

Supplementary information

CAMISIM: Simulating metagenomes and microbial communities

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1 Taxonomic profile based community design

1.1 BIOM format details

The input BIOM profiles for the "from profile" mode of CAMISIM are required to either have the lineage stored as the ID, or preferably the field "lineage" in the "metadata". The lineage should be greengenes formatted, namely semicolon separated strings $x_0_scientific\ name; x_1_scientific\ name$ with x_i being the taxonomic rank descriptor - 's' for species, 'g' for genus, 'f' for family, 'o' for order, 'c' for class, 'p' for phylum, 'k' for superkingdom - and a scientific name of the taxon.

1.2 Reference database

CAMISIM requires a reference database of available complete genomes, created by algorithm 1. Per default all genomes tagged as "Complete genome" from the RefSeq are taken into account, but arbitrary reference data bases, online or offline, can be provided.

For all genomes $g \in G_{in}$, their taxonomy is known and given as a list with 7 elements tax_g , corresponding to their taxonomic identifier on the seven main taxonomic ranks (*species, genus, family, order, class, phylum, superkingdom*).

For example, the well-known bacteria *E. coli* has the NCBI taxonomy ID 562, it's genus *Escherichia* has the ID 561 and it's taxonomy goes up to the superkingdom "bacteria" with the taxonomic ID 2, so finally *E. coli*'s list would be [562, 561, 543, 91347, 1224, 1236, 2]. Given these lists it is possible to create a set of available complete genomes per taxon G_t .

Let for example the genome of *E. coli* and the genome of *E. albertii* (taxonomic ID 208962) be part of G_{in} , then we have two available genomes on the rank of species and one for every rank above, since *E. coli* and *E. albertii* belong to the same genus. This results in the sets per taxon $G_{562} = \{562\}$, $G_{208962} = \{208962\}$, $G_{561} = \{562, 208962\}$ etc. We add all the taxa for which a set G_t exists to the collection of sets F .

Algorithm 1: *create-reference*(G_{in})

input : List of complete genomes G_{in}
output: Collection of sets F which contains sets of taxonomic IDs G_t
for every taxon t which has at least one complete genome
available

```
1  $R = [\text{species, genus, family, order, class, phylum, superkingdom}]$ 
2  $F = \emptyset$  foreach  $t \in G_{in}$  do
3   get list  $tax_t$  from NCBI
4   foreach  $i \in tax_t$  do
5      $G_t.append(tax_t[0])$ 
6      $F = F \cup G_t$ 
7   end
8 end
9 return  $F$ 
```

2 De novo community design

In addition to providing genomes, it is possible to artificially add strain variation to CAMISIM. These additional strain genomes are created with a novel version of sgEvolver. In its original implementation, the simulated strain evolution process did not model natural selection. The lack of modeled selection could then cause the Open Reading Frames (ORFs) of protein encoding genes to break. Using prodigal, these ORFs are now initially found within the genomes sampling collection and mutation rates lowered for these genomic locations: substitutions that would introduce a stop codon (assumed here to be TGA, TAA, or TAG) are rejected with a probability of 98%. Secondly, substitutions that would eliminate an existing in-frame stop codon are rejected with 100% probability. Artificial strains evolved from real genomes are added to the community genome collection until the difference between `genomes_total` and `num_real_genomes` has been reached.

2.1 Creation of the mapping file

Genomes used for the *de novo* mode of CAMISIM require a "novelty category" assigned to them. To assign a novelty category to a genome from the input genome collection, genomes from same taxon are searched for in

a reference collection created from draft and complete genomes from NCBI RefSeq (microbial part), NCBI whole bacterial genomes, NCBI draft bacterial genomes and the NCBI Human Microbiome Project are searched for. The search begins at the species rank and the continues for genus, family, order, class, phylum and superkingdom. If a genome is found, the the novelty category is set to the rank visited below. For example, if a reference genome of the same species exists for a query genome, the novelty is declared as **new_strain**. If no reference genome of the same species is found, but there is a reference genome for another species of the same genus, the novelty category is set to **new_species**, etc. OTU IDs in the mapping file are inferred by extracting small rRNAs from these genomes and clustering these with small rRNA reference databases. The exact algorithm is found in the supplement of the CAMI main paper.

