

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

The image shows a collage of web browser windows. The largest window is Flickr, displaying a photo of a child and the text 'The best way to store, search, ...'. Other windows include MySpace with its logo and the tagline 'a place for friends', and Wikipedia with its multi-language interface. A Connotea advertisement is also present at the bottom left.

Five reasons to use Connotea

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Language	Article Count
English	1 485 000+ articles
Deutsch	496 000+ Artikel
Français	393 000+ articles
Polski	315 000+ haset
Nederlands	239 000+ artikelen
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Svenska	193 000+ artiklar
Español	170 000+ artículos
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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 potential benefits from representing such information in a computer-processable format

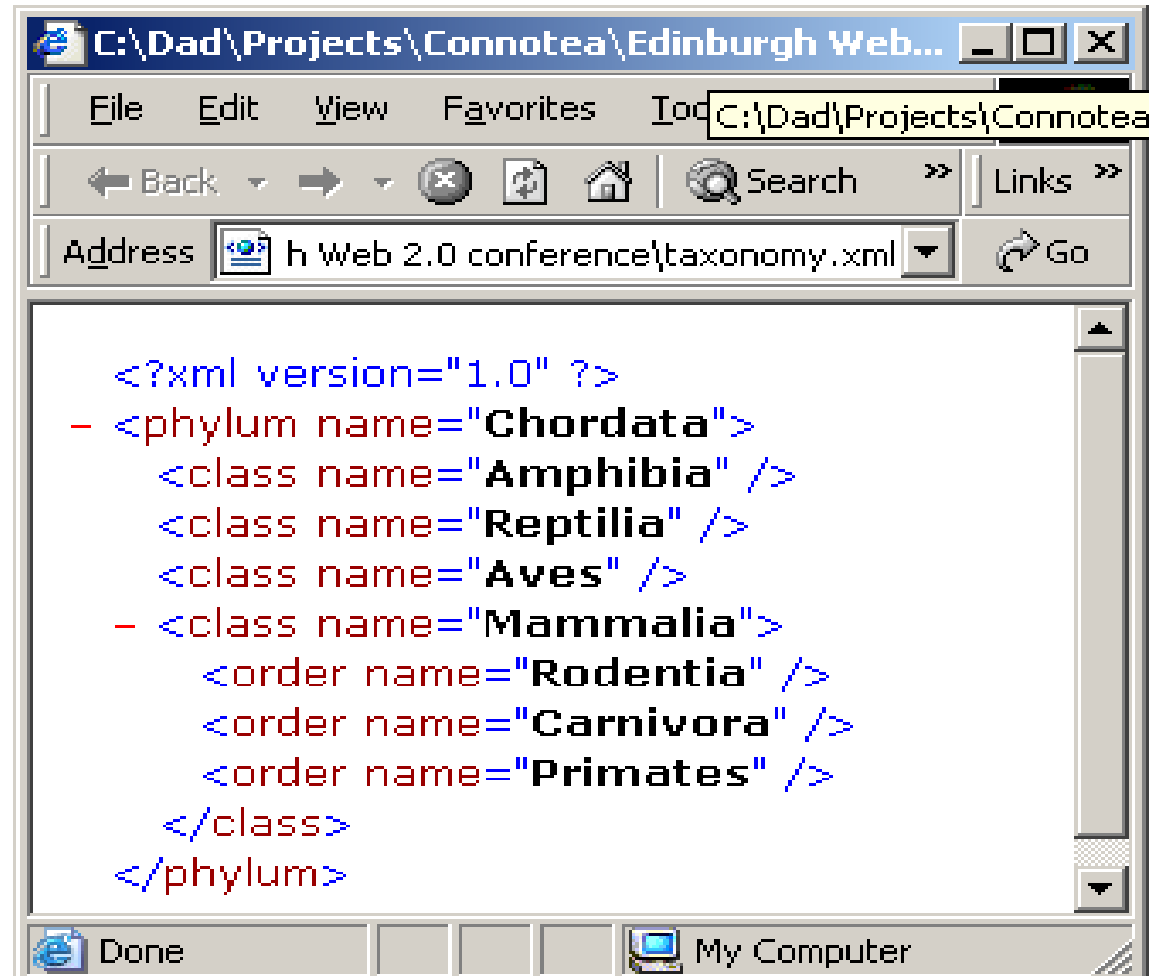
Which computer-processable format?

