

OpenCOR

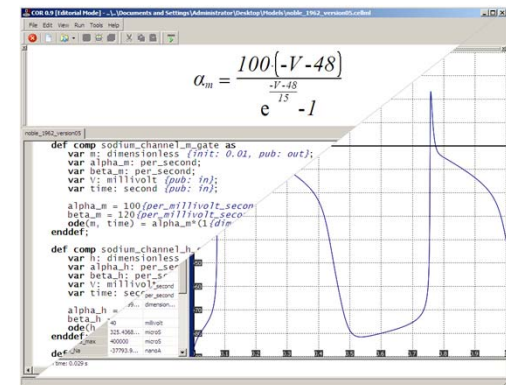
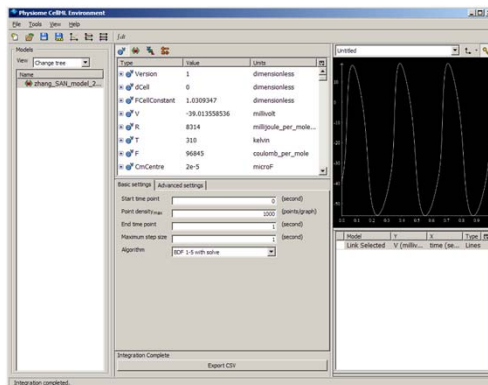
Alan Garry

alan.garry@dpag.ox.ac.uk



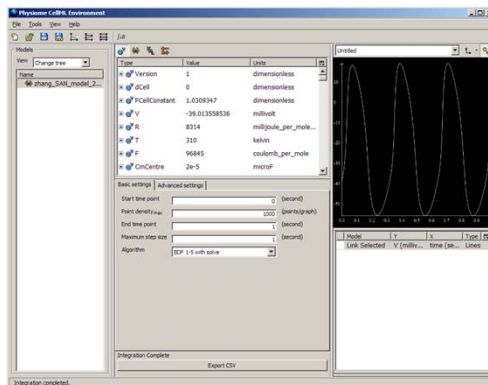
OPENCELL AND COR

- The two main CellML environments are OpenCell and COR.
- OpenCell:
 - Version 0.8 was released in October 2010.
 - Support for both CellML 1.0 and 1.1.
 - Works on Windows, Linux and Mac OS X.
 - Now officially discontinued.
- COR:
 - Version 0.9.31.1409 was released in November 2010.
 - Support for CellML 1.0.
 - Works on Windows.
 - No new major feature in years, but still maintained.

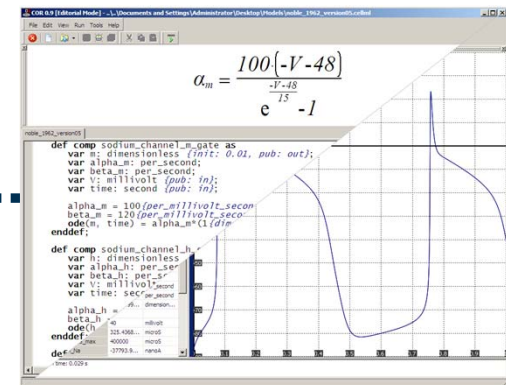


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OpenCOR
(Open COmbined Resource)



GENERAL INFORMATION

- OpenCOR is an **open source project**.
- Agreement on a (business friendly) license is yet to be reached (**3-clause BSD license?**).
- The project is hosted on **SourceForge** using **Git**.
⇒ <http://sourceforge.net/projects/opencor/> ⇐
- A (very) simple **website** has been set up.
⇒ <http://www.opencor.ws/> ⇐
- Currently being developed, built, tested and packaged on:
 - **Windows 7**;
 - **Ubuntu 10.10** (Maverick Meerkat; both the 32-bit and 64-bit versions); and
 - **Mac OS X 10.6** (Snow Leopard).

