

MERGED

Collapse All

Readme

2021-11-23 15:20

Independent Section

Contains tests that are independent of the class of modeled organism, a model's complexity or

Consistency

Stoichiometric Consistency

Stoichiometric inconsistency violates universal constraints. 1. Molecular masses are always positive, and 2. On each side of a reaction the mass is conserved. A single incorrectly defined reaction can lead to stoichiometric inconsistency in the model, and consequently to unconserved metabolites. Similar to insufficient constraints this may give rise to cycles which either produce or consume nothing or consume mass from the model. Implementation: This test uses an implementation of the algorithm presented in section 3.1 by Gevorgyan, A., M. G. P. and D. A. Fell. "Detection of Stoichiometric Inconsistency in Biomolecular Models." Bioinformatics 24, no. 19 (2008): 2245. doi: 10.1093/bioinformatics/btn425

This model's stoichiometry inconsistent

false

Mass Balance

This will exclude biomass, exchange and demand reactions as they are unbalanced by definition. It will also fail reactions where at least one metabolite does not have a formula defined. In steady state, for each metabolite the sum of influx equals the sum of efflux. Hence the masses of both sides of any model reaction have to be equal. Reactions where at least one metabolite does not have a formula are not considered to be balanced though the remaining metabolites participating in the reaction might be. Implementation: For each reaction that isn't a boundary or biomass reaction check if each metabolite has a non-zero elements attribute and calculate if the overall element balance of reactants and products is equal to zero.

A total of 1255 (46.72%) reactions are mass unbalanced with at least one of the metabolites not having a formula. The overall mass not equal to 0: r_4342, r_4343, r_4349, r_4352, ...

Specific Section

Covers general statistics and specific aspects of a metabolic network that are not universally

SBML

SBML Level and Version

Errored



This test reports if the model file is represented in the latest edition (level) of the Systems Biology Markup Language (SBML) which is Level 3, and at least version 1. Implementation: The level and version are parsed directly from the SBML document.

null

FBC enabled

Errored



The Flux Balance Constraints (FBC) Package extends SBML with structured and semantic descriptions for domain-specific model components such as flux bounds, multiple linear objective functions, gene-protein-reaction associations, metabolite chemical formulas, charge and related annotations which are relevant for parameterized GEMs and FBA models. The SBML and constraint-based modeling communities collaboratively develop this package and update it based on user input. Implementation: Parse the state of the FBC plugin from the SBML document.

null

Basic Information

Model Identifier

MERGED



The MIRIAM guidelines require a model to be identified via an ID. Further, the ID will be displayed on the memote snapshot report, which helps to

MERGED

Collapse All

Readme

2021-11-23 15:20

Charge Balance

This will exclude biomass, exchange and demand as they are unbalanced by definition. It will also fail reactions where at least one metabolite does not have a charge defined. In steady state, for each metabolite the sum of influx equals the sum of efflux. Hence the net change of both sides of any model reaction have to be equal. Reactions where at least one metabolite does not have a charge are not considered to be balanced, even though the remaining metabolites participating in the reaction are balanced. Implementation: For each reaction that isn't a biomass or exchange reaction check if each metabolite has a charge attribute and if so calculate if the overall sum of charges of reactants and products is equal to zero.

A total of 686 (25.54%) reactions are charge unbalanced with at least one of the metabolites not having a charge. The overall charge not equal to 0: r_4342, r_4344, r_4352, r_0477, r_0490, r_0502, r_0503, r_0512, r_0525, r_0530, r_0531, r_0534, r_0535, ...

```
["r_4342", "r_4344", "r_4352", "r_0477", "r_0490", "r_0502", "r_0503", "r_0512", "r_0525", "r_0530", "r_0531", "r_0534", "r_0535"]
```

Metabolite Connectivity

Disconnected metabolites are not part of any reaction in the model. They are most likely left-over from the reconstruction process, but may also point to network and knowledge gaps. Implementation: Check for any metabolites in the cobra.Model object with empty reaction attribute.

A total of 1 (0.04%) metabolites are not associated with any reaction of the model: m_0035

```
["m_0035"]
```

Unbounded Flux In Default Medium

A large fraction of model reactions able to carry unbounded flux under default conditions indicates problems with reaction directionality, missing cofactors, incorrect stoichiometry, transport reactions and more. Implementation: When changing the default constraints run flux variability analysis. From the FVA results identify those reactions that have a flux equal to the model's maximal or minimal flux.