How about XML?

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

```
?<?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>
```



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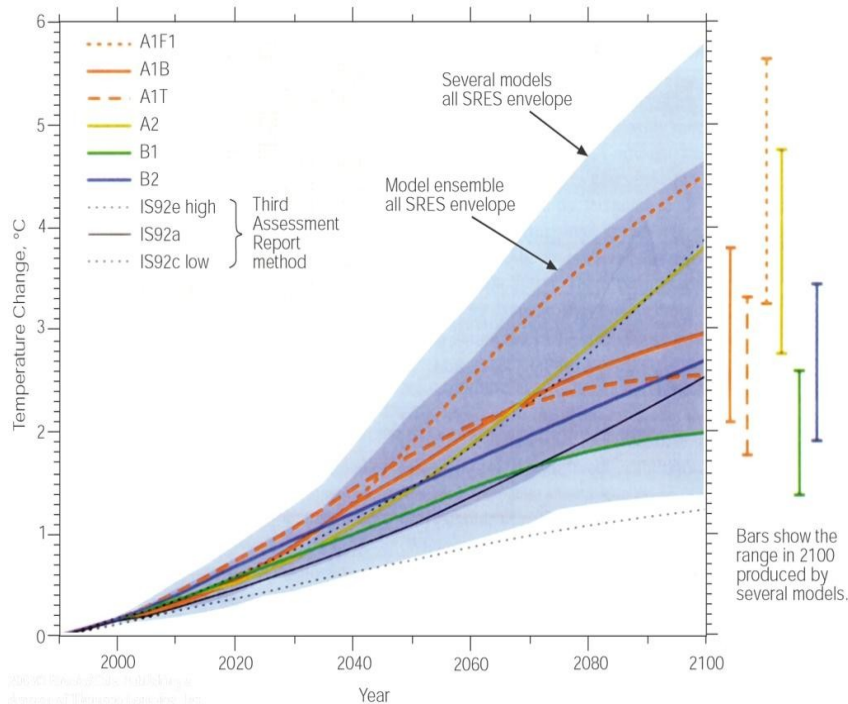
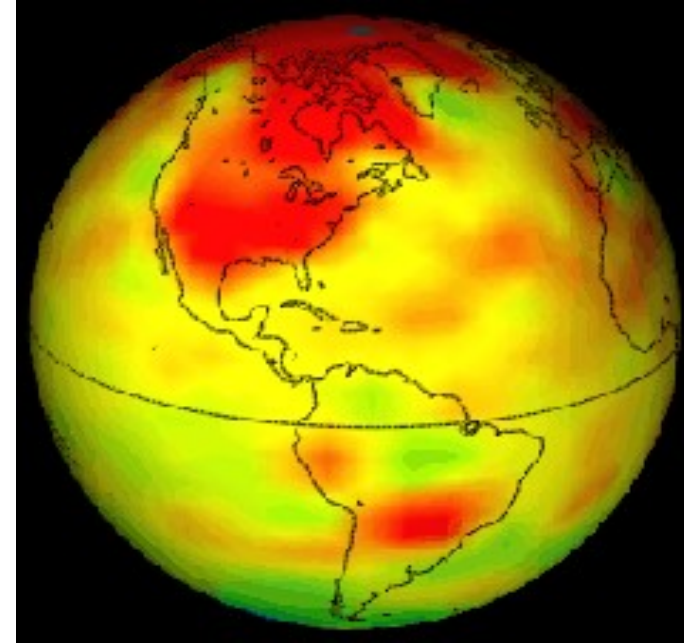
There are probably hundreds of XML-based “ markup languages” in use in academia

