

National University of Singapore



Singapore's  
Global  
University

# Machine Interpretable Mathematical Model Descriptions

David Nickerson & Martin Buist



# The Problem

- **Mathematical models used in biology are getting more realistic.**
- **Traditional peer-reviewed articles rarely contain enough information to accurately reproduce or validate future model implementations.**
- **Required information often buried in complex computational code.**
- **Quantitative validation is generally impossible without full cooperation of original authors.**

# The Answer

- **Encode mathematical models in standard formats.**
- **Unambiguously annotate the encoded model with as much information as possible, preferably using community defined standard annotations.**
- **Develop tools capable of rendering the annotated models into a human readable format.**
- **Integrate such annotated models into the model development and publication workflows.**

# Our solution

- **Encode models in CellML.**
- Use standard CellML Metadata for base annotation with the goal being MIRIAM compliance at the minimum.
- CellML Simulation metadata to annotate specific “*experiments*” with numerical methods data.
- CellML Graphing metadata to collate and extract specific numerical data from multiple “*experiments*”, as well as provide the connection to experimental data.

# CellML

- <http://www.cellml.org>
- An XML-based, open standard.
- Designed for the archiving and exchange of computer-based mathematical models.
- Originally intended for describing models of cellular physiology, but now used to describe a wide variety of mathematical models (<http://www.cellml.org/models/>).
- Primarily provides the means to annotate MathML with relevant data.

# Our solution

- Encode models in CellML.
- **Use standard CellML Metadata for base annotation with the goal being MIRIAM compliance at the minimum.**
- CellML Simulation metadata to annotate specific “*experiments*” with numerical methods data.
- CellML Graphing metadata to collate and extract specific numerical data from multiple “*experiments*”, as well as provide the connection to experimental data.

# CellML Metadata

- **Combination of existing standards plus CellML specific data to fill in the gaps**
  - RDF from the W3C Semantic Web;
  - Dublin Core Metadata Initiative;
  - vCard to describe people;
  - Bibliographic Query Service.
- **CellML Metadata adds biology-related attributes and various missing properties.**