DEVELOP, BUILD, TEST AND PACKAGE

- Some pre-requirements:

- **Git** (the git package on Ubuntu):

- \$ git clone git://opencor.git.sourceforge.net/gitroot/opencor/opencor

(Read Only)

- \$ git clone ssh://l@ogin@opencor.git.sourceforge.net/gitroot/opencor/opencor

(Read/write)

DEVELOP, BUILD, TEST AND PACKAGE

- Some pre-requisites:

- Git (

\$ G
\$ G

```
3rdparty // Various third-party libraries used by OpenCOR
├── LibQxt // The LibQxt library
├── QScintilla // The QScintilla library
├── QtMmlWidget // The QtMmlWidget library
└── QtSingleApplication // The QtSingleApplication library
build // Where OpenCOR-related build files are generated
distrib // Various files used for the packaging of OpenCOR
doc // User and developer documentation
├── 3rdparty // Third-party library used for the documentation
│   └── googleCodePrettify // The Google Code Prettify library
├── developer // Developer documentation
├── res // Various resource files used by the documentation
└── user // User documentation
i18n // Internationalisation files
res // Various resource files used by OpenCOR
├── boomy // The Boomy multiplatform icon library
├── flags // The Printable world flags icon library
└── oxygen // The Oxygen icon library
src // Source code files for OpenCOR
├── misc // Files that do not fit anywhere else
├── ui // User interfaces
│   ├── edit // User interfaces for the editing side of things
│   └── organise // User interfaces for the organisation side of things
└── widget // Widgets
    ├── edit // Widgets for the editing side of things
    ├── misc // Widget files that do not fit anywhere else
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winConsole // Console version of OpenCOR (Windows only)
├── build // Where the build files are generated
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(Read Only)
or (Read/write)

DEVELOP, BUILD, TEST AND PACKAGE

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(Read/write)

- **CMake 2.8+** (the `cmake` package on Ubuntu);

- **C++ toolchain:**

- Windows: MinGW 4.4.0;

- Ubuntu: the `g++` package; and

- Mac OS X: Xcode.

- **Qt 4.7.2:**

- Windows and Mac OS X: binaries available; and

- Ubuntu: it has to be built from its source code which requires some additional packages.

- **Qt Creator 2.1.0;** and

- **NSIS** (Windows only).

Note: the above pre-requirements are meant for someone who wants to develop, build, test and package OpenCOR in the exact same way as it is done by the OpenCOR team. However, when it comes to Qt and Qt Creator, older versions may also work (e.g. on Ubuntu, you might just want to install the `qtcreator` package).

⇒ <http://www.opencor.ws/developer/developBuildTestAndPackage.html> ⇐

DEVELOP, BUILD, TEST AND PACKAGE

- Development is currently **single-handed**.
- This will, however, change once the project has reached a **certain level of maturity**.
- Best practices:
 - **File structure**; and

DEVELOP, BUILD, TEST AND PACKAGE

- Development is currently **single-headed**

- This will be **multi-headed**

certain

- Best practice

- File

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DEVELOP, BUILD, TEST AND PACKAGE

- Development is currently **single-handed**.
- This will, however, change once the project has reached a **certain level of maturity**.
- Best practices:
 - **File structure**; and
 - **Coding style**: the rules were unashamedly taken (paraphrased, if not simply copied/pasted) from the coding style document written by the developers of Qt Creator.

⇒ <http://www.opencor.ws/developer/bestPractices.html> ⇐

DEVELOP, BUILD, TEST AND PACKAGE

- OpenCOR uses various **third-party libraries**.
- However, all the required files are in our **Git repository**.
- For the relevant software libraries, a/the **CMakeLists.txt** file was created/modified so that the library can be built as part of our build process.
- Third-party libraries currently being used:
 - Software:
 - **Google Code Prettify** (Apache v2.0);
 - **LibQxt 0.6.1** (CPL v1.0 and LGPL v2.1);
 - **QScintilla 2.4.6** (GPL v2.0, GPL v3.0 and commercial);
 - **QtMmlWidget 2.4** (LGPL v2.1); and
 - **QtSingleApplication** (BSD).
 - Image:
 - **Printable world flags** (no specific license);  
 - **Boomy multiplatform** (no specific license); and
 - **Oxygen 4.6.1** (LGPL v3.0).



⇒ <http://www.opencor.ws/developer/thirdPartyLibraries.html> ⇐

DEVELOP, BUILD, TEST AND PACKAGE

- OpenCOR can be built either from the **command line** or using **Qt Creator**.
 - **Command line:**
 - **cleanproj [. bat]**: cleans the OpenCOR environment;
 - **cleanproj all [. bat]**: cleans all of the OpenCOR environment (i.e. including third-party libraries);
 - **makeproj [. bat]**: compiles and links everything that is required to get a release version of OpenCOR; and
 - **runproj [. bat | . vbs]**: runs OpenCOR.
 - **Qt Creator:**
 - It's pretty much a matter of just opening the main **CMakeLists.txt** file and of clicking the **Run** button.
 - Support for **parallel compilation** and **debugging** (using **gdb** under the hood).
- ⇒ <http://www.opencor.ws/developer/developBuildTestAndPackage.html> ⇐

DEVELOP, BUILD, TEST AND PACKAGE

- Packaging is done from the **command line**, using **packageproj [. bat]**:
 - Windows: both a **NSIS setup program** and a **ZIP file** are generated;
 - Linux: a **. tar. gz file** is generated; and
 - Mac OS X: both a **PackageManager solution** and a **ZIP file** are generated.

Note: though built on Ubuntu, OpenCOR should also work with other versions of Ubuntu, as well as other Linux distributions though additional libraries may be required in this particular case.

⇒ <http://www.opencor.ws/developer/developBuildTestAndPackage.html> ⇐

GENERAL PHILOSOPHY

- OpenCOR can be used both as a **command line tool** and through a **graphical user interface**.

