

Modelling with CellML 1.1

David Nickerson Division of Bioengineering National University of Singapore



CellML 1.1

- Initial release 6 November 2002 and specification frozen 28 February 2006.
- Two main new features added to CeIML 1.0
 - ability to use one variable to set another variable's initial_value attribute; and
 - the import element for importing units and components from one model into another model.
- To date, only tools based on the CellML API support 1.1 models.
- No support currently in the model repository for 1.1 models.



initial_value="bob"

- Provides the mechanism by which differential equation variables can have their initial_value set outside the component in which they are defined.
- Allows modular component descriptions independent of parameter values and boundary conditions.



Units and component imports

- Define once and re-use common units and mathematics
 - error control and correction;
 - → community standards and repositories (unit dictionaries).
- Build complex models from the combination of well defined and understood sub-models.
- Clear separation of mathematical model description from specific use instantiation.



Example: the Nernst equation









Importing with encapsulation

- Encapsulated components always come along for the ride
 - → ensures components remain valid.







CellML model instances

- Given a CelIML description of a mathematical model you probably want to run multiple simulations with different experimental protocols, parameter sets, and boundary conditions.
- Its useful to define default parameter and boundary condition "models" to ease the load on the model developer.
- Experimental protocols are generally just mathematical models describing some applied boundary condition(s)
 - can be imported from standard descriptions/repositories.



Modelling with CellML 1.1



CellML Workshop 200

Auckland, New Zealand



Example: Noble 1962 model













potassium_channel_n_gate



Example: ten Tusscher et al 2004













MANIIC













25



Whats next?

- CellML 1.1 support in the cellml.org model repository.
- More tools supporting CellML 1.1 models.
- Establish a community repository of re-usable standard units and components.
- Guidelines on the use of CellML 1.1 to ensure we all create models suitable for re-use by the community wherever possible...



Best Practice (???)

- Components should only contain one equation.
- A component with math in it should define no initial_value attributes with a numerical value.
- As a mathematical model is assembled, all components should be encapsulated by a sensible interface component.
- All variables should be exposed via the encapsulating interface component.