3 Genome assembly metrics

Evaluation of the assemblies was performed using quast, or metaquast in the case of the evolutionary relatedness evaluation, for quast default parameters were chosen. For metaquast two options of `-ambiguity-usage` were used (one and all), namely allowing single contigs to only map to a single reference genome or all (both), to explain the difference between strain and consensus contigs.

The metrics which are shown for the plot, Genome fraction, NGA50 and number of contigs should in combination yield a good picture of the assembly quality, while the individual metrics might not draw the complete picture: Genome fraction just describes the percentage of the reference genome which is covered by at least one contig. So having a lot of (overlapping) contigs results in the Genome fraction to look relatively well. This is complemented by the number of contigs metric, which punishes a high number of contigs. A low number of contigs is not a good measure for assembly quality alone since it does not include the measure how long these contigs are. This is why we chose NGA50 as the final metric to show. NGA50 describes the length of the aligned contig with which 50% of the reference genome is covered, so it is basically the combination of the first two metrics: Few and long contigs are similarly bad as many short ones and both result in the NGA50 to decline.

4 Methods

4.1 iTol

The 191 iTol genomes from the itol Nexus tree (Table 4.1) were mapped to the NCBI RefSeq data base and genomes downloaded accordingly, sequences shorter than 450k bp were filtered and all genomes which did not have an exact matching complete genome, resulting in 152 genomes with their NCBI ID (Table 4.1)

iTol Nexus tree

#NEXUS

Begin trees; [Treefile created Wed May 25 12:58:12 2016]

Translate

- 1 *Escherichia coli* EDL933,
- 2 *Escherichia coli* O157:H7,
- 3 *Escherichia coli* O6,
- 4 *Escherichia coli* K12,
- 5 *Shigella flexneri* 2a 2457T,
- 6 *Shigella flexneri* 2a 301,
- 7 *Salmonella enterica*,
- 8 *Salmonella typhi*,
- 9 *Salmonella typhimurium*,
- 10 *Yersinia pestis* Medievalis,
- 11 *Yersinia pestis* KIM,
- 12 *Yersinia pestis* C092,
- 13 *Photobacterium luminescens*,
- 14 *Blochmannia floridanus*,
- 15 *Wigglesworthia brevipalpis*,
- 16 *Buchnera aphidicola* Bp,
- 17 *Buchnera aphidicola* APS,
- 18 *Buchnera aphidicola* Sg,
- 19 *Pasteurella multocida*,
- 20 *Haemophilus influenzae*,
- 21 *Haemophilus ducreyi*,
- 22 *Vibrio vulnificus* YJ016,

23 *Vibrio vulnificus* CMCP6,
24 *Vibrio parahaemolyticus*,
25 *Vibrio cholerae*,
26 *Photobacterium profundum*,
27 *Shewanella oneidensis*,
28 *Pseudomonas putida*,
29 *Pseudomonas syringae*,
30 *Pseudomonas aeruginosa*,
31 *Xylella fastidiosa* 700964,
32 *Xylella fastidiosa* 9a5c,
33 *Xanthomonas axonopodis*,
34 *Xanthomonas campestris*,
35 *Coxiella burnetii*,
36 *Neisseria meningitidis* A,
37 *Neisseria meningitidis* B,
38 *Chromobacterium violaceum*,
39 *Bordetella pertussis*,
40 *Bordetella parapertussis*,
41 *Bordetella bronchiseptica*,
42 *Ralstonia solanacearum*,
43 *Nitrosomonas europaea*,
44 *Agrobacterium tumefaciens* Cereon,
45 *Agrobacterium tumefaciens* WashU,
46 *Rhizobium meliloti*,
47 *Brucella suis*,
48 *Brucella melitensis*,
49 *Rhizobium loti*,
50 *Rhodopseudomonas palustris*,
51 *Bradyrhizobium japonicum*,
52 *Caulobacter crescentus*,
53 *Wolbachia* sp. wMel,
54 *Rickettsia prowazekii*,
55 *Rickettsia conorii*,
56 *Helicobacter pylori* J99,
57 *Helicobacter pylori* 26695,
58 *Helicobacter hepaticus*,
59 *Wolinella succinogenes*,
60 *Campylobacter jejuni*,