A fraction of 14.32% of the non-blocked reactions

attribute, this value is parsed from the "id" attribute of the <model> tag in the SBML file e.g. <model fbc:strict="true" id="iJO1366">.

The model ID is MERGED

```
"MERGED"
```

Total Metabolites

2,338

To be useful a metabolic model should consist at least of a few metabolites that are converted by reactions. This test simply checks if there are more than zero metabolites. Implementation: Check if the cobra.Model object has non-empty "metabolites" attribute, this list is populated from the list of sbml:listOfSpecies which should contain at least one sbml:species.

2338 metabolites are defined in the model.

```
["m_0001", "m_0002", "m_0003", "m_0004", "m_0005", "m_0006", "m_0007", "m_0008", "m_0009", "m_0010", "m_0011", "m_0012", "m_0013", "m_0014", "m_0015", "m_0016", "m_0017", "m_0018", "m_0019", "m_0020", "m_0021", "m_0022", "m_0023", "m_0024", "m_0025", "m_0026", "m_0027", "m_0028", "m_0029", "m_0030", "m_0031", "m_0032", "m_0033", "m_0034", "m_0035", "m_0036", "m_0037", "m_0038", "m_0039", "m_0040", "m_0041", "m_0042", "m_0043", "m_0044", "m_0045", "m_0046", "m_0047", "m_0048", "m_0049", "m_0050", "m_0051", "m_0052", "m_0053", "m_0054", "m_0055", "m_0056", "m_0057", "m_0058", "m_0059", "m_0060", "m_0061", "m_0062", "m_0063", "m_0064", "m_0065", "m_0066", "m_0067", "m_0068", "m_0069", "m_0070", "m_0071", "m_0072", "m_0073", "m_0074", "m_0075", "m_0076", "m_0077", "m_0078", "m_0079", "m_0080", "m_0081", "m_0082", "m_0083", "m_0084", "m_0085", "m_0086", "m_0087", "m_0088", "m_0089", "m_0090", "m_0091", "m_0092", "m_0093", "m_0094", "m_0095", "m_0096", "m_0097", "m_0098", "m_0099", "m_0100", "m_0101", "m_0102", "m_0103", "m_0104", "m_0105", "m_0106", "m_0107", "m_0108", "m_0109", "m_0110", "m_0111", "m_0112", "m_0113", "m_0114", "m_0115", "m_0116", "m_0117", "m_0118", "m_0119", "m_0120", "m_0121", "m_0122", "m_0123", "m_0124", "m_0125", "m_0126", "m_0127", "m_0128", "m_0129", "m_0130", "m_0131", "m_0132", "m_0133", "m_0134", "m_0135", "m_0136", "m_0137", "m_0138", "m_0139", "m_0140", "m_0141", "m_0142", "m_0143", "m_0144", "m_0145", "m_0146", "m_0147", "m_0148", "m_0149", "m_0150", "m_0151", "m_0152", "m_0153", "m_0154", "m_0155", "m_0156", "m_0157", "m_0158", "m_0159", "m_0160", "m_0161", "m_0162", "m_0163", "m_0164", "m_0165", "m_0166", "m_0167", "m_0168", "m_0169", "m_0170", "m_0171", "m_0172", "m_0173", "m_0174", "m_0175", "m_0176", "m_0177", "m_0178", "m_0179", "m_0180", "m_0181", "m_0182", "m_0183", "m_0184", "m_0185", "m_0186", "m_0187", "m_0188", "m_0189", "m_0190", "m_0191", "m_0192", "m_0193", "m_0194", "m_0195", "m_0196", "m_0197", "m_0198", "m_0199", "m_0200", "m_0201", "m_0202", "m_0203", "m_0204", "m_0205", "m_0206", "m_0207", "m_0208", "m_0209", "m_0210", "m_0211", "m_0212", "m_0213", "m_0214", "m_0215", "m_0216", "m_0217