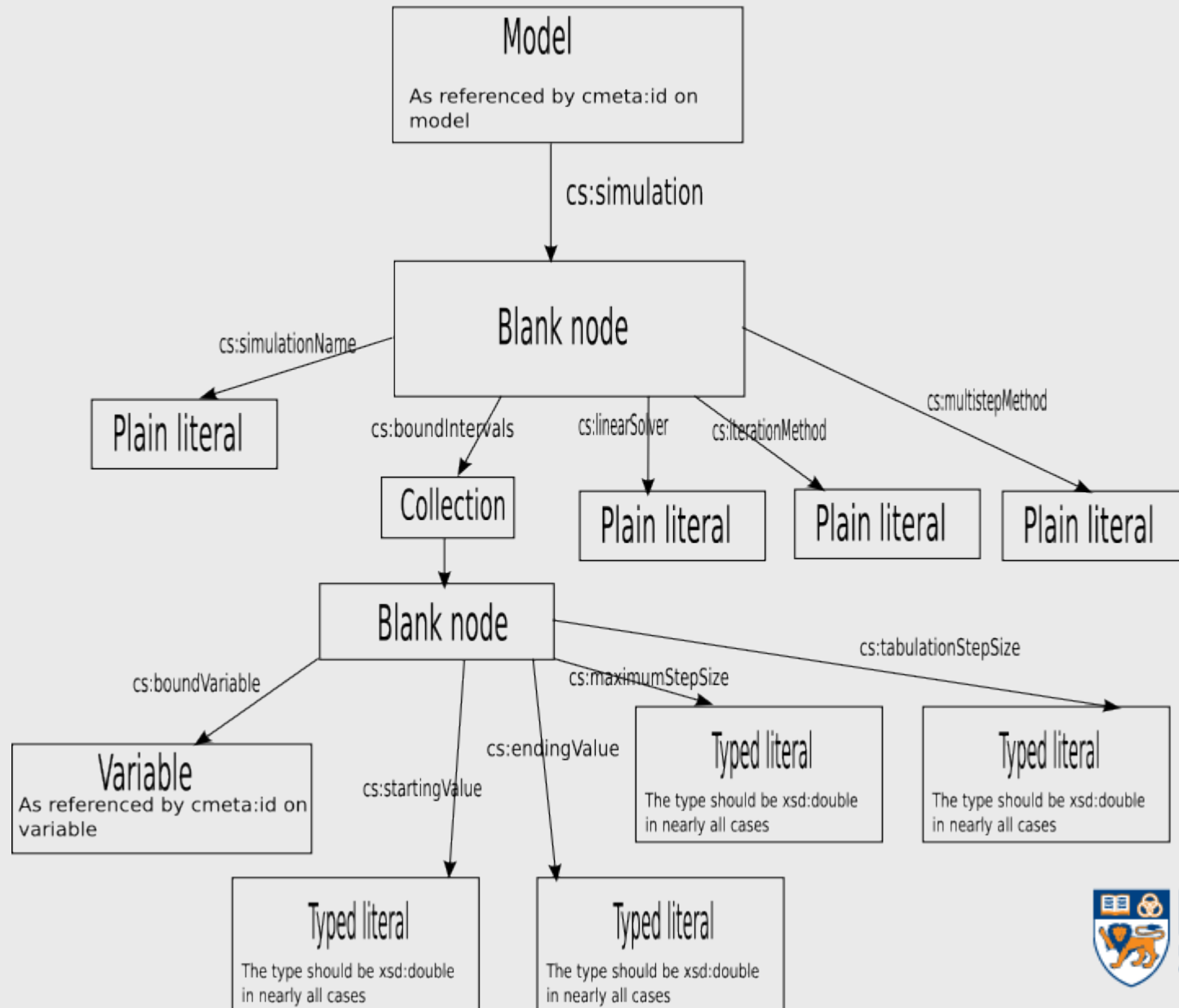
# Our solution

- Encode models in CellML.
- Use standard CellML Metadata for base annotation with the goal being MIRIAM compliance at the minimum.
- **CellML Simulation metadata to annotate specific “*experiments*” with numerical methods data.**
- CellML Graphing metadata to collate and extract specific numerical data from multiple “*experiments*”, as well as provide the connection to experimental data.



