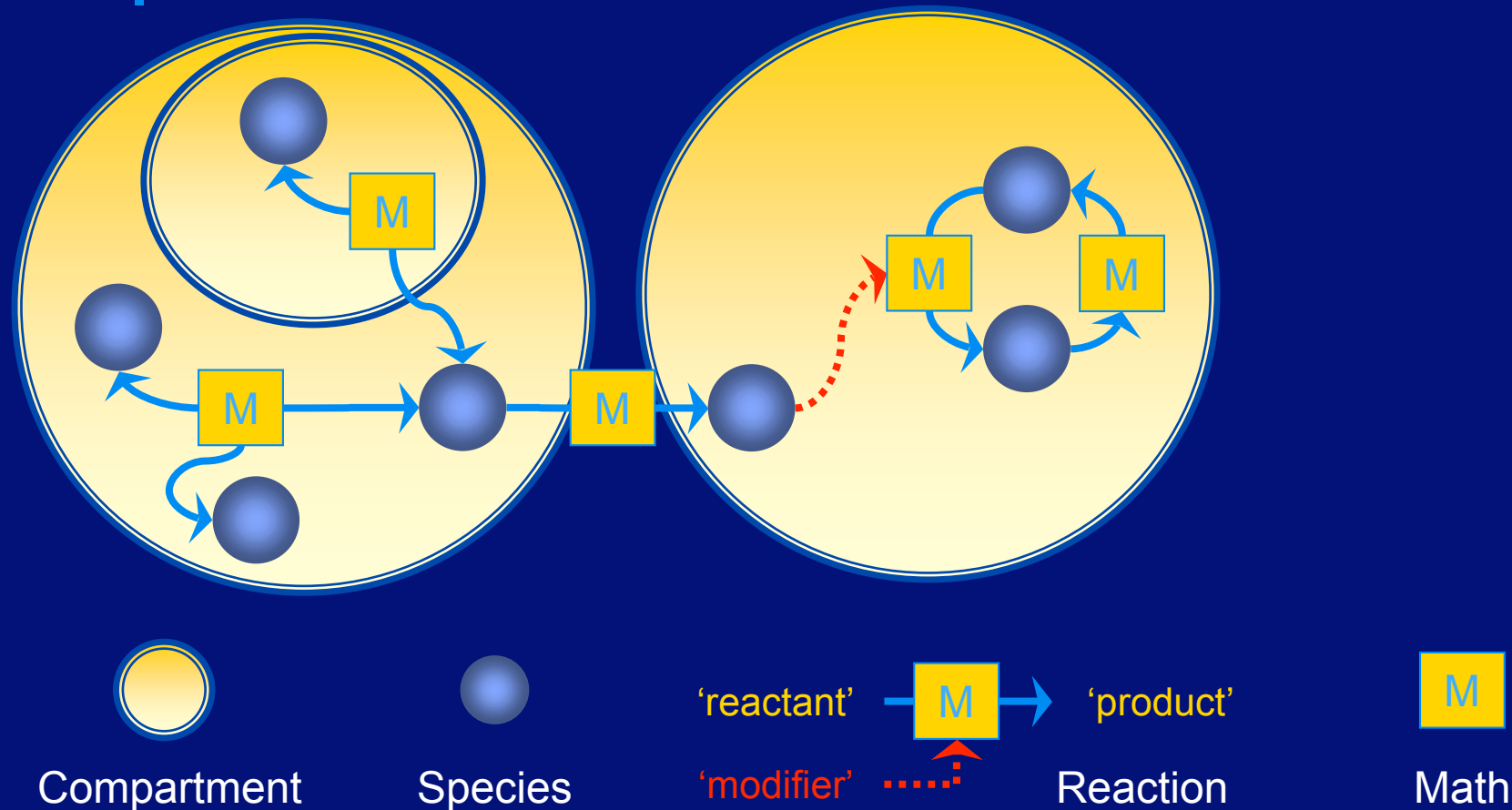


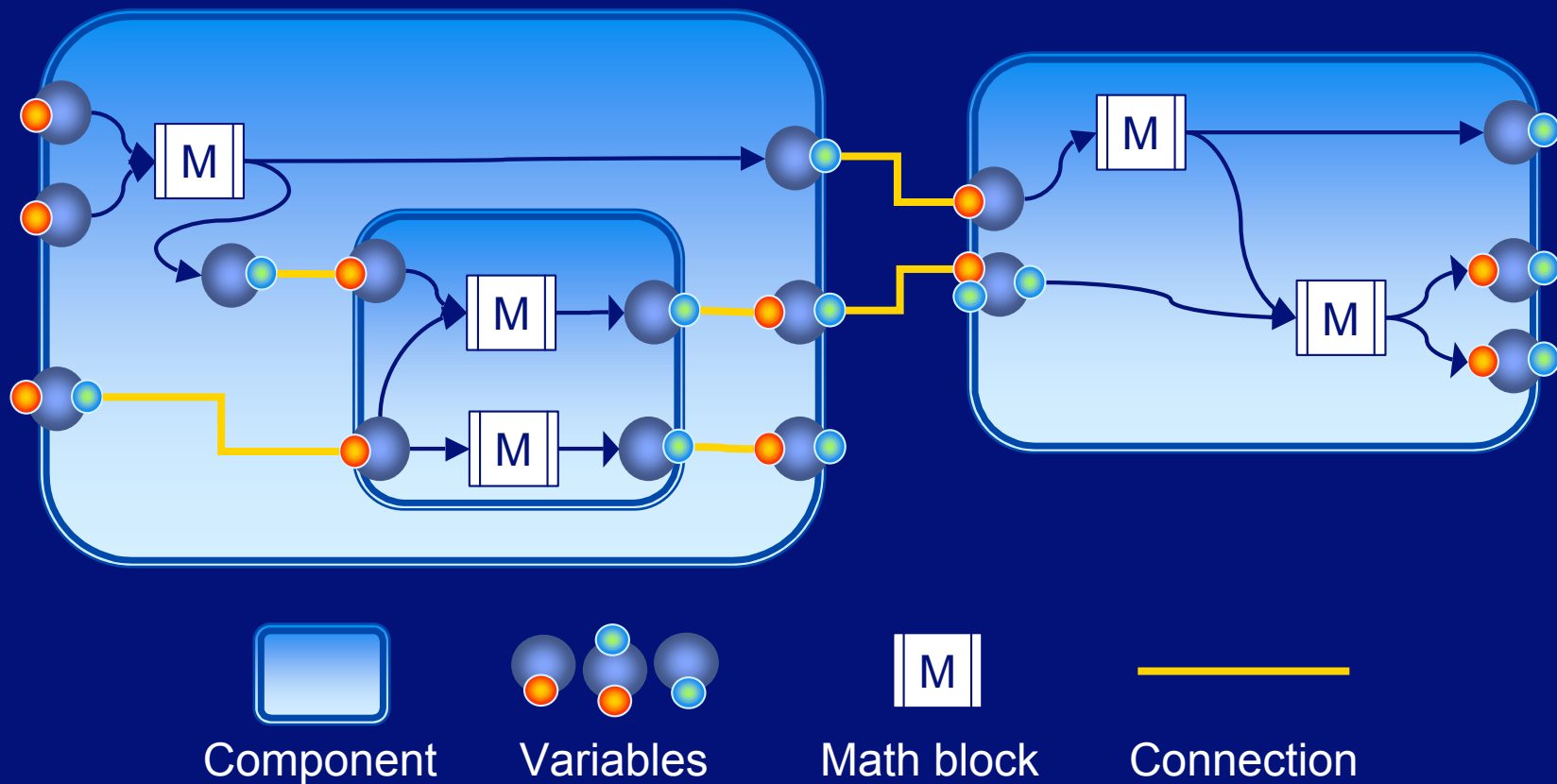
CellML2SBML

Maria J Schilstra
Biological & Neural Computation Group
Science & Technology Research Institute
University of Hertfordshire, Hatfield, UK

