Overview of data (types) in the Matlab model

molecules (species in SBML)

molecule	attributes
Transcriptional Units	ro rw
RNAs	ro rw
Protein Monomers	ro rw
Protein Complexes	ro rw
Metabolites	ro rw req roreq

ro read only rw read/write req requirement

roreq read only + requirement

parameters

- fixed for the simulation
- see also

https://simtk.org/project/xml/downloads.xml?group_id=714 https://simtk.org/frs/download.php?file_id=3757

variables (state)

• 83 states

states *MetabolicReaction*, *Metabolite*, *ProteinComplex*, *ProteinMonomer*, *Rna*, *Stimulus* are separately described in more detail

- changed (written) during simulation by at least one process
- see also

https://simtk.org/project/xml/downloads.xml?group_id=714 https://simtk.org/frs/download.php?file_id=3759 https://simtk.org/frs/download.php?file_id=3760

Naming scheme

molecules (species in SBML)

 connect the MoleculeName by double underscores ('___') with a CompartmentName and/or a MoleculeState

```
MoleculeName__CompartmentName__MoleculeState
MoleculeName__CompartmentName
MoleculeName__MoleculeState
```

- list of CompartmentNames
 - o m (membrane)
 - o e (extracellular)

The cytosol ('c') can be ignored. If no CompartmentName is used it is assumed the molecule is in the cytosol.

- list of possible MoleculeStates
 - o aminoacylated
 - o bound
 - o damaged
 - o folded
 - o inactivated
 - intergenic
 - o mature
 - o misfolded
 - nascent
 - o processed
 - $\circ \quad processed I$
 - o processedII
 - o signalsequence

from StatePropertyRowCollDs.xlsx

(https://simtk.org/frs/download.php?file_id=3760)

The state 'activated' can be ignored. If no MoleculeState is used it is assumed the molecule is in the state 'activated'.

If you have to use other states please don't use a dash ('-') in the state name. This might cause problems in the further processing of the files.

- examples: ATP, ATP__e, MG_001_MONOMER__inactivated, MG_001_MONOMER_ m__inactivated
- MoleculeNames can be found in five lists (files) on GitHub https://github.com/whole-cell-tutors/wholecell/tree/master/wholecell-integration
 - Molecules_names_TUs.csv

- Molecules names RNAs.csv
- o Molecules names Monomers.csv
- Molecules_names_Complex.csv
- Molecules names Metabolites.csv
- make a local copy of these files for each process and update the files example: Molecules_names_Metabolites_translation.csv

put an 'x' in the respective column you can remove lines from these files and just keep the ones for your process

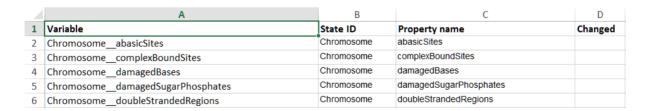
parameters

If a model needs a parameter the team who is implementing this model has to take care of this parameter (the Integration team won't provide it, sorry!).

variables (state)

- connect the StateID by double underscores ('___') with the PropertyName
 StateID__PropertyName
- example: StateID Metabolite with PropertyName counts -> variable Metabolite__counts
- VariableNames can be found in a list (file) on GitHub
 https://github.com/whole-cell-tutors/wholecell/tree/master/wholecell-integration
 - Variables.csv
- make a local copy of this file for each process and update the file example: Variables_translation.csv

you can remove lines from this file and just keep the ones the process changes (writes) or you put an 'x' in the fourth column (*Changed*)



requirement parameters

 make sure your model has a requirement parameter for each molecule (species) that is a requirement

- the requirement itself has to be calculated by the model (the Integration team won't do it for you, sorry!)
- connect the name you have made up for a molecule by two underscores ('__') with the text *requirement*
- example: ATP__requirement or ATP__e__requirement