Moving from COR to PCEnv/COR

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INTRODUCTION

PCEnv and COR: two CellML environments with similar goals.



AIM



anything **bad** about YAPE is the result of my own thinking...

PHILOSOPHY

A three-step process:

- 1. Organising;
- 2. Editing; and

3. Simulating.

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Models			
	aw Interpreted Raw COR Math Graph		
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	Messages		Console

ORGANISER

- Repository Explorer, File Explorer and Models organiser.
- Repository Explorer: 'link' to the CellML repository.
- File Explorer: mainly for consistency.
- Models organiser: organise models independently of their physical location.
- Drag/drop files from the Repository and File Explorers to the Models organiser and Editor.
- Diff' between two models.

EDITOR

- Viewer, Metadata, Editor and Messages.
- Viewer: graphically render units definitions, variable declarations and mathematical equations.
- Metadata: edit metadata using either a raw or interpreted view.
- Editor: edit CelIML files using either a raw, COR like, mathematical or graphical view (or any other view).
- Messages: list any message related to the editing of CelIML files and their metadata.

SIMULATOR

- Simulation, Parameters, Results, SVG and Console.
- Simulation: access to simulation parameters, including the integrator to use (e.g. CVODE).
- Parameters: access to the model parameters.
- Results: one or several graph panels for rendering simulation data.
- SVG: place holder for a SVG diagram.
- Console: list simulation information (e.g. computational time).
- 'Diff' between current simulation and default.

MISCELLANEOUS (I)

General:

 Concept of add-on (e.g. for computing electrophysiological parameters or for testing/refining a particular equation).

Organiser:

 To query the CellML repository for *I*_{Ca,L} would not only return results for *I*_{Ca,L}, but also for *Cav1.3* (through ontology). Import of a given result would involve automatic mapping of parameters, conversion of units, etc.

MISCELLANEOUS (II)

Editor:

- Use Scintilla as the main editor (syntax highlighting, code folding, bookmarks, view splitting, etc.).
- COR like view should keep things in the same order as in the CelIML file.
- Ability to comment a model (through metadata?).
- Export to various languages (with or without lookup table (for any parameter) and/or partial evaluation).

Simulator:

- Debug mode (i.e. trace into a model).
- Hijack mode (i.e. apply any protocol to one or several parameters; e.g. to create an IV curve).
- Render complex parameters (e.g. $I_{Na}+I_{K}$).

CONCLUSION

- COR's strong point is on the editing of CellML files while PCEnv's is on simulating them.
- It would therefore make sense to merge the two of them, as well as add new features.
- To achieve the above, we would need to give YAPE (?) a proper identity and more people on board.

preDCT Computational prediction of drug cardiotoxicity



European Union - funded grant within FP7 Virtual Physiological Human call

5 Vacancies

Modelling Drug Action on Cardiac Electrophysiology

1 Senior Postdoctoral Fellow

4 Research Assistants

Computational Biology and Cardiac Electrophysiology Groups (June 2008 - May 2011)

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