Note: Prefix cs: refers to <http://www.cellml.org/metadata/simulation/1.0#>

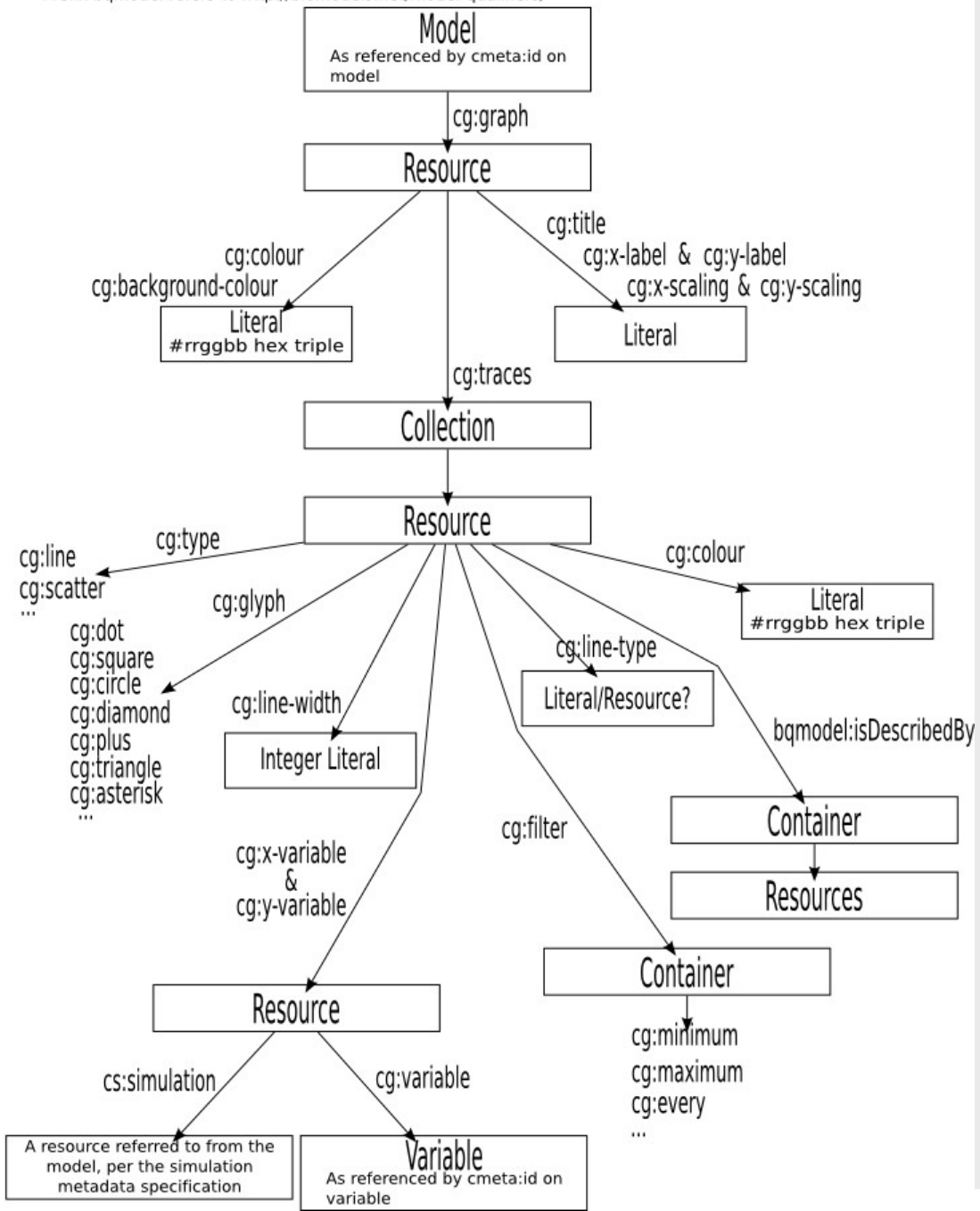
Prefix cmeta: refers to <http://www.cellml.org/metadata/1.0#>



# Our solution

- Encode models in CellML.
- Use standard CellML Metadata for base annotation with the goal being MIRIAM compliance at the minimum.
- CellML Simulation metadata to annotate specific “*experiments*” with numerical methods data.
- **CellML Graphing metadata to collate and extract specific numerical data from multiple “*experiments*”, as well as provide the connection to experimental data.**