", "m_0218", "m_0219", "m_0220", "m_0221", "m_0222", "m_0223", "m_0224", "m_0225", "m_0226", "m_0227", "m_0228", "m_0229", "m_0230", "m_0231", "m_0232", "m_0233", "m_0234", "m_0235", "m_0236", "m_0237", "m_0238", "m_0239", "m_0240", "m_0241", "m_0242", "m_0243", "m_0244", "m_0245", "m_0246", "m_0247", "m_0248", "m_0249", "m_0250", "m_0251", "m_0252", "m_0253", "m_0254", "m_0255", "m_0256", "m_0257", "m_0258", "m_0259", "m_0260", "m_0261", "m_0262", "m_0263", "m_0264", "m_0265", "m_0266", "m_0267", "m_0268", "m_0269", "m_0270", "m_0271", "m_0272", "m_0273", "m_0274", "m_0275", "m_0276", "m_0277", "m_0278", "m_0279", "m_0280", "m_0281", "m_0282", "m_0283", "m_0284", "m_0285", "m_0286", "m_0287", "m_0288", "m_0289", "m_0290", "m_0291", "m_0292", "m_0293", "m_0294", "m_0295", "m_0296", "m_0297", "m_0298", "m_0299", "m_0300", "m_0301", "m_0302", "m_0303", "m_0304", "m_0305", "m_0306", "m_0307", "m_0308", "m_0309", "m_0310", "m_0311", "m_0312", "m_0313", "m_0314", "m_0315", "m_0316", "m_0317", "m_0318", "m_0319", "m_0320", "m_0321", "m_0322", "m_0323", "m_0324", "m_0325", "m_0326", "m_0327", "m_0328", "m_0329", "m_0330", "m_0331", "m_0332", "m_0333", "m_0334", "m_0335", "m_0336", "m_0337", "m_0338", "m_0339", "m_0340", "m_0341", "m_0342", "m_0343", "m_0344", "m_0345", "m_0346", "m_0347", "m_0348", "m_0349", "m_0350", "m_0351", "m_0352", "m_0353", "m_0354", "m_0355", "m_0356", "m_0357", "m_0358", "m_0359", "m_0360", "m_0361", "m_0362", "m_0363", "m_0364", "m_0365", "m_0366", "m_0367", "m_0368", "m_0369", "m_0370", "m_0371", "m_0372", "m_0373", "m_0374", "m_0375", "m_0376", "m_0377", "m_0378", "m_0379", "m_0380", "m_0381", "m_0382", "m_0383", "m_0384", "m_0385", "m_0386", "m_0387", "m_0388", "m_0389", "m_0390", "m_0391", "m_0392", "m_0393", "m_0394", "m_0395", "m_0396", "m_0397", "m_0398", "m_0399", "m_0400", "m_0401", "m_0402", "m_0403", "m_0404", "m_0405", "m_0406", "m_0407", "m_0408", "m_0409", "m_0410", "m_0411", "m_0412", "m_0413", "m_0414", "m_0415", "m_0416", "m_0417", "m_0418", "m_0419", "m_0420", "m_0421", "m_0422", "m_0423", "m_0424", "m_0425", "m_0426", "m_0427", "m_0428", "m_0429", "m_0430", "m_0431", "m_0432", "m_0433", "m_0434", "m_0435", "m_0436", "m_0437", "m_0438", "m_0439", "m_0440", "m_0441", "m_0442", "m_0443", "m_0444", "m_0445", "m_0446", "m_0447", "m_0448", "m_0449", "m_0450", "m_0451", "m_0452", "m_0453", "m_0454", "m_0455", "m_0456", "m_0457", "m_0458", "m_0459", "m_0460", "m_0461", "m_0462", "m_0463", "m_0464", "m_0465", "m_0466", "m_0467", "m_0468", "m_0469", "m_0470", "m_0471", "m_0472", "m_0473", "m_0474", "m_0475", "m_0476", "m_0477", "m_0478", "m_0479", "m_0480", "m_0481", "m_0482", "m_0483", "m_0484", "m_0485", "m_0486", "m_0487", "m_0488", "m_0489", "m_0490", "m_0491", "m_0492", "m_0493", "m_0494", "m_0495", "m_0496", "m_0497", "m_0498", "m_0499", "m_0500", "m_0