OpenCell software: CellML Libraries

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About OpenCell (briefly)

- Current developers:
  - Auckland Bioengineering Institute
    - Andrew Miller
    - Justin Marsh
  - Oxford:
    - Alan Garny

- Free and Open Source
- Windows, Linux, MacOS
- Based on CellML API
- Previously known as
- "Physiome CellML Environment" (PCEnv).

OpenCell

File View Tools Help

Kinetics of L-dopa and 3-OMD

Type	Value	Units
▲ Components		
▷ environment		
▲ gastrointestinal_compart...		
▷ F_b_dopa		dimensionless
▷ A_dopa_b	101	umole
▷ ka_b_dopa	2.11	per_hour
▷ F_G		dimensionless
▷ F_H		dimensionless
▷ CL_H		liter_per_hour

F_H = 1 {unit: dimensionless} - CL_H / Q;

F_G = 0.244 {unit: dimensionless};

CL_H = f_H * CL_dopa_0;

F_b_dopa = F_H * F_G;

d(A_dopa_b)/d(time) = -(ka_b_dopa) * A_dopa_b;

$$F\_H = 1 - \left(\frac{CL\_H}{Q}\right)$$

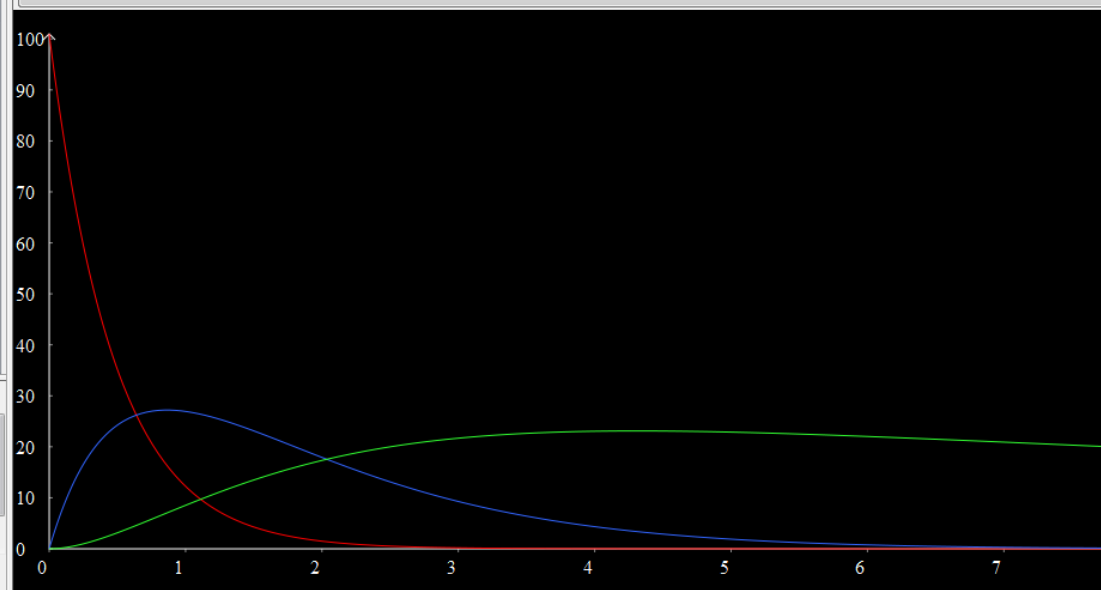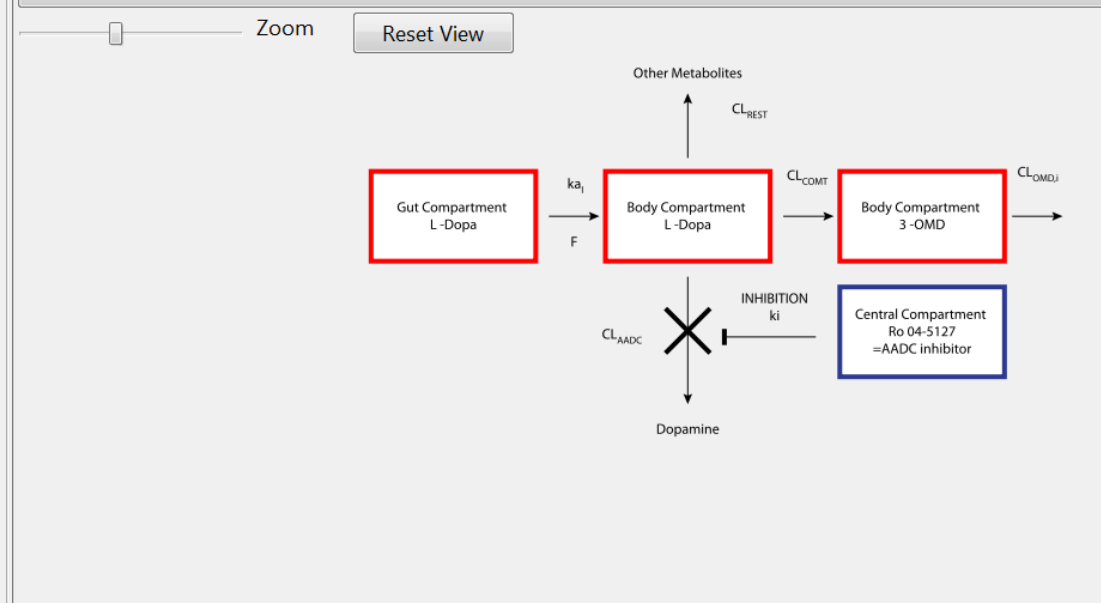$$F\_G = 0.244$$
$$CL\_H = f\_H \times CL\_dopa\_0$$
$$F\_b\_dopa = F\_H \times F\_G$$
$$\frac{d(A\_dopa\_b)}{dtime} = (-ka\_b\_dopa) \times A\_dopa\_b$$