```
agarny@pc-hbl i n: ~/OpenCOR$ ./OpenCOR -h
Usage: OpenCOR [OPTION]... [FILE]...
Start OpenCOR and open the FILE(s) passed as argument(s).
```

```
-a, --about      Display OpenCOR about information
-h, --help      Display this help information
-v, --version    Display OpenCOR version information
```

Mandatory or optional arguments to long options are also mandatory or optional for any corresponding short options.

```
agarny@pc-hbl i n: ~/OpenCOR$ ./OpenCOR -a
OpenCOR 0.1
GNU/Linux 2.6.35-28-generic
```

OpenCOR is a cross-platform CellML-based modelling environment which can be used to organise, edit, simulate and analyse CellML files.

```
agarny@pc-hbl i n: ~/OpenCOR$ ./OpenCOR -v
OpenCOR 0.1
agarny@pc-hbl i n: ~/OpenCOR$
```


GENERAL PHILOSOPHY

- OpenCOR can be used both as a **command line tool** and through a **graphical user interface**. Some general features:
 - **Fully customisable** (an on-going process);
 - **Multi-lingual** (English and French at the moment);
 - **Auto updates** (both for development versions and release versions);
 - **Crash report** (still need to think a bit more about this one);
 - **Plugin approach** (to allow for community involvement); and
 - **User friendly** (as much as possible!).
- OpenCOR will be used to **organise, edit, simulate and analyse** CellML and, in the long-term future, SBML files:
 - CellML and SBML support will be through the **Auckland CellML API** and the **SBML API**, respectively;