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

Environmental modelling

Hugely important

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

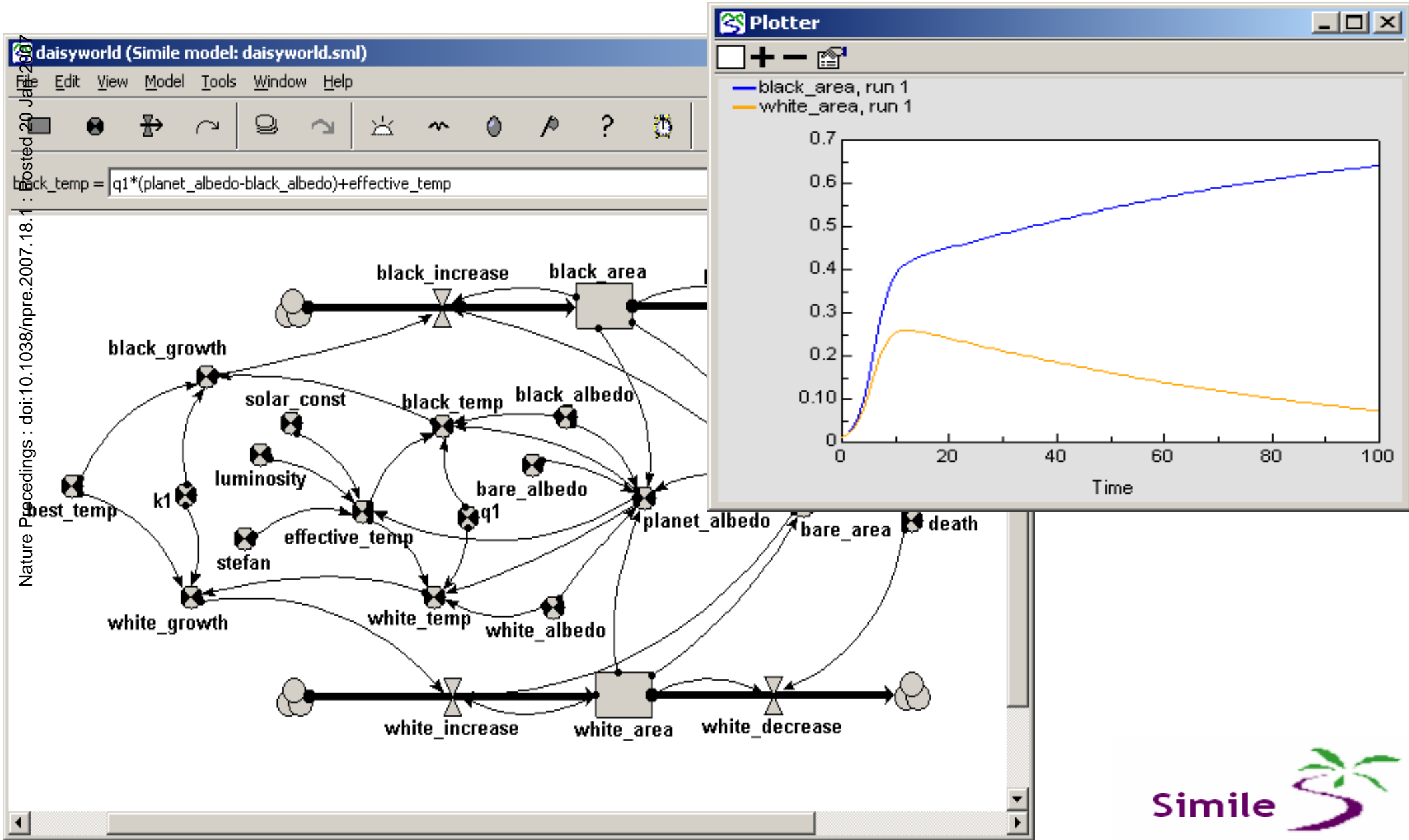


Current practice

- 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



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```

<?xml version="1.0" ?>
- <model url="http://www.similette.com/models/daisyworld/daisyworld.xml">
+ <source>
- <properties>
  <complete>true</complete>
  <file_name>C:/examplemodels/models/bob/daisyworld1/daisyworld1.ame</file_name>
  <name>Desktop</name>
  <title>The Watson and Lovelock DaisyWorld model</title>
  <description>This model is intended to demonstrate how the presence of living organisms on a
  planet can buffer the effect of changes in solar luminosity. The planet without life gradually
  gets hotter as luminosity increases. The planet with life (black and white daisies) is able to
  maintain the planet at an almost-constant temperature over a range of
  luminosities.</description>
  <link>http://www.pik-potsdam.de/~bloh/</link>
  <diagram_gif>images/daisyworld.gif</diagram_gif>
</properties>
- <submodel id="top">
+ <graphics>
- <nodes>
+ <clouds>
- <compartments>
  - <compartment id="node00002">
    - <infos>
      <complete>true</complete>
      <name>black_area</name>
    </infos>
    + <graphics>
  </compartment>
  - <compartment id="node00003">
    <infos>

```

MultiGuise

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

- Javascript generator
- MathML display
- Model summary**
- Raw XML display
- Simple simulator

Display



The Watson and Lovelock DaisyWorld model

This model is intended to demonstrate how the presence of living organisms on a planet can buffer the effect of changes in solar luminosity. The planet without life gradually gets hotter as luminosity increases. The planet with life (black and white daisies) is able to maintain the planet at an almost-constant temperature over a range of luminosities.

For more information, please click [here](#)

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- Summary statistics**
- SVG model diagram

Display

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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- McMurtrie model of vegetation bioma