61 *Desulfovibrio vulgaris*,
62 *Geobacter sulfurreducens*,
63 *Bdellovibrio bacteriovorus*,
64 *Acidobacterium capsulatum*,
65 *Solibacter usitatus*,
66 *Fusobacterium nucleatum*,
67 *Aquifex aeolicus*,
68 *Thermotoga maritima*,
69 *Thermus thermophilus*,
70 *Deinococcus radiodurans*,
71 *Dehalococcoides ethenogenes*,
72 *Nostoc* sp. PCC 7120,
73 *Synechocystis* sp. PCC6803,
74 *Synechococcus elongatus*,
75 *Synechococcus* sp. WH8102,
76 *Prochlorococcus marinus* MIT9313,
77 *Prochlorococcus marinus* SS120,
78 *Prochlorococcus marinus* CCMP1378,
79 *Gloeobacter violaceus*,
80 *Gemmata obscuriglobus*,
81 *Rhodopirellula baltica*,
82 *Leptospira interrogans* L1-130,
83 *Leptospira interrogans* 56601,
84 *Treponema pallidum*,
85 *Treponema denticola*,
86 *Borrelia burgdorferi*,
87 *Tropheryma whipplei* TW08/27,
88 *Tropheryma whipplei* Twist,
89 *Bifidobacterium longum*,
90 *Corynebacterium glutamicum* 13032,
91 *Corynebacterium glutamicum*,
92 *Corynebacterium efficiens*,
93 *Corynebacterium diphtheriae*,
94 *Mycobacterium bovis*,
95 *Mycobacterium tuberculosis* CDC1551,
96 *Mycobacterium tuberculosis* H37Rv,
97 *Mycobacterium leprae*,
98 *Mycobacterium paratuberculosis*,

99 *Streptomyces avermitilis*,
100 *Streptomyces coelicolor*,
101 *Fibrobacter succinogenes*,
102 *Chlorobium tepidum*,
103 *Porphyromonas gingivalis*,
104 *Bacteroides thetaiotaomicron*,
105 *Chlamydophila pneumoniae* TW183,
106 *Chlamydia pneumoniae* J138,
107 *Chlamydia pneumoniae* CWL029,
108 *Chlamydia pneumoniae* AR39,
109 *Chlamydophila caviae*,
110 *Chlamydia muridarum*,
111 *Chlamydia trachomatis*,
112 *Thermoanaerobacter tengcongensis*,
113 *Clostridium tetani*,
114 *Clostridium perfringens*,
115 *Clostridium acetobutylicum*,
116 *Mycoplasma mobile*,
117 *Mycoplasma pulmonis*,
118 *Mycoplasma pneumoniae*,
119 *Mycoplasma genitalium*,
120 *Mycoplasma gallisepticum*,
121 *Mycoplasma penetrans*,
122 *Ureaplasma parvum*,
123 *Mycoplasma mycoides*,
124 *Phytoplasma* Onion yellows,
125 *Listeria monocytogenes* F2365,
126 *Listeria monocytogenes* EGD,
127 *Listeria innocua*,
128 *Oceanobacillus iheyensis*,
129 *Bacillus halodurans*,
130 *Bacillus cereus* ATCC 14579,
131 *Bacillus cereus* ATCC 10987,
132 *Bacillus anthracis*,
133 *Bacillus subtilis*,
134 *Staphylococcus aureus* MW2,
135 *Staphylococcus aureus* N315,
136 *Staphylococcus aureus* Mu50,