 - Access to the **CellML Model Repository** and **BioModels Database** (through Web services);
 - Support for **ontologies** (through Web services to **RICORDO**);
 - Support for **SED-ML** (through the CellML and SBML APIs?); and
 - 2D and 3D representation of a model (using **SVG** and **cmgui**, respectively).

ORGANISE

- Access to:
 - The **CellML Model Repository** and **BioModels Database** to search, download, upload, etc. a model;
 - A **file browser** and therefore local files (be they CellML/SBML documents or not); and
 - A **file organiser** to virtually arrange files (e.g. a virtual folder that contains a symbolic link to all the CellML files used in a modelling study).

EDITING (CELLML FILES INITIALLY)

- Editing of a CellML file using one of **several views**:
 - **Raw XML view**;
 - **COR-like view** (i.e. a compact format);
 - **Improved COR-like view** (i.e. COR-like view without CellML-specific concepts such as public/private interfaces, encapsulation hierarchy and connections);
 - **Tree-like view** (with the ability to show/hide various CellML features); and
 - **Graphical view** (using SVG or cmgui, and based on the metadata/ontology information present in a CellML file).
- Some other editing features:
 - **Graphical rendering** of unit/variable definitions, mathematical equations, etc.;
 - **CellML validation** (list of warnings/errors highlighting a particular problem);
 - **Basic metadata support** (i.e. model authors/description/curators, etc.);