- Simple ecosystem - trophics.xml
- Simple individual-tree-based model
- Soil component of the Century mode**
- Very simple ecosystem model, with

Stylesheets

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Display



Number of submodels 10
 Number of compartments 12
 Total number of flows 31
 - of which interflows 16
 Number of variables 91
 Number of influences 166

Each submodel below contains:	Sub model	Comp	Flow	Inter flow	Var	Infl
main	2	.	.	.	1	4
-- Litterlayer	1	5	12	5	25	59
---- MetabolicFractionModel	5	4
-- SoilLayer	7	7	19	11	12	60
---- MetabolicFractionModel	5	4
---- dddt_passive	6	3
---- dddt_metabolic	6	5
---- dddt_LigninStructural	8	7
---- dddt_slow	6	5
---- dddt_active	9	8
---- dddt_NonLigninStructural	8	7

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MultiGuise

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Load

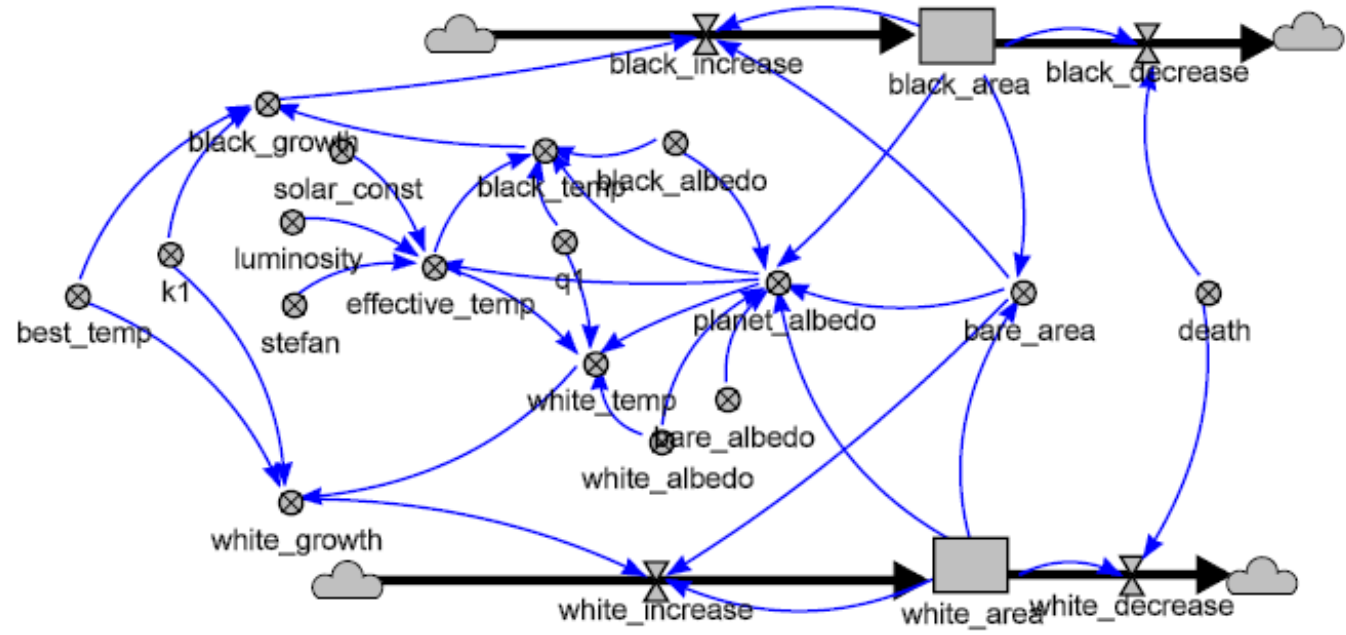
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- Simple ecosystem: 3 trophic layers
- Soil component of the Century model (i

Stylesheets

- C generator for MODCOM framework
- C# generator for MODCOM framework
- Code generator for TIME framework
- Equation listing**
- Fortran generator for BFG framework

Display



The Watson and Lovelock DaisyWorld model

compartments

black_area = 0.01

white_area = 0.01

variables

death = 0.3

black_growth = Math.pow(1-k1*(best_temp-black_temp),2)

best temp, black temp, k1,

white_growth = Math.pow(1-k1*(best_temp-white_temp),2)

best temp, white temp, k1,

black_temp = q1*(planet_albedo-black_albedo)+effective_temp

black albedo, effective temp, planet albedo, q1,

effective_temp = Math.pow(solar_const*luminosity*(1-planet_albedo)/stefan,0.25)-273

solar const, luminosity, stefan, planet albedo,

white_temp = q1*(planet_albedo-white_albedo)+effective_temp

planet albedo, q1, effective temp, white albedo,

black_albedo = 0.25

white_albedo = 0.75

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Stylesheets

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

Display



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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Display



