Replication Initiation

Harold Gómez
Jens Hahn
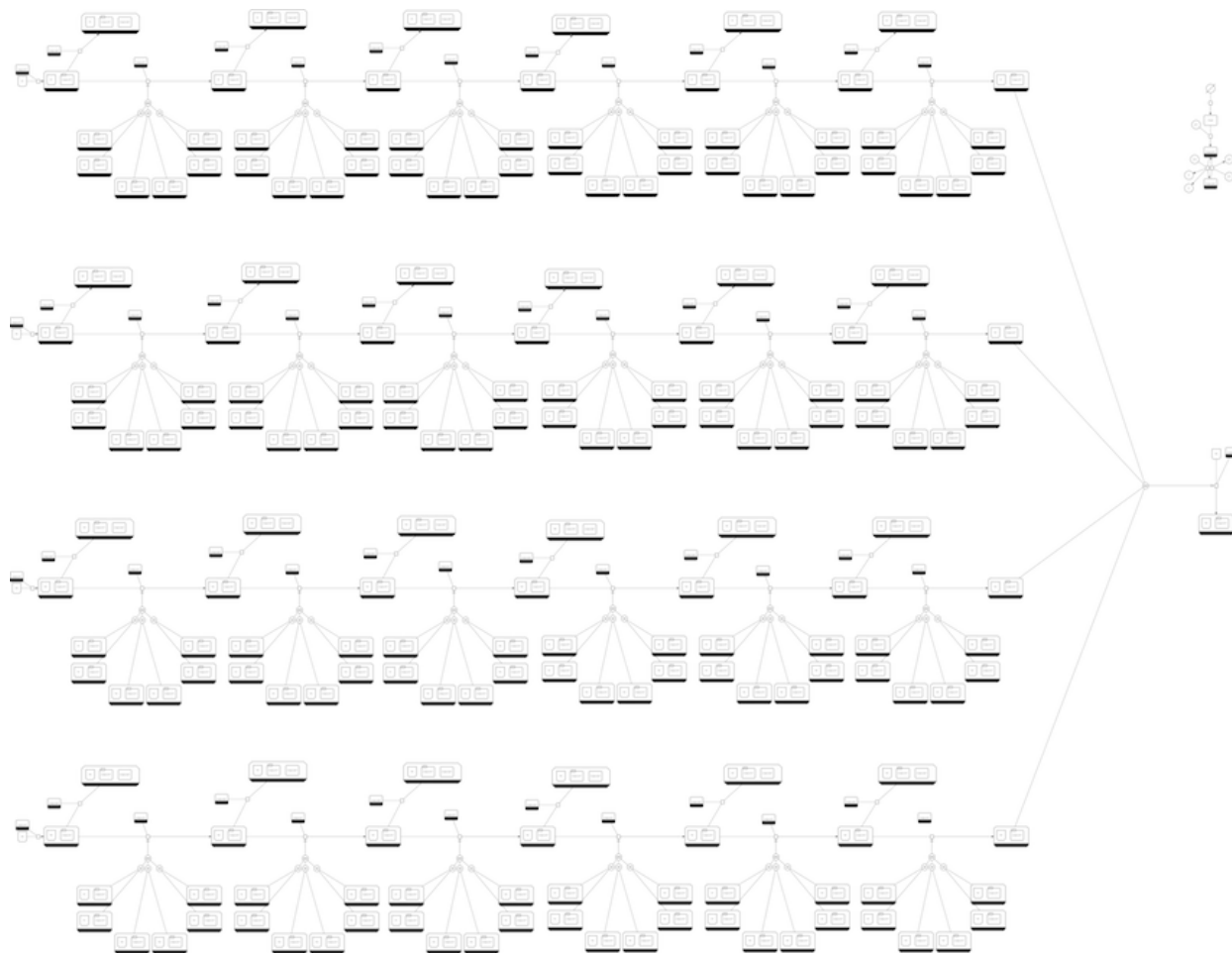Nikita Mandrik
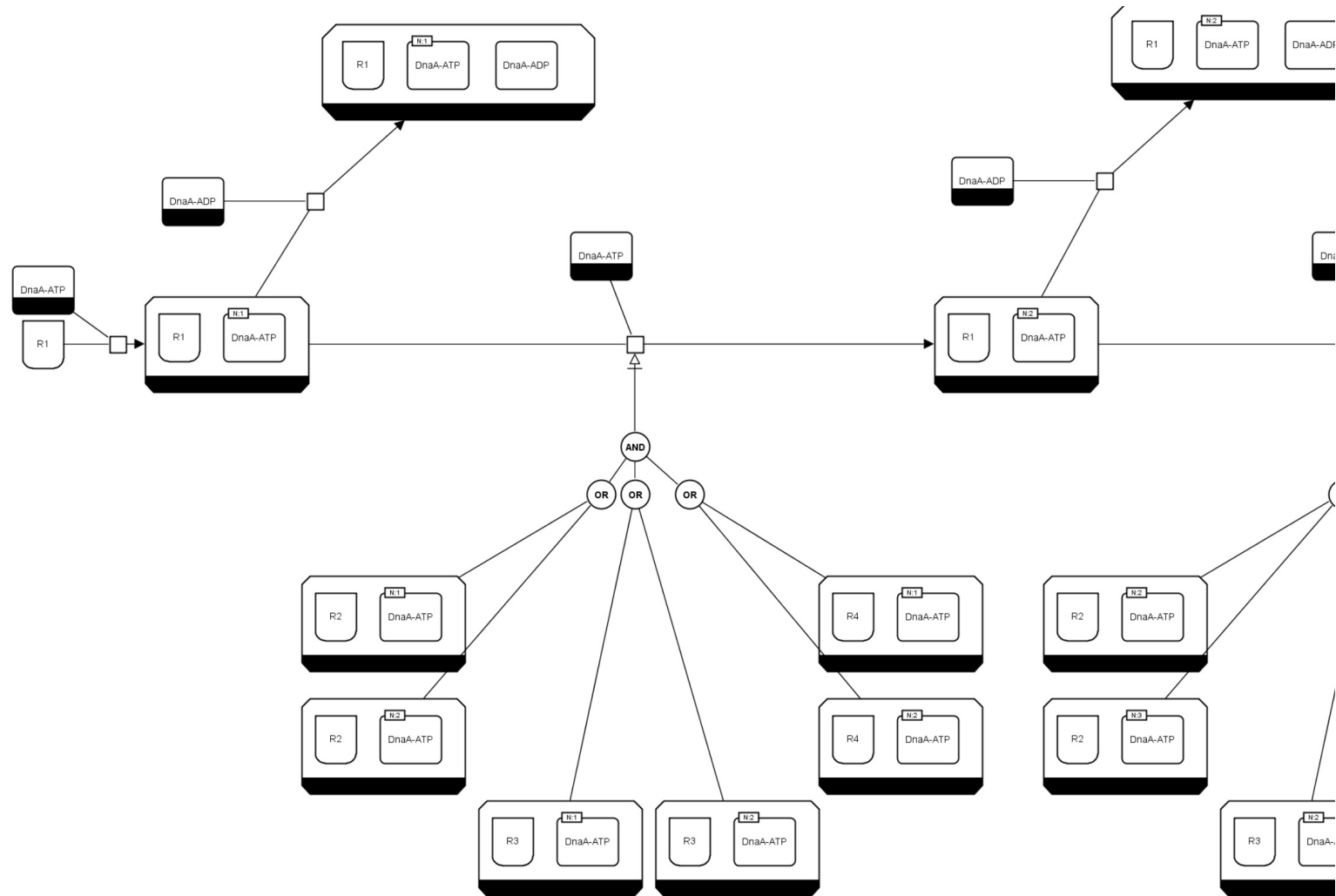