 - **Advanced metadata support** so that, using domain-specific ontologies (RICORDO), models can be comprehensively annotated;
 - **Diff** of two CellML files (only for text-based views); and
 - **Export of CellML files** to various programming (e.g. C/C++, F77, Java MATLAB, Python) and word processing languages (MS Word 2007/2010 and TeX); and
 - **Import/export** from/to SBML.

SIMULATE

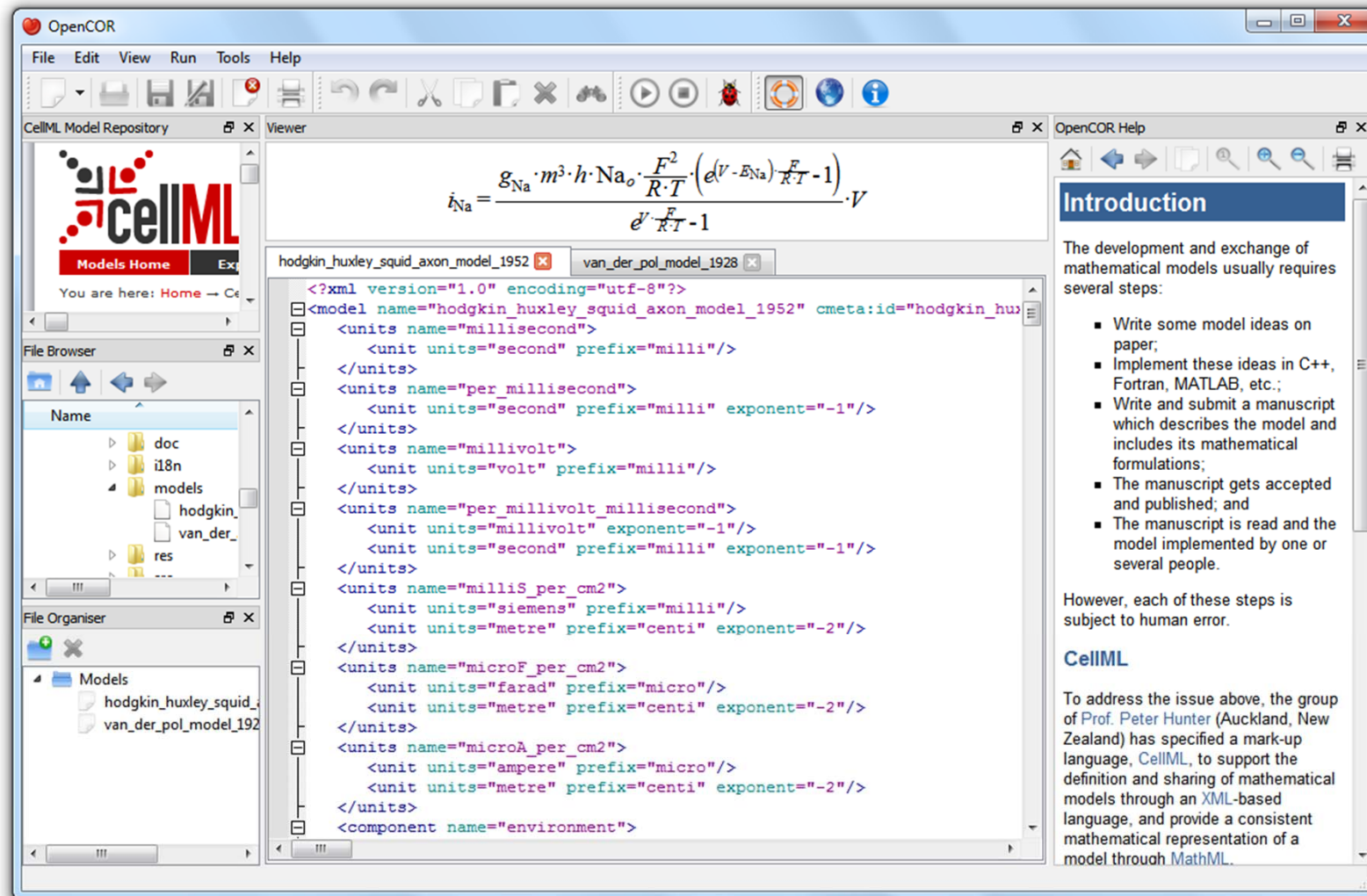
- Some general features include:
 - Editing of simulation (e.g. start/end points) and numerical solver parameters (dependent on the solver to be used);
 - Editing of model parameters (using a tree-like view);
 - Support for models consisting of differential algebraic equations (**CVODE** and **IDA** as default solvers);
 - Run/pause/stop a simulation;
 - Plotting of simulation results (against any model param.);
 - Export of simulation results to the CSV format; and
 - Create a new or update an existing CellML file based on the results of a simulation.

ANALYSE

- Analysis features will mainly be provided by the community through the use of plugins.
- For example, a plugin to analyse cardiac action potentials and extract some key parameters from them (e.g. upstroke velocity, action potential amplitude, action potential duration at 90% repolarisation).

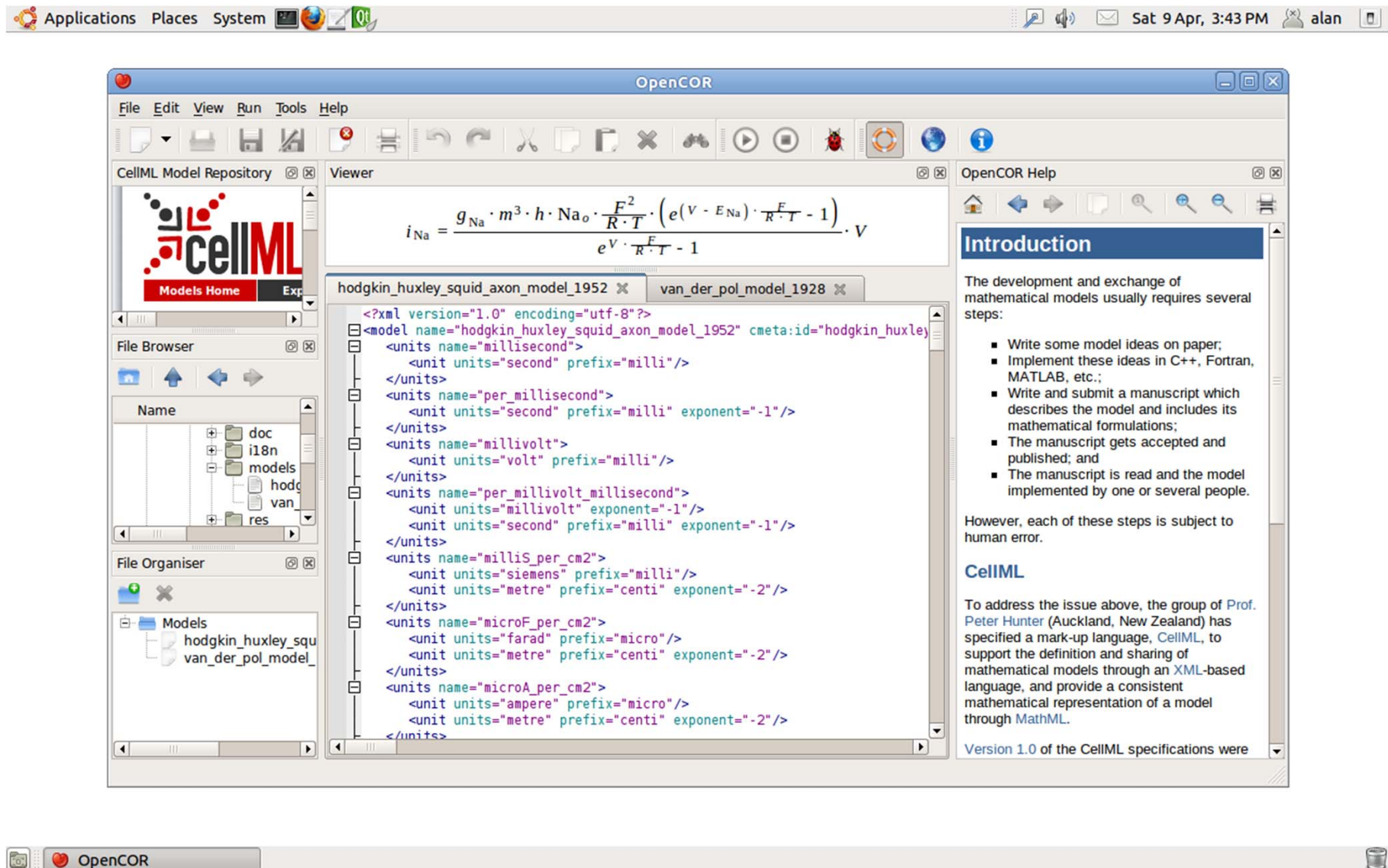
WHAT OPENCOR CURRENTLY LOOKS LIKE...

... on Windows



WHAT OPENCOR CURRENTLY LOOKS LIKE...

... on Linux



WHAT OPENCOR CURRENTLY LOOKS LIKE...

... on Mac OS X

OpenCOR File Edit View Run Tools Help