```
const VarInfo params[] =
{
  {"death","description","units"},
  {"black_albedo","description","units"},
  {"white_albedo","description","units"},
  {"q1","description","units"},
  {"solar_const","description","units"},
  {"luminosity","description","units"},
  {"stefan","description","units"},
  {"bare_albedo","description","units"},
  {"best_temp","description","units"},
  {"k1","description","units"},
}

void model(double* state, double* param, double* signal,
double* deriv) {
  black_area = state[0]
  white_area = state[1]

  death = param[0]
  black_albedo = param[1]
  white_albedo = param[2]
  q1 = param[3]
  solar_const = param[4]
  luminosity = param[5]
  stefan = param[6]
  bare_albedo = param[7]
  best_temp = param[8]
  k1 = param[9]

  bare_area = 1-black_area-white_area;
  black_decrease = death*black_area;
  white_decrease = death*white_area;
  planet_albedo =
  black_albedo*black_area+white_albedo*white_area+bare_albedo*bare
```

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Javascript generator
 MathML display
 Model summary

Simulistics

```
// Javascript code for simulating the behaviour of "The Watson
and Lovelock DaisyWorld model"
// 20th Nov 2006
```

```
// Initial compartment values:
black_area = 0.01
white_area = 0.01
```

```
// Constant flows:
```

```
// Parameters:
death = 0.3
black_albedo = 0.25
white_albedo = 0.75
q1 = 20
solar_const = 917
luminosity = 0.8
stefan = 0.0000000567
bare_albedo = 0.5
best_temp = 22.5
k1 = 0.003265
```