Martin Scharm
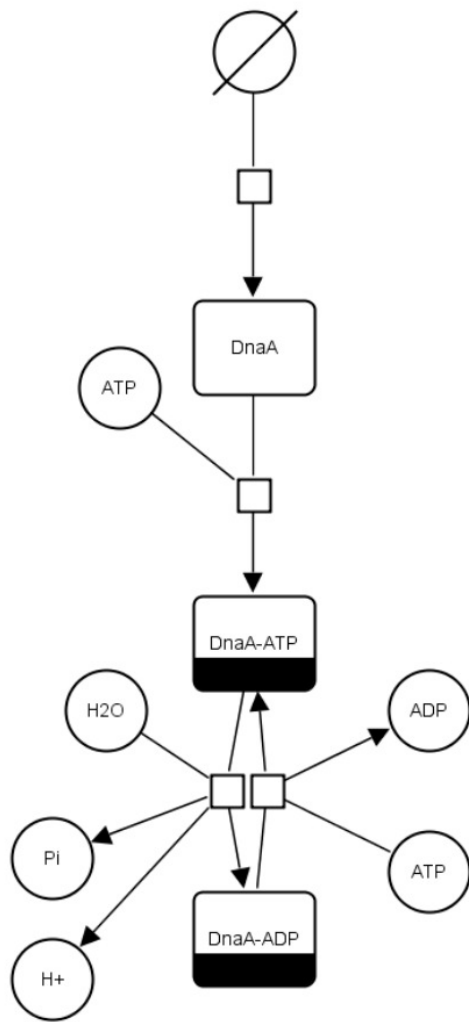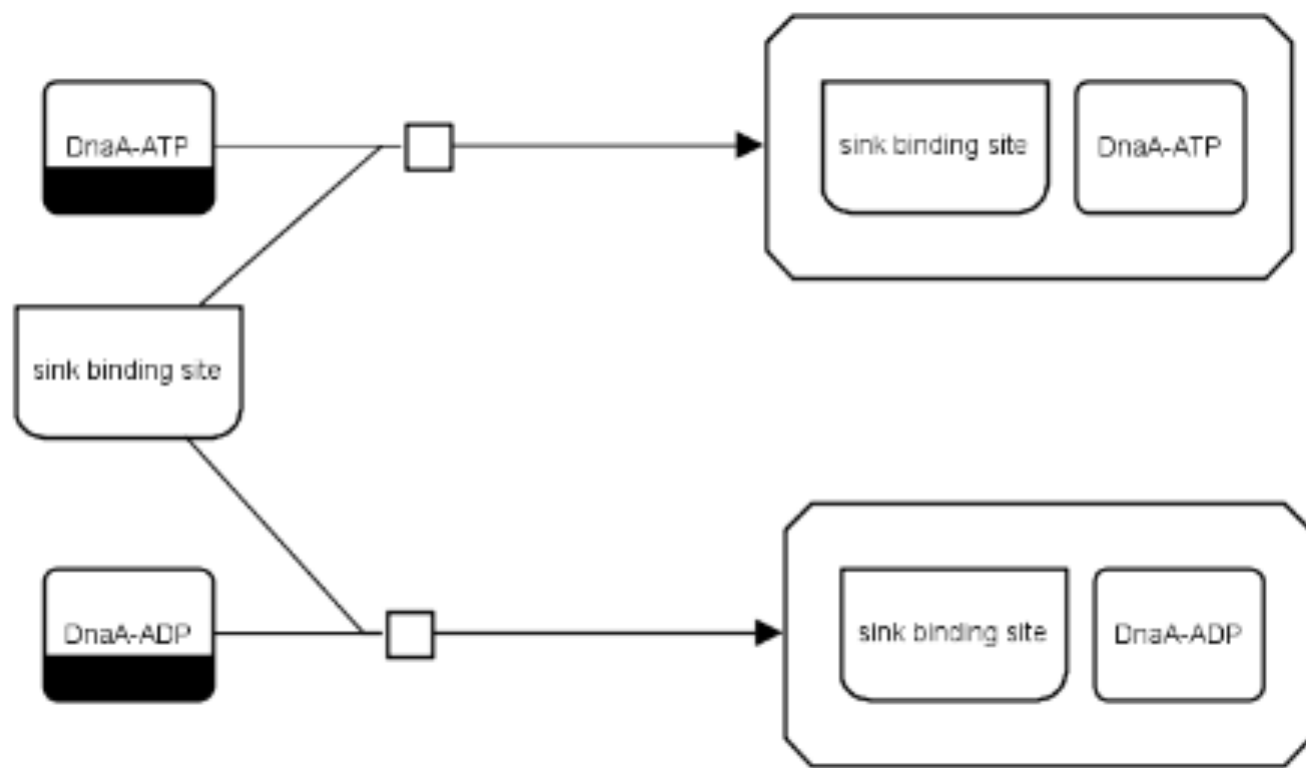Florian Wendland