501", "m_0502", "m_0503", "m_0504", "m_0505", "m_0506", "m_0507", "m_0508", "m_0509", "m_0510", "m_0511", "m_0512", "m_0513", "m_0514", "m_0515", "m_0516", "m_0517", "m_0518", "m_0519", "m_0520", "m_0521", "m_0522", "m_0523", "m_0524", "m_0525", "m_0526", "m_0527", "m_0528", "m_0529", "m_0530", "m_0531", "m_0532", "m_0533", "m_0534", "m_0535", "m_0536", "m_0537", "m_0538", "m_0539", "m_0540", "m_0541", "m_0542", "m_0543", "m_0544", "m_0545", "m_0546", "m_0547", "m_0548", "m_0549", "m_0550", "m_0551", "m_0552", "m_0553", "m_0554", "m_0555", "m_0556", "m_0557", "m_0558", "m_0559", "m_0560", "m_0561", "m_0562", "m_0563", "m_0564", "m_0565", "m_0566", "m_0567", "m_0568", "m_0569", "m_0570", "m_0571", "m_0572", "m_0573", "m_0574", "m_0575", "m_0576", "m_0577", "m_0578", "m_0579", "m_0580", "m_0581", "m_0582", "m_0583", "m_0584", "m_0585", "m_0586", "m_0587", "m_0588", "m_0589", "m_0590", "m_0591", "m_0592", "m_0593", "m_0594", "m_0595", "m_0596", "m_0597", "m_0598", "m_0599", "m_0600", "m_0601", "m_0602", "m_0603", "m_0604", "m_0605", "m_0606", "m_0607", "m_0608", "m_0609", "m_0610", "m_0611", "m_0612", "m_0613", "m_0614", "m_0615", "m_0616", "m_0617", "m_0618", "m_0619", "m_0620", "m_0621", "m_0622", "m_0623", "m_0624", "m_0625", "m_0626", "m_0627", "m_0628", "m_0629", "m_0630", "m_0631", "m_0632", "m_0633", "m_0634", "m_0635", "m_0636", "m_0637", "m_0638", "m_0639", "m_0640", "m_0641", "m_0642", "m_0643", "m_0644", "m_0645", "m_0646", "m_0647", "m_0648", "m_0649", "m_0650", "m_0651", "m_0652", "m_0653", "m_0654", "m_0655", "m_0656", "m_0657", "m_0658", "m_0659", "m_0660", "m_0661", "m_0662", "m_0663", "m_0664", "m_0665", "m_0666", "m_0667", "m_0668", "m_0669", "m_0670", "m_0671", "m_0672", "m_0673", "m_0674", "m_0675", "m_0676", "m_0677", "m_0678", "m_0679", "m_0680", "m_0681", "m_0682", "m_0683", "m_0684", "m_0685", "m_0686", "m_0687", "m_0688", "m_0689", "m_0690", "m_0691", "m_0692", "m_0693", "m_0694", "m_0695", "m_0696", "m_0697", "m_0698", "m_0699", "m_0700", "m_0701", "m_0702", "m_0703", "m_0704", "m_0705", "m_0706", "m_0707", "m_0708", "m_0709", "m_0710", "m_0711", "m_0712", "m_0713", "m_0714", "m_0715", "m_0716", "m_0717", "m_0718", "m_0719", "m_0720", "m_0721", "m_0722", "m_0723", "m_0724", "m_0725", "m_0726", "m_0727", "m_0728", "m_0729", "m_0730", "m_0731", "m_0732", "m_0733", "m_0734", "m_0735", "m_0736", "m_0737", "m_0738", "m_0739", "m_0740", "m_0741", "m_0742", "m_0743", "m_0744", "m_0745", "m_0746", "m_0747", "m_0748", "m_0749", "m_0750", "m_0751", "m_0752", "m_0753", "m_0754", "m_0755", "m_0756", "m_0757", "m_0758", "m_0759", "m_0760", "m_0761", "m_0762", "m_0763", "m_0764", "m_0765", "m_0766", "m_0767", "m_0768", "m_0769", "m_0770", "m_0771", "m_0772", "m_0773", "m_0774", "m_0775", "m_0776", "m_0777", "m_0778", "m_0779", "m_0780", "m_0781", "m_0782", "m_0783", "m_0784", "m_0