137 *Staphylococcus epidermidis*,
138 *Streptococcus agalactiae* III,
139 *Streptococcus agalactiae* V,
140 *Streptococcus pyogenes* M1,
141 *Streptococcus pyogenes* MGAS8232,
142 *Streptococcus pyogenes* MGAS315,
143 *Streptococcus pyogenes* SSI-1,
144 *Streptococcus mutans*,
145 *Streptococcus pneumoniae* R6,
146 *Streptococcus pneumoniae* TIGR4,
147 *Lactococcus lactis*,
148 *Enterococcus faecalis*,
149 *Lactobacillus johnsonii*,
150 *Lactobacillus plantarum*,
151 *Thalassiosira pseudonana*,
152 *Cryptosporidium hominis*,
153 *Plasmodium falciparum*,
154 *Oryza sativa*,
155 *Arabidopsis thaliana*,
156 *Cyanidioschyzon merolae*,
157 *Dictyostelium discoideum*,
158 *Eremothecium gossypii*,
159 *Saccharomyces cerevisiae*,
160 *Schizosaccharomyces pombe*,
161 *Anopheles gambiae*,
162 *Drosophila melanogaster*,
163 *Takifugu rubripes*,
164 *Danio rerio*,
165 *Rattus norvegicus*,
166 *Mus musculus*,
167 *Homo sapiens*,
168 *Pan troglodytes*,
169 *Gallus gallus*,
170 *Caenorhabditis elegans*,
171 *Caenorhabditis briggsae*,
172 *Leishmania major*,
173 *Giardia lamblia*,
174 *Nanoarchaeum equitans*,

```

175 Sulfolobus tokodaii,
176 Sulfolobus solfataricus,
177 Aeropyrum pernix,
178 Pyrobaculum aerophilum,
179 Thermoplasma volcanium,
180 Thermoplasma acidophilum,
181 Methanobacterium thermautotrophicum,
182 Methanopyrus kandleri,
183 Methanococcus maripaludis,
184 Methanococcus jannaschii,
185 Pyrococcus horikoshii,
186 Pyrococcus abyssi,
187 Pyrococcus furiosus,
188 Archaeoglobus fulgidus,
189 Halobacterium sp. NRC-1,
190 Methanosarcina acetivorans,
191 Methanosarcina mazei
;
tree iTOL_exported_tree = [&R] (((((((((((((((((((((((1:0.00000,2:0.00000):0.00044[9
End;

```

Genome Table

NCBI_ID	Scientific_Name
240015	Acidobacterium capsulatum ATCC 51196
56636	Aeropyrum pernix
63363	Aquifex aeolicus
2234	Archaeoglobus fulgidus
198094	Bacillus anthracis str. Ames
222523	Bacillus cereus ATCC 10987
226900	Bacillus cereus ATCC 14579
86665	Bacillus halodurans
1423	Bacillus subtilis
818	Bacteroides thetaiotaomicron
959	Bdellovibrio bacteriovorus
216816	Bifidobacterium longum
518	Bordetella bronchiseptica
519	Bordetella parapertussis

