

2023 HARMONY breakout session

"Rule-based modeling and SBML Multi Package"

Session information:

1. Time: Tue, April 25, 2023, seattle local time 11:00 - 12:30 PDT/UTC-7

Room: 403

Zoom:

Track C [zoom link](#)

Meeting ID: 924 1346 1326

Passcode: 424005

Content: flexible and I may start with reviewing the general structure of the current multi package more detailed than my lightning talk. Welcome any suggestions.

Thank everyone for joining the session. It will great for everyone to add your name and contact to [Session 1 \(4/25/2023\)](#). Also add things of your questions/comments in the discussion to the minutes.

2. We will have session 2 and I will walk through some examples. Bring any questions you have to the session. If necessary, we could add more sessions.

Time: Wed, April 26, 2023, seattle local time 11:00 - 12:30 PDT/UTC-7

Room: 403

Zoom: same as Tue

Related resources:

1. HARMONY 2023:
<https://co.mbine.org/events/>
2. Link to this google doc:
https://docs.google.com/document/d/1cWrHW9h58THla6NGdTCNCOs5Jw_tPjZuafoajhlpSQ/edit?usp=sharing
Or <https://tinyurl.com/mrynwzzv>
3. SBML Multi Package Spec, V1R2:
<https://sbml.org/documents/specifications/level-3/version-1/multi/>
4. Simmune:
<https://www.niaid.nih.gov/research/simmune-project>
5. BioNetGen:
<https://bionetgen.org/>
6. Kappa
7. Biochemical space <https://github.com/sybila/eBCSgen/wiki>
8. Morpheus:
<https://morpheus.gitlab.io/>

Related publications:

1. [Zhang, F., and Meier-Schellersheim, M. \(2020\) Multistate, Multicomponent and Multicompartment Species Package for SBML Level 3. Retrieved from COMBINE. https://identifiers.org/combine.specifications/sbml.level-3.version-1.multi.version-1.release-2](https://identifiers.org/combine.specifications/sbml.level-3.version-1.multi.version-1.release-2)
- 2.

Discussion minutes:

Session 1 (4/25/2023):

Participants:

- Fengkai Zhang, NIH, zhangfen@nih.gov
- Michael Blinov
- Martin Meier-Schellersheim
- Leonard Haris
- Matej Trojak
- T.J Sego
- Daniel Weindl
- Branislav Brozmann
-
-
-

Items discussed or reviewed:

- Review of current Multi package, mainly UML diagrams
 - Components, speciesType and instances
 - Feature type, values and feature
- Transportation of species? Multi “can” handle by defining different levels of compartment “types”. Need real change of “locations/compartments”?
- Change of compartment of species?
- Conversion between species types and compartment types (for tissue simulations)
- Port in BioNetGen and Simmune, but not in current Multi yet
- Why species type and compartment type are defined in different ways: SpeciesType class and isType boolean attribute
- Also touch “spatially resolved” simulation, how to populate different concentrations in different regions of a cell.

Session 2 (4/26/2023)

Participants:

- Fengkai Zhang
- Michael Blinov

- Daniel Weindl
- Branislav Brozmann
-

Items:

- Simmune support to SBML: export Ecad model and import the sbml model to Simmune
- Clarify the validation functions in SBML core and SBML Multi package
- Rule-based modeling tools: recreate Simmune Ecad model in vcell (partially successful, cis and trans configuration in simmune not available in vcell yet)