785", "m_0786", "m_0787", "m_0788", "m_0789", "m_0790", "m_0791", "m_0792", "m_0793", "m_0794", "m_0795", "m_0796", "m_0797", "m_0798", "m_0799", "m_0800", "m_0801", "m_0802", "m_0803", "m_0804", "m_0805", "m_0806", "m_0807", "m_0808", "m_0809", "m_0810", "m_0811", "m_0812", "m_0813", "m_0814", "m_0815", "m_0816", "m_0817", "m_0818", "m_0819", "m_0820", "m_0821", "m_0822", "m_0823", "m_0824", "m_0825", "m_0826", "m_0827", "m_0828", "m_0829", "m_0830", "m_0831", "m_0832", "m_0833", "m_0834", "m_0835", "m_0836", "m_0837", "m_0838", "m_0839", "m_0840", "m_0841", "m_0842", "m_0843", "m_0844", "m_0845", "m_0846", "m_0847", "m_0848", "m_0849", "m_0850", "m_0851", "m_0852", "m_0853", "m_0854", "m_0855", "m_0856", "m_0857", "m_0858", "m_0859", "m_0860", "m_0861", "m_0862", "m_0863", "m_0864", "m_0865", "m_0866", "m_0867", "m_0868", "m_0869", "m_0870", "m_0871", "m_0872", "m_0873", "m_0874", "m_0875", "m_0876", "m_0877", "m_0878", "m_0879", "m_0880", "m_0881", "m_0882", "m_0883", "m_0884", "m_0885", "m_0886", "m_0887", "m_0888", "m_0889", "m_0890", "m_0891", "m_0892", "m_0893", "m_0894", "m_0895", "m_0896", "m_0897", "m_0898", "m_0899", "m_0900", "m_0901", "m_0902", "m_0903", "m_0904", "m_0905", "m_0906", "m_0907", "m_0908", "m_0909", "m_0910", "m_0911", "m_0912", "m_0913", "m_0914", "m_0915", "m_0916", "m_0917", "m_0918", "m_0919", "m_0920", "m_0921", "m_0922", "m_0923", "m_0924", "m_0925", "m_0926", "m_0927", "m_0928", "m_0929", "m_0930", "m_0931", "m_0932", "m_0933", "m_0934", "m_0935", "m_0936", "m_0937", "m_0938", "m_0939", "m_0940", "m_0941", "m_0942", "m_0943", "m_0944", "m_0945", "m_0946", "m_0947", "m_0948", "m_0949", "m_0950", "m_0951", "m_0952", "m_0953", "m_0954", "m_0955", "m_0956", "m_0957", "m_0958", "m_0959", "m_0960", "m_0961", "m_0962", "m_0963", "m_0964", "m_0965", "m_0966", "m_0967", "m_0968", "m_0969", "m_0970", "m_0971", "m_0972", "m_0973", "m_0974", "m_0975", "m_0976", "m_0977", "m_0978", "m_0979", "m_0980", "m_0981", "m_0982", "m_0983", "m_0984", "m_0985", "m_0986", "m_0987", "m_0988", "m_0989", "m_0990", "m_0991", "m_0992", "m_0993", "m_0994", "m_0995", "m_0996", "m_0997", "m_0998", "m_0999", "m_1000", "m_1001", "m_1002", "m_1003", "m_1004", "m_1005", "m_1006", "m_1007", "m_1008", "m_1009", "m_1010", "m_1011", "m_1012", "m_1013", "m_1014", "m_1015", "m_1016", "m_1017", "m_1018", "m_1019", "m_1020", "m_1021", "m_1022", "m_1023", "m_1024", "m_1025", "m_1026", "m_1027", "m_1028", "m_1029", "m_1030", "m_1031", "m_1032", "m_1033", "m_1034", "m_1035", "m_1036", "m_1037", "m_1038", "m_1039", "m_1040", "m_1041", "m_1042", "m_1043", "m_1044", "m_1045", "m_1046", "m_1047", "m_1048", "m_1049", "m_1050", "m_1051", "m_1052", "m_1053", "m_1054", "m_1055", "m_1056", "m_1057", "m_1058", "m_1059", "m_1060", "m_1061", "m_1062", "m_1063", "m_1064", "m_1065", "m_1066", "m_1067", "m_1068", "m_