```
// Time settings:
duration = 20;
timestep = 0.1;
```

```
for (var t = 0; t <= duration; t=t+1){
for (var tstep=0.0; tstep<1.0; tstep=tstep+timestep){
bare_area = 1-black_area-white_area;
black_decrease = death*black_area;
white_decrease = death*white_area;
planet_albedo =
black_albedo*black_area+white_albedo*white_area+bare_albedo*bare
effective_temp = Math.pow(solar_const*luminosity*(1-
```

MultiGuise

Packages

- Archelogos: Charmides
- Business Dynamics models (SimileXML)
- Business Dynamics models (SimileXML)
- Connotea models package (1)
- Connotea models package (2)

Load

Documents

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

Transforms

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

Display

Initial compartment values

black_area

white_area

Parameter values

death

black_albedo

white_albedo

q1

solar_const

luminosity

stefan

bare_albedo

best_temp

k1

Run control

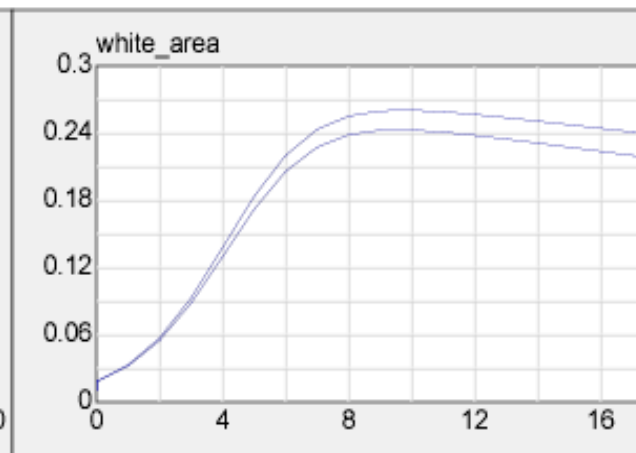
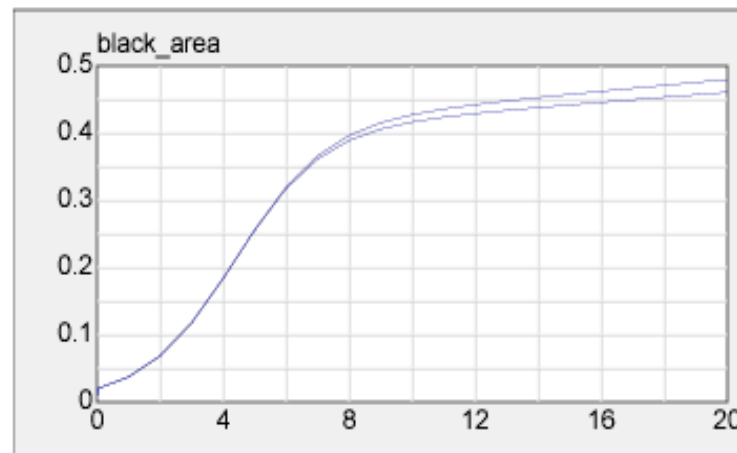
Time step

Run duration

Display interval

Run

Run: 1 2



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MultiGuise

Packages

- Archelogos: Charmides
- Business Dynamics models (SimileXML)
- Business Dynamics models (SimileXML)
- Connotea models package (1)**
- Connotea models package (2)

Documents

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- McMurtrie model of vegetation biomass**
- Simple ecosystem - trophics.xml
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- Graphical simulator**
- Javascript generator (on similette.com)
- Model summary (on similette.com)
- Model summary statistics (on similette.com)
- Simile-XML transform: displays the network

Initial compartment values

biomass

Parameter values

kloss

SLA

k

r

Pmax

leaf_fraction

efficiency

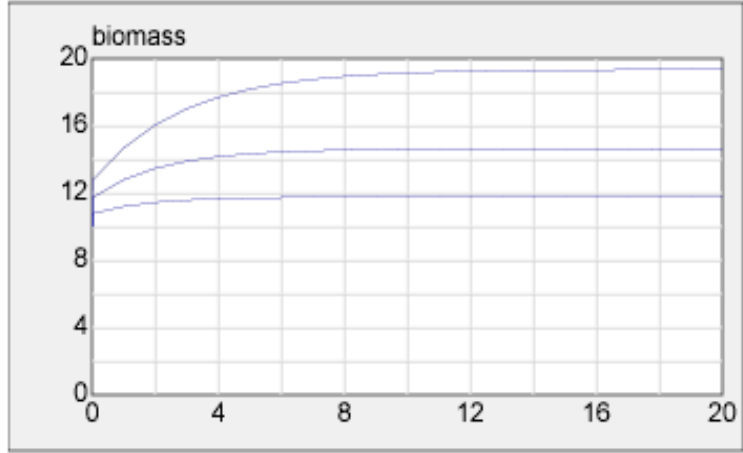
Run control

Time step

Run duration

Display interval

Run: 1 2 3



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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.

Search My library

Find results



you are logged in as robertm

My library Log out

Home Latest News About Connotea Site Guide Community pages

- robertm's groups: connomultiquise, Declarative modelling, Ecosystem services

- robertm's tags: By Usage A-Z Find: allosteric transitions, archelogos, biomass, cdc2, cdc2 kinase

robertm's bookmarks matching tag Simile-XML EXPORT LIST RSS ? Number of bookmarks per page: 10 | 25 | 50 | 100

Simple ecosystem: 3 trophic layers www.similette.com Posted by robertm to Simile-XML on Tue Nov 14 2006 at 15:27 UTC | info

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

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, Report a problem