520 *Bordetella pertussis*
 139 *Borrelia burgdorferi*
 375 *Bradyrhizobium japonicum*
 118099 *Buchnera aphidicola* (*Acyrtosiphon pisum*)
 135842 *Buchnera aphidicola* (*Baizongia pistaciae*)
 98794 *Buchnera aphidicola* (*Schizaphis graminum*)
 6238 *Caenorhabditis briggsae*
 197 *Campylobacter jejuni*
 203907 *Candidatus Blochmannia floridanus*
 155892 *Caulobacter vibrioides*
 83560 *Chlamydia muridarum*
 813 *Chlamydia trachomatis*
 83557 *Chlamydomonas caviae*
 115711 *Chlamydomonas pneumoniae* AR39
 115713 *Chlamydomonas pneumoniae* CWL029
 182082 *Chlamydomonas pneumoniae* TW-183
 1097 *Chlorobaculum tepidum*
 536 *Chromobacterium violaceum*
 1488 *Clostridium acetobutylicum*
 1502 *Clostridium perfringens*
 1513 *Clostridium tetani*
 1717 *Corynebacterium diphtheriae*
 152794 *Corynebacterium efficiens*
 196627 *Corynebacterium glutamicum* ATCC 13032
 1718 *Corynebacterium glutamicum*
 777 *Coxiella burnetii*
 45157 *Cyanidioschyzon merolae*
 243164 *Dehalococcoides ethenogenes* 195
 882 *Desulfovibrio vulgaris* subsp. *vulgaris* str. Hildenborough
 1351 *Enterococcus faecalis*
 562 *Escherichia coli*
 155864 *Escherichia coli* O157:H7 EDL933
 83334 *Escherichia coli* O157:H7
 59374 *Fibrobacter succinogenes* subsp. *succinogenes* S85
 76856 *Fusobacterium nucleatum* subsp. *nucleatum*
 35554 *Geobacter sulfurreducens*
 33072 *Gloeobacter violaceus*
 730 *Haemophilus ducreyi*

727 *Haemophilus influenzae*
32025 *Helicobacter hepaticus*
210 *Helicobacter pylori*
85963 *Helicobacter pylori* J99
33959 *Lactobacillus johnsonii*
1590 *Lactobacillus plantarum*
1360 *Lactococcus lactis* subsp. *lactis*
5664 *Leishmania major*
1642 *Listeria innocua*
1639 *Listeria monocytogenes*
265669 *Listeria monocytogenes* str. 4b F2365
381 *Mesorhizobium loti*
2190 *Methanocaldococcus jannaschii*
39152 *Methanococcus maripaludis*
2320 *Methanopyrus kandleri*
2214 *Methanosarcina acetivorans*
2209 *Methanosarcina mazei*
187420 *Methanothermobacter thermautotrophicus* str. Delta H
1770 *Mycobacterium avium* subsp. *paratuberculosis*
1765 *Mycobacterium bovis*
1769 *Mycobacterium leprae*
83331 *Mycobacterium tuberculosis* CDC1551
83332 *Mycobacterium tuberculosis* H37Rv
2096 *Mycoplasma gallisepticum*
2097 *Mycoplasma genitalium*
267748 *Mycoplasma mobile* 163K
44101 *Mycoplasma mycoides* subsp. *mycoides* SC
28227 *Mycoplasma penetrans*
2104 *Mycoplasma pneumoniae*
2107 *Mycoplasma pulmonis*
160232 *Nanoarchaeum equitans*
65699 *Neisseria meningitidis* serogroup A
491 *Neisseria meningitidis* serogroup B
915 *Nitrosomonas europaea*
182710 *Oceanobacillus iheyensis*
100379 *Onion yellows phytoplasma*
747 *Pasteurella multocida*
141679 *Photobacterium luminescens* subsp. *laumondii*

