Merging and Visualisation of SBML Models

Karthik Raman and Nagasuma Chandra

Supercomputer Education and Research Centre

Indian Institute of Science

Bangalore, INDIA

Merging of SBML Models

- Models are available from several sources on the web, e.g. KEGG
- Possible to construct genomic scale models from KEGG
- Possible to simulate – if kinetic laws are embedded
- SBML is structured – affords easy merging !
- KEGG models are easier to merge …

Components of SBML Models

- **Compartments**
- **Specie(s)**
- **Reactions**
- Kinetic Laws
- Parameters

Merging KEGG Models

- KEGG SBML Models are available at

  http://www.systems-biology.org/001/

- Merging involves
  - concatenation of individual component definitions
  - removal of duplicate entries
- Requires
  - Unique specie names
  - Unique reaction ids

} True for KEGG

Visualisation of Models

- Possible – using graph layout software
- XSL transformation to 'dot' format can be done offline too using an XSLT script from *sbml.org*
- *dotty* (*Graphviz* suite) can be used for visualisation – can render even JPEG output
- Also available online at *sbml.org*; online visualisation limited to 100 reactions

Example – *Mycobacterium tuberculosis H37Rv*

- SBML Level 2 Version 1 models available at
  http://www.systems-biology.org/001/SBML.nocd-e.l2v1.20040616.tgz
- Scripts available at (for cygwin)
  http://rishi.serc.iisc.ernet.in/~karthik/sbml/sbmlmerge.htm
- Model validated online (sbml.org)
- 1384 species & 975 reactions
- *dotty* performs 'aesthetic' layout
- Output: very large file

Advantages

- Sub-models can be separately curated and validated
- Merging/Compilation is then easy – and can be automated
- Simulation of large systems can give profound results

Disadvantage

- Rigidity in reaction/species names

Discussion

- Guidelines for reaction IDs/ species names and sub-model creation in general?
- Kinetic parameters and Kinetic laws?
- Incorporation of layout information in SBML?
- Dedicated SBML visualisation software?