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 CellML 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 CellML description of a mathematical model you probably want to run multiple simulations with different experimental protocols, parameter sets, and boundary conditions.
- It's 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.
Example: Noble 1962 model
file:///home/andre/data-new/cellml/models/1962_noble/experiments/free-running.xml

interface

membrane  
sodium_channel  
potassium_channel  
leakage_current

sodium_channel_m_gate  
sodium_channel_h_gate  
potassium_channel_n_gate
Example: ten Tusscher et al 2004
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.