837 *Porphyromonas gingivalis*
 1219 *Prochlorococcus marinus*
 74547 *Prochlorococcus marinus* str. MIT 9313
 59919 *Prochlorococcus marinus* subsp. *pastoris* str. CCMP1986
 287 *Pseudomonas aeruginosa*
 160488 *Pseudomonas putida* KT2440
 323 *Pseudomonas syringae* pv. *tomato*
 13773 *Pyrobaculum aerophilum*
 29292 *Pyrococcus abyssi*
 2261 *Pyrococcus furiosus*
 53953 *Pyrococcus horikoshii*
 305 *Ralstonia solanacearum*
 1076 *Rhodopseudomonas palustris*
 781 *Rickettsia conorii*
 782 *Rickettsia prowazekii*
 209261 *Salmonella enterica* subsp. *enterica* serovar *Typhi* Ty2
 601 *Salmonella typhi*
 70863 *Shewanella oneidensis*
 198215 *Shigella flexneri* 2a str. 2457T
 623 *Shigella flexneri*
 382 *Sinorhizobium meliloti*
 234267 *Solibacter usitatus* Ellin6076
 158878 *Staphylococcus aureus* subsp. *aureus* Mu50
 196620 *Staphylococcus aureus* subsp. *aureus* MW2
 158879 *Staphylococcus aureus* subsp. *aureus* N315
 1282 *Staphylococcus epidermidis*
 216495 *Streptococcus agalactiae* serogroup III
 216466 *Streptococcus agalactiae* serogroup V
 1309 *Streptococcus mutans*
 1313 *Streptococcus pneumoniae*
 171101 *Streptococcus pneumoniae* R6
 1314 *Streptococcus pyogenes*
 198466 *Streptococcus pyogenes* MGAS315
 186103 *Streptococcus pyogenes* MGAS8232
 193567 *Streptococcus pyogenes* SSI-1
 33903 *Streptomyces avermitilis*
 1902 *Streptomyces coelicolor*
 2287 *Sulfolobus solfataricus*

111955 *Sulfolobus tokodaii*
 32046 *Synechococcus elongatus*
 84588 *Synechococcus* sp. WH 8102
 1148 *Synechocystis* sp. PCC 6803
 119072 *Thermoanaerobacter tengcongensis*
 2303 *Thermoplasma acidophilum*
 50339 *Thermoplasma volcanium*
 2336 *Thermotoga maritima*
 262724 *Thermus thermophilus* HB27
 158 *Treponema denticola*
 160 *Treponema pallidum*
 203267 *Tropheryma whipplei* str. Twist
 218496 *Tropheryma whipplei* TW08/27
 134821 *Ureaplasma parvum*
 666 *Vibrio cholerae*
 36870 *Wigglesworthia glossinidia* endosymbiont of *Glossina brevipalpis*
 66077 *Wolbachia* sp. wMel
 844 *Wolinella succinogenes*
 92829 *Xanthomonas axonopodis* pv. citri
 340 *Xanthomonas campestris* pv. campestris
 2371 *Xylella fastidiosa*
 183190 *Xylella fastidiosa* Temecula1
 632 *Yersinia pestis*
 187410 *Yersinia pestis* KIM

4.2 Parameters

The varying genome coverage samples were created with CAMISIM, with config-files as well as genomes and all output provided upon request, with *XX* being the desired coverage:

```
./metagenomesimulation configXX.ini
```

The genome similarity samples were also created with CAMISIM and the provided config-files, mapping files and genomes, where *XX* is a number corresponding to one of the 152 iTol genomes:

```
./metagenomesimulation configXX.ini
```

The iTol genomes were evolved manually using the sgEvolver using a specific template tree available on request:

```
./sgEvolver template.tree genome.fa genome.fa evolved_genome.bam
```

evolved_genome.fa

MEGAHIT 1.0.3/1.12 was run with default parameters on all the read sets:

```
./megahit --12 anonymous_reads.fq -o Assembly/
```

SPAdes was called with the `--meta` flag (from here on called metaSPAdes) and `lsthline!-phred-offset!` parameter set to 33 in case quality information on the reads was missing (and on 48 cores with `-t 48`):

```
./spades.py --12 anonymous_reads.fq --meta -t 48 --phred-offset 33 -o metaSPAdes
```

quast 3.1 was run for the coverage experiment:

```
./quast.py -R e_coli_k12.fa -o quast contigs.fasta
```

(for the E.coli coverage sweep)

For the similarity experiment, metaquast was run with a small patch (now built in into newer version of quast) to allow mapping to only a single reference genome for multiple best hits ("strain contigs") or to multiple reference genomes ("consensus contigs") using the ambiguity-usage flag of the nucmer mapping.

```
./metaquast.py -R genome_ancestor.fa,genome_evolved.fa -o quast contigs.fasta
```

```
./metaquast.py.OLD -R genome_ancestor.fa,genome_evolved.fa -o quast contigs.fasta
```

Where the latter is the unpatched evaluating consensus contigs and the first the patched evaluating strain contigs.