Schematic Diagram

Zoom   Reset View

Other Metabolites

CL_{REST}

| Gut Compartment L-Dopa | ka_I → F | Body Compartment L-Dopa | CL_{COMT} → | Body Compartment 3-OMD | $CL_{OMD,I}$ → |

CL_{AADC}

INHIBITION
ki

Central Compartment
Ro 04-5127
=AADC inhibitor

Dopamine
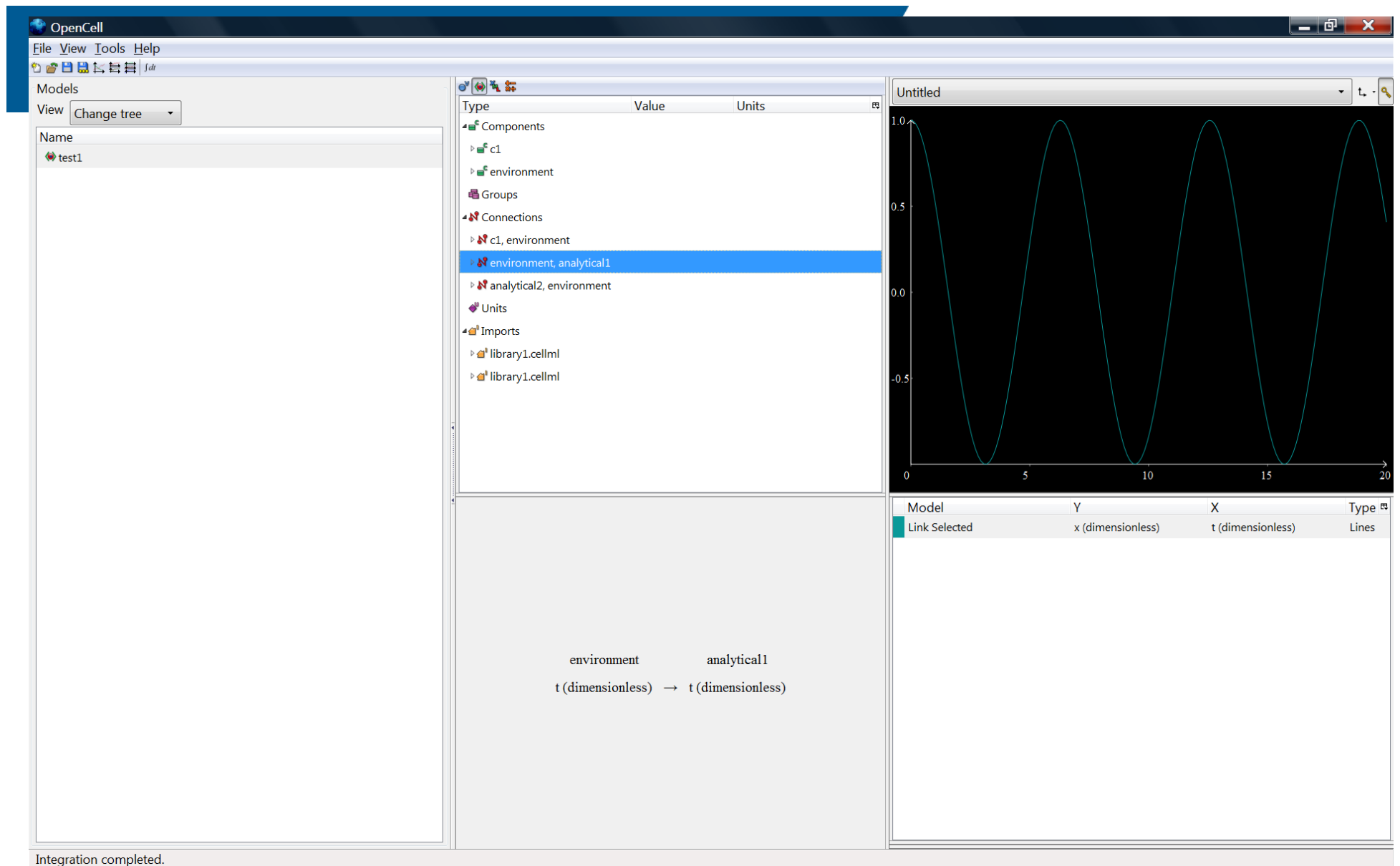
