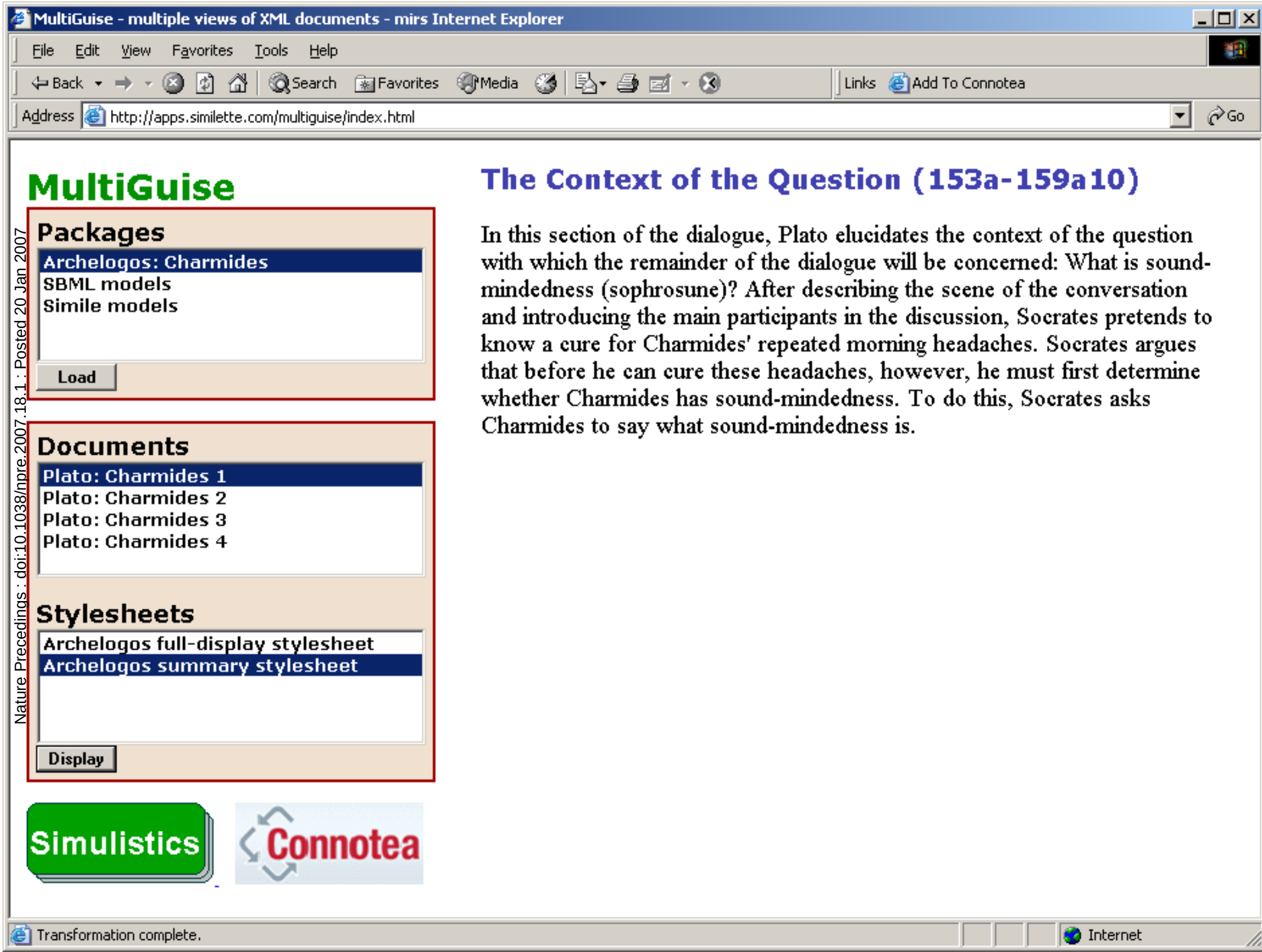
Reference:Goldbeter A (1991)*A minimal cascade model for the mitotic oscillator involving cyclin and cdc2 kinase*, PNAS 88:9107-9111

Web Reference:http://www.pnas.org/cgi/content/abstract/88/20/9107

This model represents the inactive forms of CDC-2 Kinase and Cyclin Protease as separate species, unlike the ODEs in the published paper, in which the equations for the inactive forms are substituted into the equations for the active forms using a mass conservation rule M+MI=1,X+XI=1. Mass is still conserved in this model through the explicit reactions M<->MI and X<->XI. The terms in the kinetic laws are identical to the corresponding terms in the kinetic laws in the published paper.

This is a Systems Biology Markup Language (SBML) file, generated by MathSBML 2.4.6 (14-January-2005) 14-January-2005 18:37:35.503857. SBML is a form of XML, and most XML files will not display properly in an internet browser. To view the contents of an XML file use the "Page Source" or equivalent button on you browser.





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Documents

Plato: Charmides 1
Plato: Charmides 2
Plato: Charmides 3
Plato: Charmides 4

Stylesheets

Archelogos full-display stylesheet
Archelogos summary stylesheet

Display

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The Context of the Question (153a-159a10)

1. Setting
    1.1. Introduction of Socrates and Chaerephon
    1. Chaerephon asks about the battle at Potidaea
    1.2. Introduction of Critias
    1. Socrates asks about philosophy, the young, wisdom, and beauty
    1.3. Introduction of Charmides
2. Concern for the Soul
    1. Charmides will be irresistible, if his soul is good natured
        1. Charmides' face is fine
        2. Charmides' body or
        3. [A fine face, a fine body, and a good-natured soul are required for irresistibility]
    2. Critias maintains that Charmides' soul is good-natured
        1. Because it is fine and good (
    3. Socrates proposes to examine Charmides' soul by conversing with him
        1. [Because] being philosophical and being poetical are (the only?) two ways in which a soul is fine and good.
3. Pretense of the Cure for the Headache
    3.1. An argument that Charmides' headaches cannot be cured until it is determined whether or not Charmides is sound-minded
    1. If Charmides is sound-minded, he will not need the incantations and the drug for the headache can be applied

Conclusions

The practice of environmental modelling would be greatly improved if the environmental research community adopted a standard, XML-based language for publishing models.

More generally, there are numerous academic disciplines that could benefit from sharing research information in XML.

Connotea provides a great, social environment for sharing information published in XML.

Much more can be done to develop, promote and support the uptake of XML in a Web 2.0 world.

Acknowledgements:
- Ben Lund (Web Publishing, Nature)
- Pierre Lindenbaum (IntegraGen)