The data sets (mousegut and HMP) where created using the `from_profile` script of CAMISIM versions 0.2, 0.2.1 and 0.2.2 respectively:

```
./metagenome_from_profile -p profile.biom -o out
```

All scripts for creating tables, plots, config files are also available, either upon request or already under data.cami-challenge.org/participate.

4.3 PICRUST

We created functional profiles with PICRUST, using a prediction model from 3772 KEGG genomes and corresponding 16S rRNA sequences according the PICRUST "Genome Prediction Tutorial": 1) The determination of 16S rRNA copy numbers was performed by rrnDB Estimate version 5.2.2) KEGG Orthology (KO) profiles of the genomes were extracted from the KEGG database Release 77. 3) A tree was created from GreenGenes reference alignment (Version 13.5 OTU-RepSet 97) and the 16S rRNA of the KEGG genomes to build a integrated prediction model.

4.4 Config file

Due to its flexibility, CAMISIM requires an extensive configuration file. A default config for both short and long reads is shipped within CAMISIM and is exemplary shown here:

```
[Main]
# maximum number of processes
max_processors=8

# 0: community design + read simulator,
# 1: read simulator only
phase=0

# output directory, where the output will be stored (will be
#   overwritten if set in from_profile)
output_directory=

# temporary directory
temp_directory=/tmp

# gold standard assembly
gsa=True

# gold standard for all samples combined
pooled_gsa=True

# anonymize sequences?
anonymous=True

# id of dataset, used in folder names and is prefix in anonymous
#   sequences
dataset_id=RL

# Read Simulation settings, relevant also for from_profile
[ReadSimulator]
# which readsimulator to use:
# Choice of 'art', 'wgsim', 'nanosim', 'pbsim'
```

```

type=art

# Samtools (http://www.htslib.org/) takes care of sam/bam files
. Version 1.0 or higher required!
# file path to executable
samtools=tools/samtools-1.3/samtools

# file path to read simulation executable
readsim=tools/art_illumina-2.3.6/art_illumina

#error profiles:
#for ART:
#HiSeq 150bp: hi150
#MBARC-26 150bp: mbarc
#for wgsim:
#error rate as <float> (e.g. 0.05 for 5% error rate)
#blank for nanosim and wgsim
profile=mbarc

# Directory containing error profiles (can be blank for wgsim)
error_profiles=tools/art_illumina-2.3.6/profiles/

#paired end read, insert size (not applicable for nanosim)
fragments_size_mean=270
fragment_size_standard_deviation=27

# Everything in this section is only required for de novo
simulation:
[CommunityDesign]
# specify the samples size in Giga base pairs
size=5

# how many different samples?
number_of_samples=1

# how many communities
num_communities=1

```

```

# directory containing the taxdump of ncbi, version from
  22.02.2017 is shipped
# "nodes.dmp"
# "merged.dmp"
# "names.dmp"
ncbi_taxdump=tools/ncbi-taxonomy_20170222.tar.gz

# the strain simulator for de novo strain creation
strain_simulation_template=scripts/StrainSimulationWrapper/
  sgEvolver/simulation_dir/

# define communities: [community<integer>]
[community0]
# information about all included genomes:
# can be used for multiple samples
metadata=
id_to_genome_file=

# how many genomes do you want to sample overall?
genomes_total=
num_real_genomes=

# how many genomes per species taxon
# (species taxon will be replaced by OTU-cluster later on)
max_strains_per_otu=1
ratio=1

# which kind of different samples do you need?
# replicates / timeseries_lognormal / timeseries_normal /
  differential
mode=

# Part: community design
# Set parameters of log-normal and normal distribution, number
  of samples
# sigma > 0; influences shape (higher sigma -> smaller peak and
  longer tail),
log_sigma=2