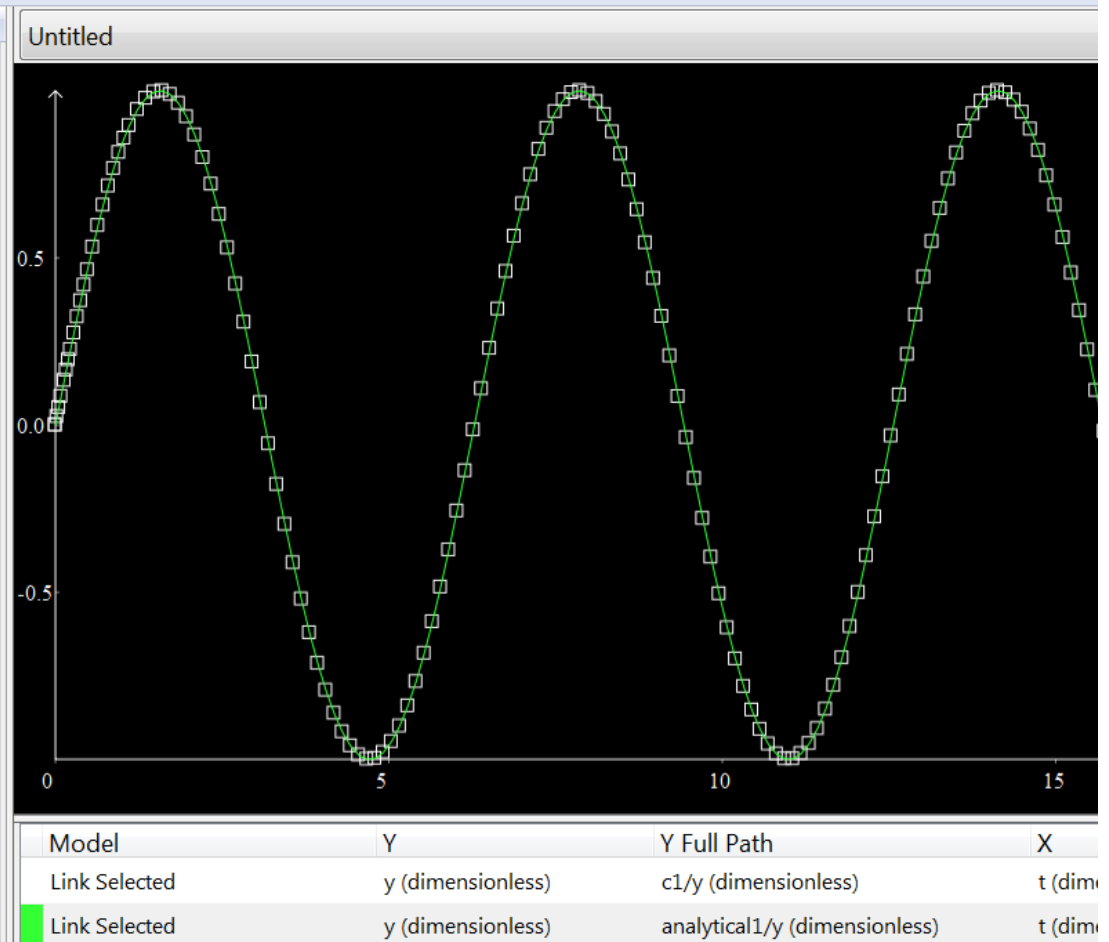Script Message: Displaying flux of A_dopa_b, C_dopa_b, C_OMD_b

Features of OpenCell that support CellML 1.1

- Supports files that use imports
  - Relative URLs
  - Absolute URLs

- Uses CellML API
  - Subtleties of encapsulation: instantiate encapsulated connected components.