Bluetooth Wi-Fi Audio UK (Charged) Sat 9 Apr 15:41:39 Q

CellML Model Repository

Viewer

OpenCOR Help

Introduction

The development and exchange of mathematical models usually requires several steps:

- Write some model ideas on paper;
- Implement these ideas in C++, Fortran, MATLAB, etc.;
- Write and submit a manuscript which describes the model and includes its mathematical formulations;
- The manuscript gets accepted and published; and
- The manuscript is read and the model implemented by one or several people.

However, each of these steps is subject to human error.

CellML

To address the issue above, the group of Prof. Peter Hunter (Auckland, New Zealand) has specified a mark-up language, CellML, to support the definition and sharing of mathematical models through an XML-based language, and provide a consistent mathematical representation of a model through MathML.

Version 1.0 of the CellML specifications were released in August 2001. These specifications were subsequently refined to support model evolution and re-use, and were released in February 2006 as version 1.1. The inherent nature of CellML means that CellML models are independent of the operating system or

CellML Model Repository

Models Home

You are here: Home → CellML

File Browser

Name

- makepr
- makepr
- models
- hodg
- van
- package
- package

File Organiser

Models

- hodgkin_huxley_sq
- van_der_pol_model

Viewer

hodgkin_huxley_squid_axon_model_1952

van_der_pol_model_1928