1069", "m_1070", "m_1071", "m_1072", "m_1073", "m_1074", "m_1075", "m_1076", "m_1077", "m_1078", "m_1079", "m_1080", "m_1081", "m_1082", "m_1083", "m_1084", "m_1085", "m_1086", "m_1087", "m_1088", "m_1089", "m_1090", "m_1091", "m_1092", "m_1093", "m_1094", "m_1095", "m_1096", "m_1097", "m_1098", "m_1099", "m_1100", "m_1101", "m_1102", "m_1103", "m_1104", "m_1105", "m_1106", "m_1107", "m_1108", "m_1109", "m_1110", "m_1111", "m_1112", "m_1113", "m_1114", "m_1115", "m_1116", "m_1117", "m_1118", "m_1119", "m_1120", "m_1121", "m_1122", "m_1123", "m_1124", "m_1125", "m_1126", "m_1127", "m_1128", "m_1129", "m_1130", "m_1131", "m_1132", "m_1133", "m_1134", "m_1135", "m_1136", "m_1137", "m_1138", "m_1139", "m_1140", "m_1141", "m_1142", "m_1143", "m_1144", "m_1145", "m_1146", "m_1147", "m_1148", "m_1149", "m_1150", "m_1151", "m_1152", "m_1153", "m_1154", "m_1155", "m_1156", "m_1157", "m_1158", "m_1159", "m_1160", "m_1161", "m_1162", "m_1163", "m_1164", "m_1165", "m_1166", "m_1167", "m_1168", "m_1169", "m_1170", "m_1171", "m_1172", "m_1173", "m_1174", "m_1175", "m_1176", "m_1177", "m_1178", "m_1179", "m_1180", "m_1181", "m_1182", "m_1183", "m_1184", "m_1185", "m_1186", "m_1187", "m_1188", "m_1189", "m_1190", "m_1191", "m_1192", "m_1193", "m_1194", "m_1195", "m_1196", "m_1197", "m_1198", "m_1199", "m_1200", "m_1201", "m_1202", "m_1203", "m_1204", "m_1205", "m_1206", "m_1207", "m_1208", "m_1209", "m_1210", "m_1211", "m_1212", "m_1213", "m_1214", "m_1215", "m_1216", "m_1217", "m_1218", "m_1219", "m_1220", "m_1221", "m_1222", "m_1223", "m_1224", "m_1225", "m_1226", "m_1227", "m_1228", "m_1229", "m_1230", "m_1231", "m_1232", "m_1233", "m_1234", "m_1235", "m_1236", "m_1237", "m_1238", "m_1239", "m_1240", "m_1241", "m_1242", "m_1243", "m_1244", "m_1245", "m_1246", "m_1247", "m_1248", "m_1249", "m_1250", "m_1251", "m_1252", "m_1253", "m_1254", "m_1255", "m_1256", "m_1257", "m_1258", "m_1259", "m_1260", "m_1261", "m_1262", "m_1263", "m_1264", "m_1265", "m_1266", "m_1267", "m_1268", "m_1269", "m_1270", "m_1271", "m_1272", "m_1273", "m_1274", "m_1275", "m_1276", "m_1277", "m_1278", "m_1279", "m_1280", "m_1281", "m_1282", "m_1283", "m_1284", "m_1285", "m_1286", "m_1287", "m_1288", "m_1289", "m_1290", "m_1291", "m_1292", "m_1293", "m_1294", "m_1295", "m_1296", "m_1297", "m_1298", "m_1299", "m_1300", "m_1301", "m_1302", "m_1303", "m_1304", "m_1305", "m_1306", "m_1307", "m_1308", "m_1309", "m_1310", "m_1311", "m_1312", "m_1313", "m_1314", "m_1315", "m_1316", "m_1317", "m_1318", "m_1319", "m_1320", "m_1321", "m_1322", "m_1323", "m_1324", "m_1325", "m_1326", "m_1327", "m_1328", "m_1329", "m_1330", "m_1331", "m_1332", "m_1333", "m_1334", "m_1335", "m_1336", "m_1337", "m_1338", "m_1339", "m_1340", "m_1341", "m_1342", "m_1343", "m_1344", "m_1345", "m_1346", "m_1347", "m_1348", "m_1349", "m_1350", "m_1351", "m_1352",
```