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Search My library [input field]

Find results



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My library

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[C# generator for MODCOM framework](#)
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MultiGuise

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- Archelogos: Charmides
- SBML models**
- 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

Display

Stylesheets

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

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 $M \leftrightarrow MI$ and $X \leftrightarrow XI$. 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.

This model originates from BioModels Database: A Database of Annotated Published Models. It is copyright (c) 2005-2006 The BioModels Team.

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Model:

Goldbeter1991_MinMitOscil_ExplInact

Main model constituents

Compartments	cell
Species	Cyclin Active CDC-2 Kinase Active Cyclin Protease Inactive CDC-2 Kinase Inactive Cyclin Protease
Parameters	V1 V3 VM1 VM3 Kc
Reactions	creation of cyclin default degradation of cyclin cdc2 kinase triggered degradation of cyclin activation of cdc2 kinase deactivation of cdc2 kinase activation of cyclin protease deactivation of cyclin protease

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MultiGuise

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- Archelogs: Charmides**
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Load

Documents

- Plato: Charmides 1**
- Plato: Charmides 2
- Plato: Charmides 3
- Plato: Charmides 4

Stylesheets

- Archelogs full-display stylesheet
- Archelogs summary stylesheet**

Display



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

In this section of the dialogue, Plato elucidates the context of the question with which the remainder of the dialogue will be concerned: What is sound-mindedness (sophrosune)? After describing the scene of the conversation and introducing the main participants in the discussion, Socrates pretends to know a cure for Charmides' repeated morning headaches. Socrates argues that before he can cure these headaches, however, he must first determine whether Charmides has sound-mindedness. To do this, Socrates asks Charmides to say what sound-mindedness is.

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Stylesheets

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Display



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

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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.

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- Pierre Lindenbaum (IntegraGen)**