# SBML/SED-ML Whole-Cell Discussion

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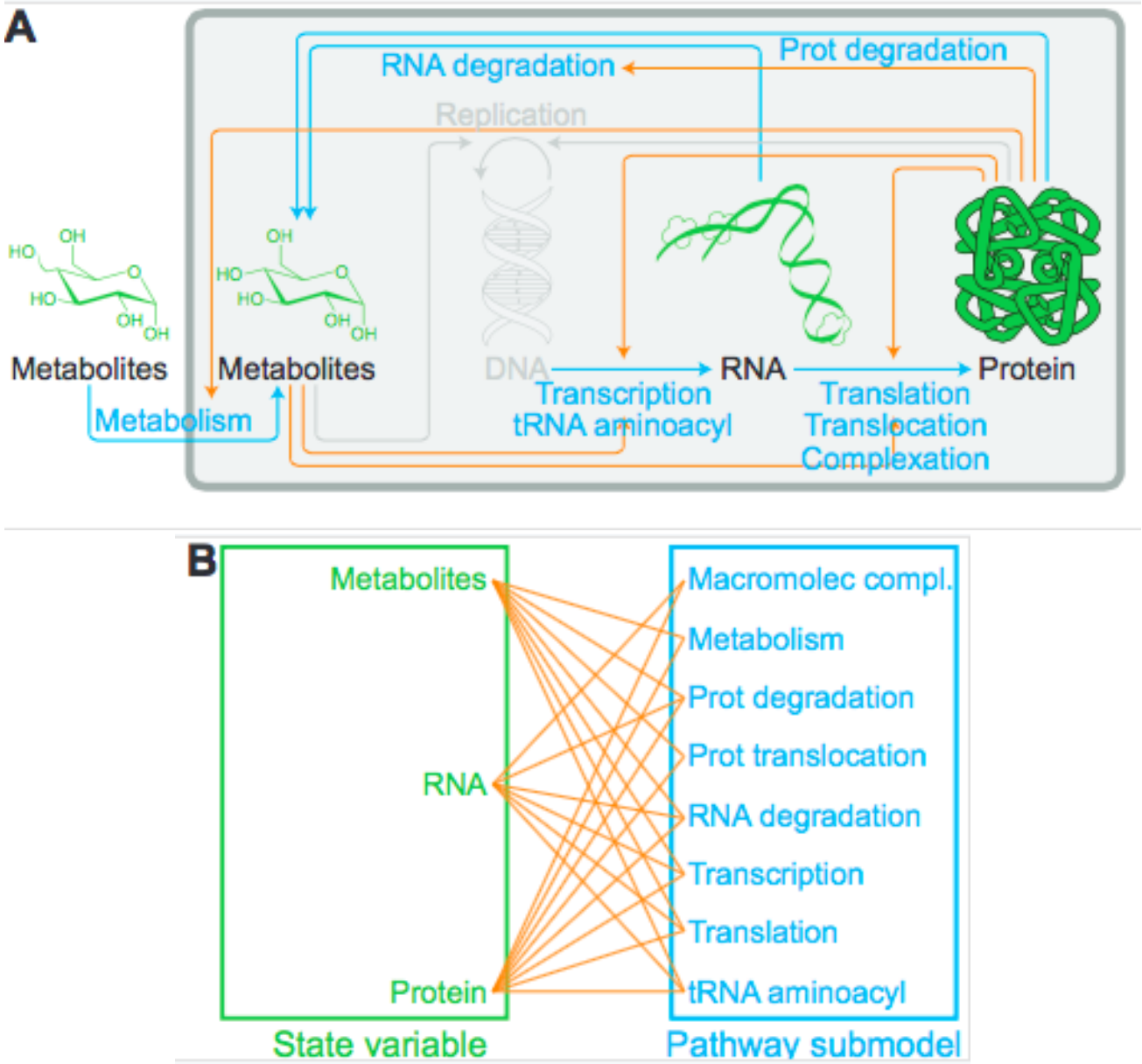
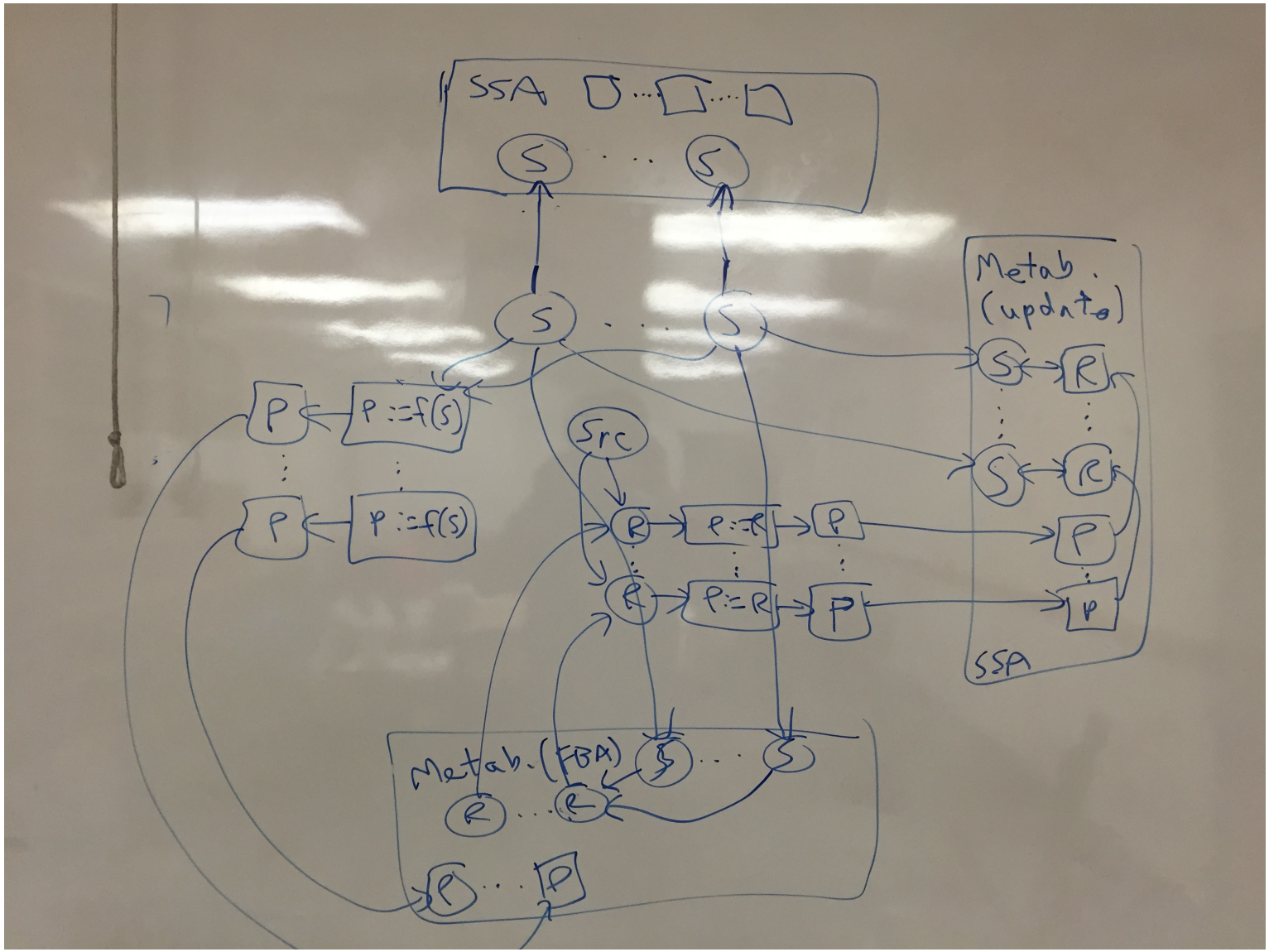
# Whole Cell 2: Reduced Model