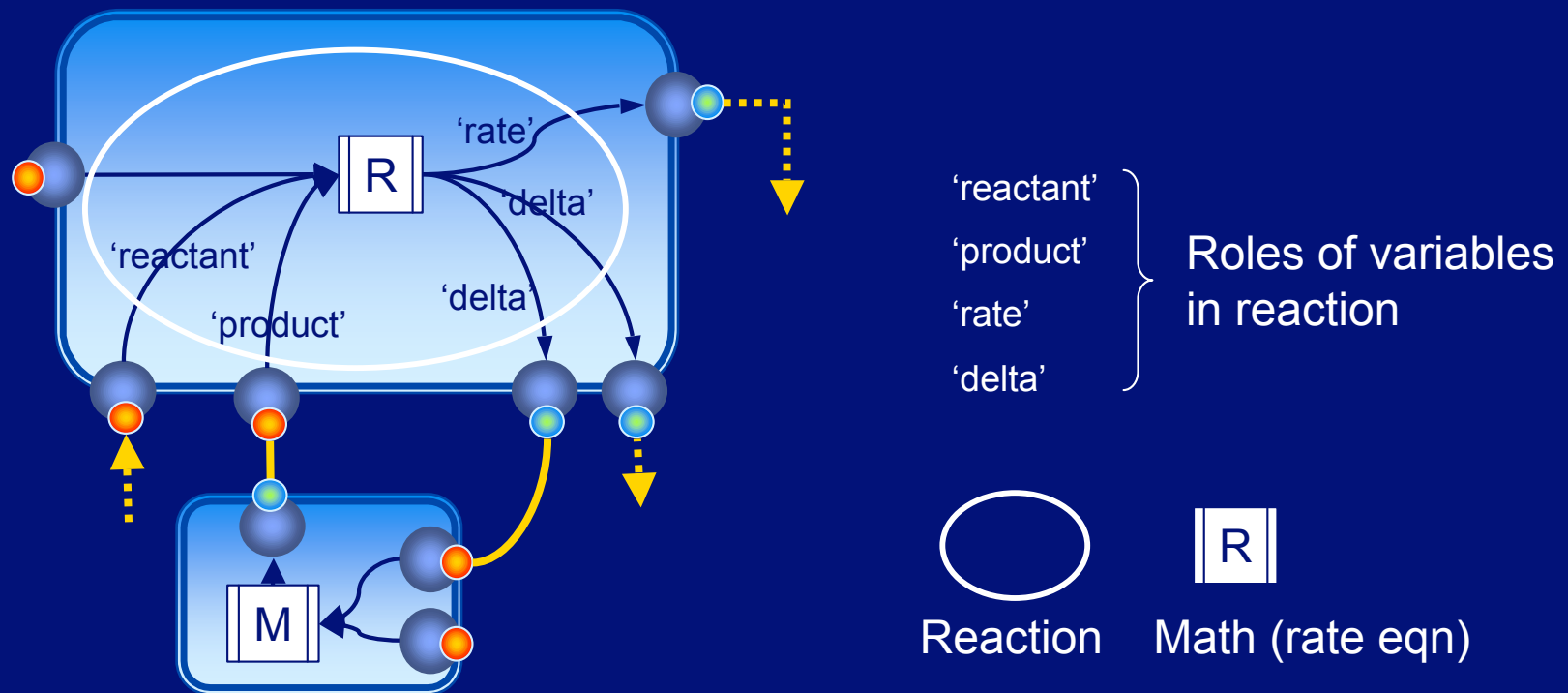
Main functional units in SBML



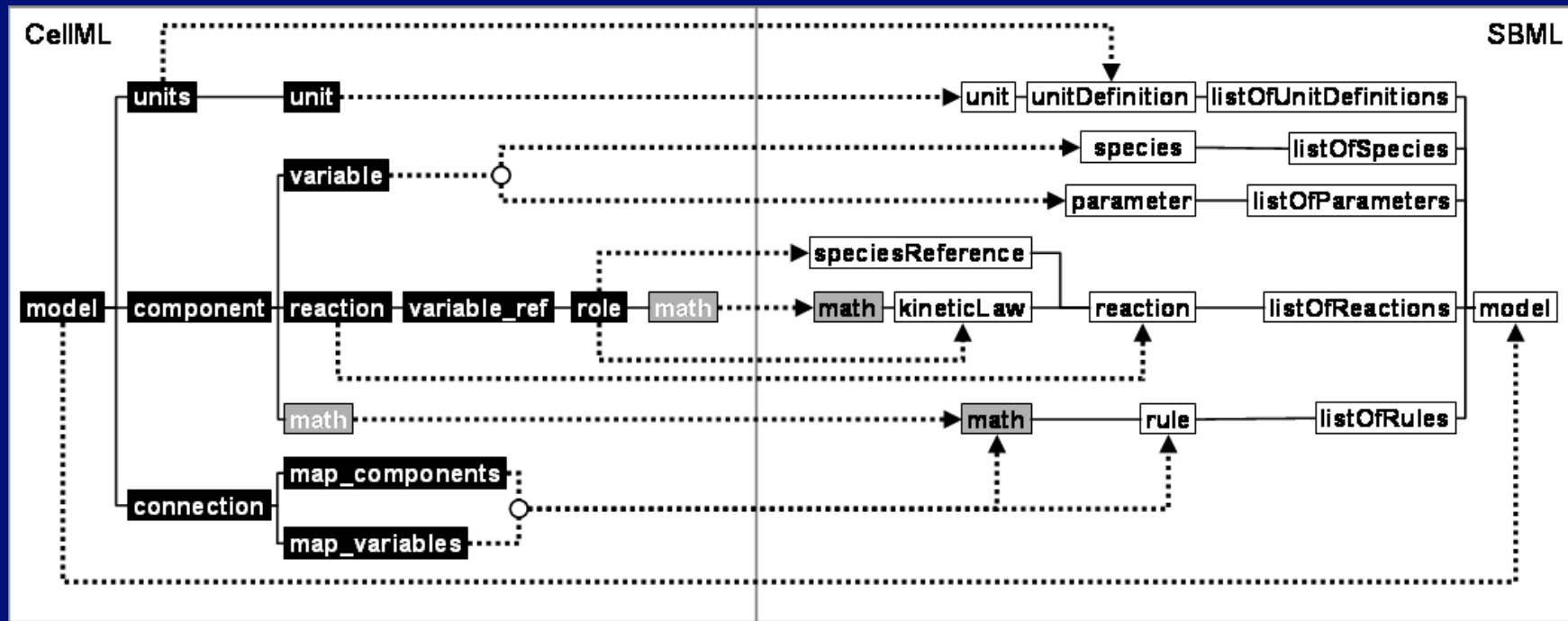
Main functional units in CellML



Reaction structure in CellML



Mapping: one (CellML) to many (SBML)