```

```

# mu (real number) is a parameter for the log-scale
log_mu=1

# do you want to see a distribution before you decide to use it
? yes/no
view=no

# second community
#[community1]
#metadata=defaults/plasmid_metadata_v2.3_filtered.tsv
#id_to_genome_file=defaults/plasmid_path.tsv
#genomes_total=20
#max_strains_per_otu=3
#ratio=2.5
#mode=differential
#log_mu=1
#log_sigma=2
#view=false

```

5 OTU mapping file

The mouse gut BIOM file and thus dataset includes metagenomic data from different mice, vendors and sites in the gut. The exact assignment of each sample in the data set to the mice/vendors (as a code) and location in the gut is found in the following mapping file:

```

biom16S-SampleID SampleID-CAMISIM Microbiota Location
500.L21 0 HZI Ileum
502.L21 1 HZI Colon
503.L21 2 N6 Ileum
504.L21 3 N6 Cecum
506.L21 4 Jan-10C Ileum
507.L21 5 Jan-10C Cecum
508.L21 6 Jan-10C Colon
509.L21 7 NCI Ileum

```

510.L21 8 NCI Cecum
511.L21 9 NCI Colon
512.L21 10 Tac-401 Ileum
513.L21 11 Tac-401 Cecum
514.L21 12 Tac-401 Colon
515.L21 13 Tac-401 Ileum
516.L21 14 Tac-401 Cecum
517.L21 15 Tac-401 Colon
518.L21 16 Tac-130 Ileum
520.L21 17 Tac-130 Colon
521.L21 18 Tac-130 Ileum
522.L21 19 Tac-130 Cecum
523.L21 20 Tac-130 Colon
524.L21 21 ChR-9 Ileum
526.L21 22 ChR-9 Colon
527.L21 23 ChR-9 Ileum
528.L21 24 ChR-9 Cecum
529.L21 25 ChR-9 Colon
530.L21 26 ChR-11 Ileum
531.L21 27 ChR-11 Cecum
532.L21 28 ChR-11 Colon
533.L21 29 ChR-11 Ileum
534.L21 30 ChR-11 Cecum
535.L21 31 ChR-11 Colon
536.L21 32 Har-2 Ileum
537.L21 33 Har-2 Cecum
538.L21 34 Har-2 Colon
539.L21 35 Har-2 Ileum
540.L21 36 Har-2 Cecum
541.L21 37 Har-2 Colon
542.L21 38 Jan-1A Ileum
543.L21 39 Jan-1A Cecum
544.L21 40 Jan-1A Colon
545.L21 41 Jan-1A Ileum
546.L21 42 Jan-1A Cecum
547.L21 43 Jan-1A Colon
548.L21 44 ChR-7 Cecum
549.L21 45 Tac-809 Cecum

550.L21 46 N6 Content
551.L21 47 NCI Content
552.L21 48 Jan-10C Content
553.L21 49 HZI Content
554.L21 50 N6 Content
555.L21 51 Jan-10C Content
556.L21 52 NCI Content
557.L21 53 Tac-809 DistalColon
559.L21 54 Tac-809 ProximalColon
560.L21 55 Tac-809 DistalColon
561.L21 56 Tac-809 ProximalColon
562.L21 57 Tac-809 Cecum
563.L21 58 ChR-7 DistalColon
564.L21 59 ChR-7 ProximalColon
565.L21 60 ChR-7 DistalColon
566.L21 61 ChR-7 ProximalColon
567.L21 62 ChR-7 Cecum
569.L21 63 ChR-7 Ileum
570.L21 64 Prevotella Culture