tutor: Mike Hucka

Say 'Hello'!

SBGN: Statistics

4480 XML nodes, defining 1034 glyphs

SBGN: Details

- Reactions with logical conditions on activation

- Used VANTED to draw SBGN
- Problems encountered:
    - Too small for scripting, but too large for clicking
    - Exporting when drawing contains non-SBGN elements
    - Double ids
    - Problems with exporting SBGN-ML

Modelling

Submodule	Antimony, exported to SBML, annotated using SBMLeditor			
	implemented	annotated	validated	tested
Activation	x	x	x	(x)
Reactivation	x	x	x	
Dissociation	x	x	x	(x)
Displacement	x		x	
Binding and polymerization				
"Glue" module				

Modelling: Details

- No reactions – only arithmetics and conditions
  - ➡ SBML Events, InitialAssigments, "Rules", Functions

- Used BioUML, writing model in Antimony syntax
- Problems encountered:
  - Never forget to 'Apply' when editing in BioUML!

Modeling: Statistics

Submodule	Nodes	Species	Parameters	Events	Functions
RI_reactivation_sbml_annotated.xml	293	4	9	2	3
RI_dissociation_sbml_annotated.xml	1108	16	12	14	0
RI_displacing_sbml.xml	1003	4	88	13	5
RI_activation_sbml_annotated.xml	211	3	5	2	1

Modelling: Easy Things

- Mathematics were easy for this module
- SBML model easy once Matlab was understood
  - But …
- Annotations
  - Thanks to Jonathan's supplementary material
- Feature requests for BioUML

Modelling: "Fiddly" Things (time sinks)

- Software tool issues, such as editor sync/save
- Copy/pasting model parts to repeat structures (e.g., lot of parameters repeated)
- SBML Events: difficult to create in correct order
- Integration team instructions changed ⇒ had to copy files to different places, etc.

Modelling: Challenges

- Chromosome binding site representation
- Expressing "if" conditions in SBML
- Understanding of Matlab code
- Stochastic selection of binding sites

Modelling: Still To Do

- Create "Glue" submodule to connect others
- Address model of binding and polymerization
  - cooperativity → many conditions
- Create tests for all submodels
- Do global integration with rest of whole cell model
  - communicating requirements
  - synchronizing chromosome access

Thanks

Mike

Dagmar & Falk

Jonathan