Tricky bits: units and compartments

□ Units

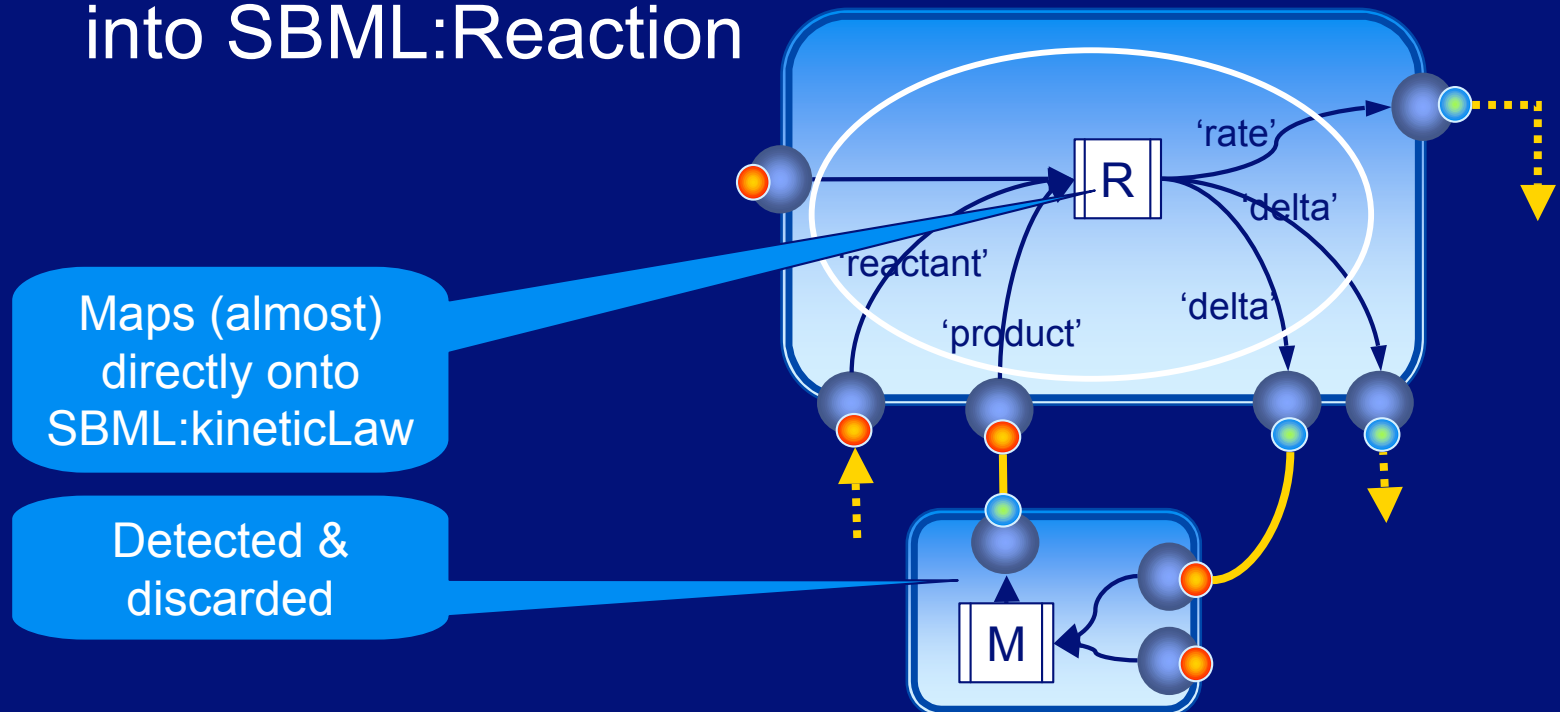
- CellML: unit definitions may be nested
- SBML (L2v1): unit definitions must be a combination of SI units
- Decomposition of nested CellML units required

□ Compartments

- CellML:Group (component grouping) conceptually different from SBML:Compartment (physical containment)
- All elements to single SBML:Compartment

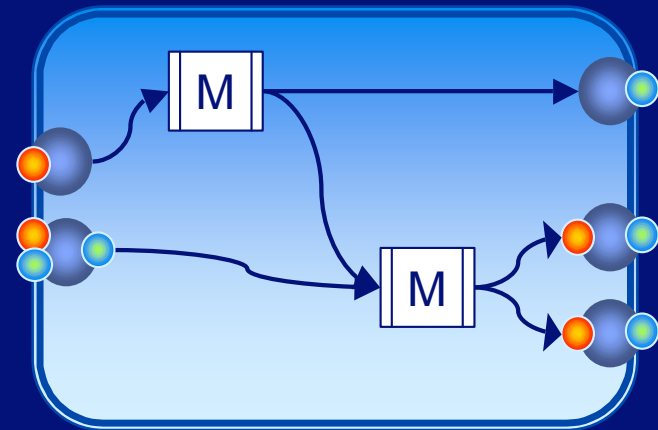
Tricky bits: math and reactions

- Only CellML:Reaction can be converted into SBML:Reaction



Tricky bits: math and reactions

- **All** other math goes to an SBML:Rule descendant
 - This includes ODEs that describe changes in concentrations (e.g. $dS/dt = f(S, P, M)$)





Tricky bits: other complications

- ❑ Extracting SBML substanceUnits and spatialSizeUnits for Species
- ❑ Converting reaction rate equation into units of substance per time
- ❑ Ordering SBML:assignmentRule elements; eliminating cyclic dependencies



Implementation

- 4 consecutive XSLT stylesheets
 - Application note submitted to Bioinformatics – major revision required
 - Challenge from “Referee 2”: “A careful use of `xsl:key` elements to index the various CellML constituents could have helped to reduce that number quite significantly (like to one?)”



Conversion

- CellML to SBML converter
 - 96% of (306) models in CellML repository convertible, minimal loss of information
 - Sometimes minor modification of CellML formulation required (e.g. elimination of new 'base units')
 - CellML models with PDEs or imports not yet convertible