- User interface displays variables via "import path"

Type	Value	Units
▲ ◼ᶜ Components		
▷ ◼ᶜ c1		
▷ ◼ᶜ environment		
🔲 Groups		
▲ 𝐍 Connections		
▷ 𝐍 c1, environment		
▷ 𝐍 environment, analytical1		
▷ 𝐍 analytical2, environment		
◆ Units		
▲ 🏠 Imports		
▷ 🏠 library1.cellml		
▷ 🏠 library1.cellml		

Untitled
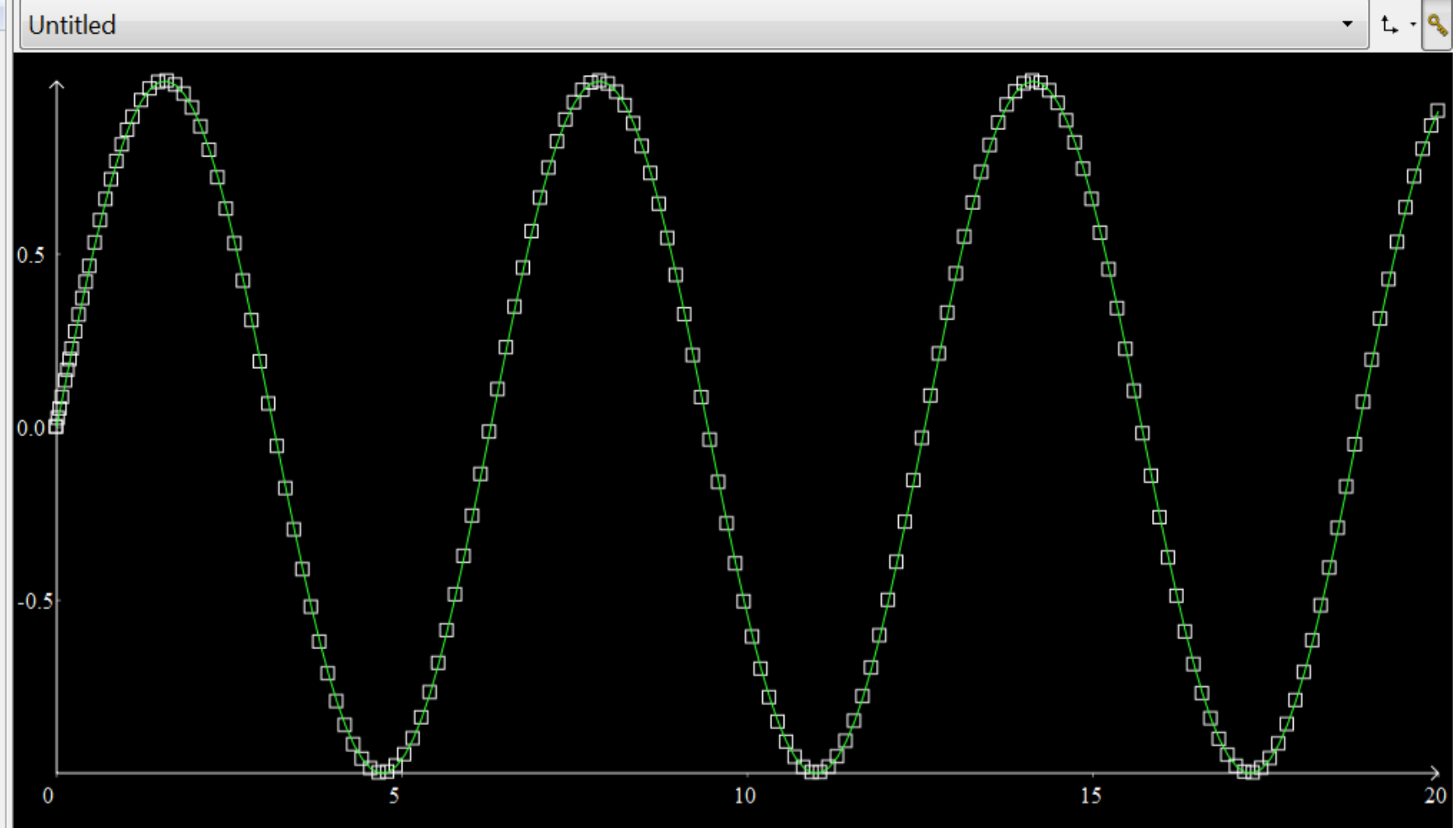
1.0

0.5

0.0

-0.5

Improvements ideas

- Components instantiated via import should appear in model tree so that "drag-n-drop" features can be used:
  - Drag to make connections
  - Drag to view graphs

- View/edit **metadata** (e.g. Variable or component annotation)

- Allow semi-automated connections to be based on **metadata**

Improvements ideas

- SBGN or other Graphical view

- Mathematical display of model including enough info to see compartmentalisation

- Link with PMR2:
  - Browse for components/libraries

Automated Refactoring

- Decompose 1.0 model into 1.1 models with imports (prototype script exists)

- To extract reusable parts of models into components and libraries

- Reconnect (e.g. change to different parameters)

Improvement ideas

- CellML API: address issues to improve uptake by developers.

- Model assemblies:
  - Currently imports refer to files.

Discussion