# Whole Cell 2: SBML Model



# Discussion Topics

- SBML Packages:
  - Arrays Package
  - Distribution Package
  - MathML Extension Packages
  - Hierarchical Model Composition Package Modification
  - Flux Balance Package (Thursday 1:30)
  - Multi Package (Wednesday 1:30)
  - Dynamic Package (Friday 1:30)
  - Other packages: groups, render, spatial?
- SED-ML Extensions:
  - Interactions with hierarchical models
  - Extending SED-ML Data Generators (Wednesday 3:30)
  - Using data with SED-ML (Friday 3:30)

# Arrays Package

- Enables representation of regular structures such as chromosome and RNA transcripts in the whole cell model.
- Avoids need to replicate attributes saving memory.
- Sparse array representations may save even more memory.
- Arrays can potentially even be used for rule-based modeling.

# Arrays Package: Status

- Specification is complete.
- JSBML implementation is complete including validation and flattening.
- libsbml implementation is complete excluding validation and flattening.
- iBioSim supports the entire package.
- Need a second implementation, Antimony?, BioUML?
- Need a decision about support of dynamic arrays.

# Distribution Package

- Provides support for random distributions and uncertainty.
- Distributions can be univariate or multivariate.
- Leverages UncertML to define them.

# Distribution Package: Status

- Decided to split into two or three packages (univariate, multivariate, and uncertainty?).
- JSBML and libsbml implementation is complete.
- Several tools at least simulate and export a subset of the univariate part (import?).
- What is left to do to approve this package?

# MathML Extension Packages

- quotient, rem, max, min and implies added to L3V2 core.
- The rest of MathML divided into several packages.
  - stats - mean, variance, mode, sdev, median, moment, momentabout
  - arrays - vector, selector
  - linear algebra - matrix, matrixrow, inverse, transpose, determinant, vectorproduct, scalarproduct, outerproduct
  - sum/product - sum, product, lowlimit, uplimit, tendsto
  - content - interval
  - logic - condition, forall, exists, equivalent
  - arithmetic - lcm, gcd, factorof, approx
  - sets - emptyset, set, list, union, intersect, in, notin, subset, notsubset, prsubset, notprsubset, setdiff, card, cartesian
  - complex - conjugate, arg, real, imaginary, complexes, imaginaryi
  - function composition - compose, domain, codomain, domainofapplication, image
  - calculus - int, diff, partialdiff, curl, divergence, laplacian, grad
  - others - ident, naturalnumbers, primes, eulergamma

# MathML Extension Packages: Status

- Proposal approved?
- Draft specifications exist?
- Implementation in libSBML?, JSBML?

# Hierarchical Model Composition Package

- Enables composition of SubModels.
- SubModels can be modified with Replacements and Deletions.
- Targets of Replacements/Deletions can optionally be identified with Ports.

# Hierarchical Model Composition Package: Ports Reboot

- Problems:
  - Ports were a highly controversial, and do add some additional complexity.
  - Replacements/ReplacedBys challenging to use due to be associated with all SBase objects.
- SBOL solution:
  - Instantiations in SBOL have Access/Direction attribute.
  - MapsTos associated with instantiations and reference a local and remote object that are considered to be the same object.
  - MapsTos have Restriction type to indicate where to get attributes (useLocal, useRemote, verifyIdentical, merge).

# SED-ML Whole-Cell Modeling Needs

- A better means for communication between submodels especially to support dynamic FBA.
- A better way of dealing with SBML+Comp (hierarchical) models.