$$i_{Na} = \frac{g_{Na} \cdot m^3 \cdot h \cdot Na_o \cdot \frac{F^2}{R \cdot T} \cdot \left(e^{(V - E_{Na}) \cdot \frac{F}{R \cdot T}} - 1 \right)}{e^{V \cdot \frac{F}{R \cdot T}} - 1} \cdot V$$

<?xml version="1.0" encoding="utf-8"?>

<model name="hodgkin_huxley_squid_axon_model_1952" cmeta:id="hodgkin_huxle

<units name="millisecond">

<unit units="second" prefix="milli"/>

</units>

<units name="per_millisecond">

<unit units="second" prefix="milli" exponent="-1"/>

</units>

<units name="millivolt">

<unit units="volt" prefix="milli"/>

</units>

<units name="per_millivolt_millisecond">

<unit units="millivolt" exponent="-1"/>

<unit units="second" prefix="milli" exponent="-1"/>

</units>

<units name="milliS_per_cm2">

<unit units="siemens" prefix="milli"/>

<unit units="metre" prefix="centi" exponent="-2"/>

</units>

<units name="microF_per_cm2">

<unit units="farad" prefix="micro"/>

<unit units="metre" prefix="centi" exponent="-2"/>

</units>

<units name="microA_per_cm2">

<unit units="ampere" prefix="micro"/>

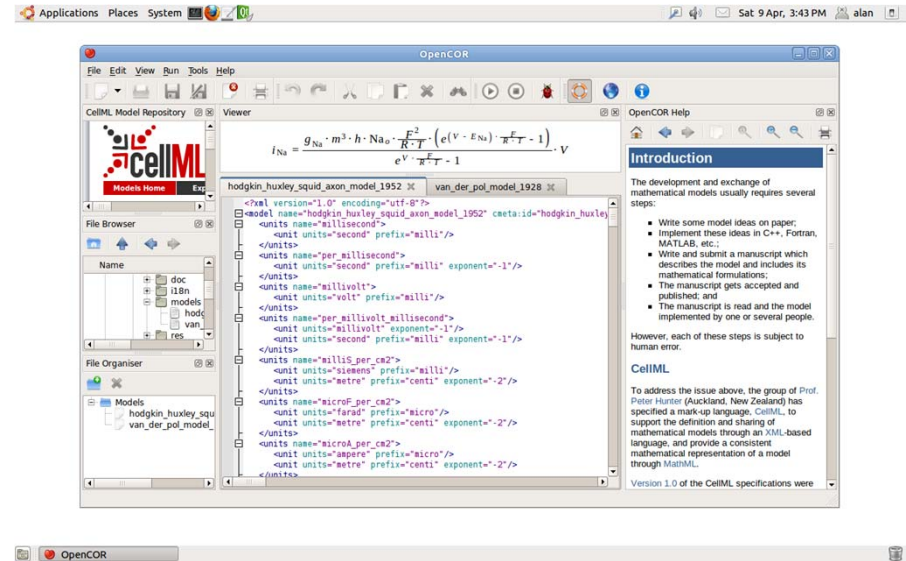
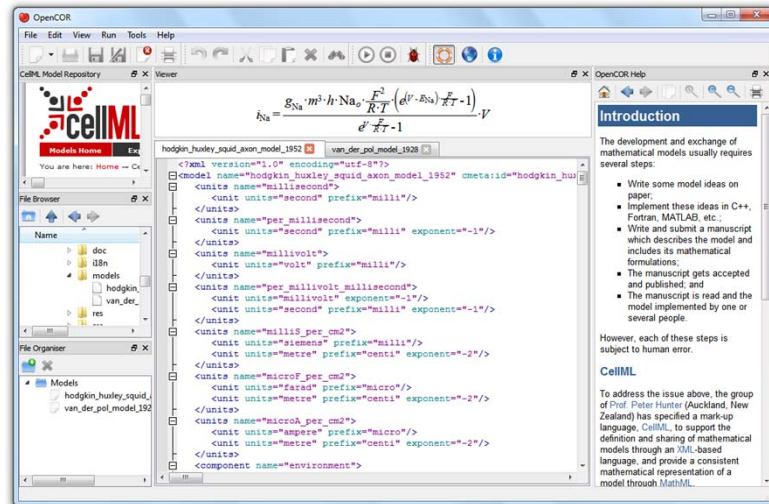
<unit units="metre" prefix="centi" exponent="-2"/>

</units>

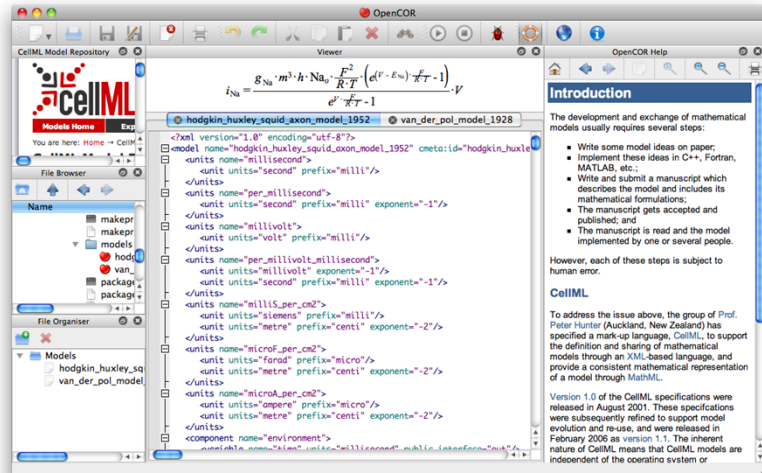
<component name="environment">

variable name="time" units="millisecond" public_interface="out"/>

WHAT OPENCOR CURRENTLY LOOKS LIKE...



OpenCOR File Edit View Run Tools Help (Charged) Sat 9 Apr 15:41:39



Still aiming at a first public release by the end of the year...

ACKNOWLEDGEMENTS