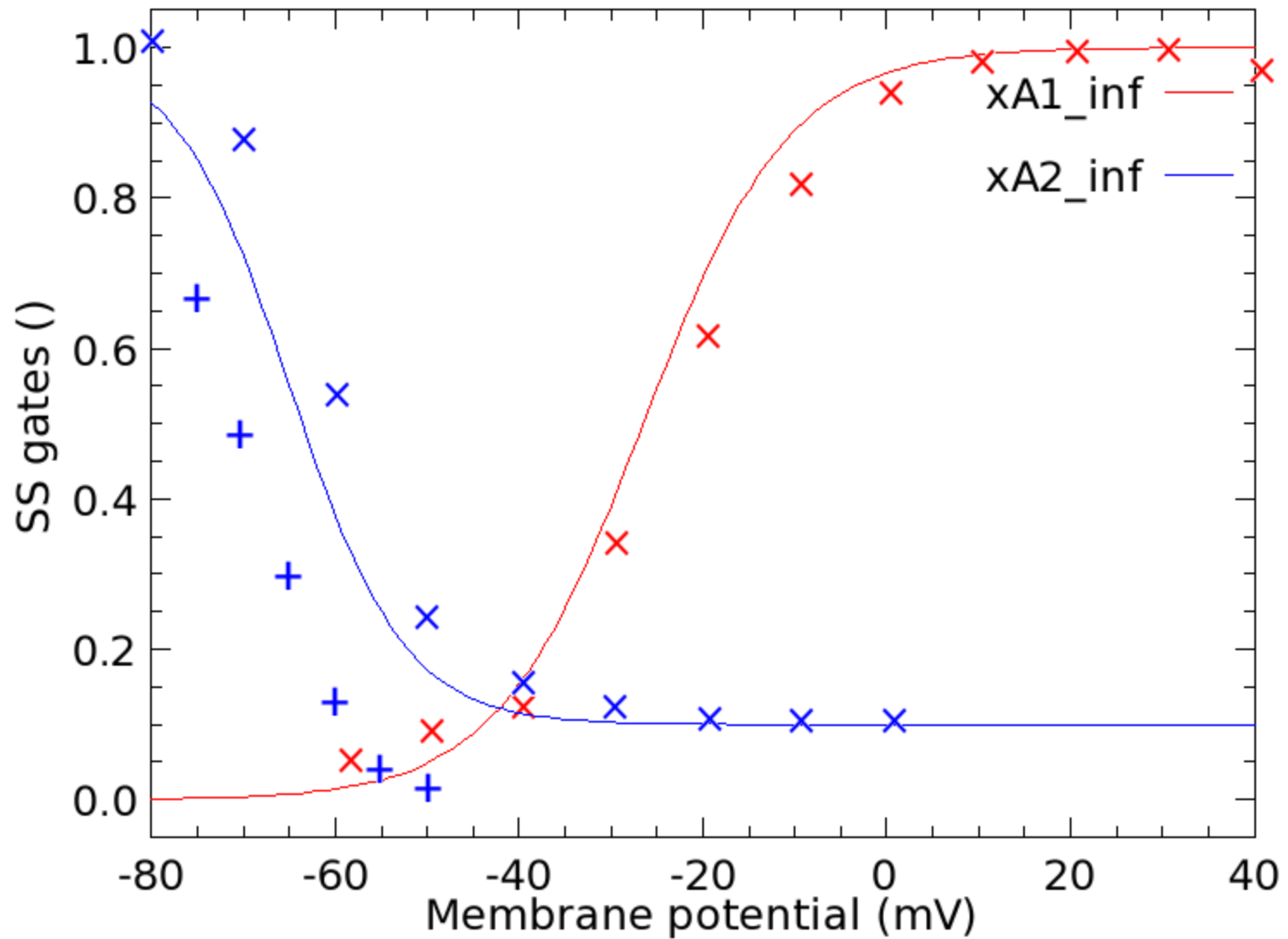
Note: Prefix cg refers to <http://www.cellml.org/metadata/graphs/1.0#>  
 Prefix cmeta refers to <http://www.cellml.org/metadata/1.0#>  
 Prefix cs refers to <http://www.cellml.org/simulation/1.0#>  
 Prefix bqmodel refers to <http://biomodels.net/model-qualifiers/>



# Our solution

- **Encode models in CellML.**
- **Use standard CellML Metadata for base annotation with the goal being MIRIAM compliance at the minimum.**
- **CellML Simulation metadata to annotate specific “*experiments*” with numerical methods data.**
- **CellML Graphing metadata to collate and extract specific numerical data from multiple “*experiments*”, as well as provide the connection to experimental data.**

## Steady-state Gating Kinetics



# Acknowledgments

- **A\*STAR BMRC Grant #05/1/21/19/383.**
- **Alberto Corrias.**
- **Members of the CellML community.**

# Links

- **<http://www.cellml.org>**
- **<http://cellml.sourceforge.net>**
- **<http://www.biomodels.net>**