Step #1 - Assembly / Binning / COG Annotation

Config file config.yaml is extended by additional config specified via the command line.

Building DAG of jobs...
Using shell: /usr/bin/bash

Provided cores: 8

Rules claiming more threads will be scaled down.

Job stats:

| job | count | min threads | max threads |
|--------------------------|-------|-------------|-------------|
| all | 1 | 1 | 1 |
| bed orfs | 1 | 1 | 1 |
| bedtools split cov | 8 | 1 | 1 |
| bowtie align | 8 | 8 | 8 |
| bowtie index | 1 | 8 | 8 |
| cat split annotation | 1 | 1 | 1 |
| compute avg cov | 1 | 1 | 1 |
| concoct | 1 | 8 | 8 |
| copy_fasta | 1 | 1 | 1 |
| coverage | 1 | 1 | 1 |
| create bin folders | 1 | 1 | 1 |
| cut contigs | 1 | 1 | 1 |
| extract SCG sequences | 1 | 1 | 1 |
| get SCG tables | 1 | 1 | 1 |
| initial_quantity_of_bins | 1 | 1 | 1 |
| merge_contigs | 1 | 8 | 8 |
| parse_cogs_annotation | 1 | 1 | 1 |
| prodigal | 1 | 1 | 1 |
| reads_yaml | 1 | 1 | 1 |
| refine | 1 | 8 | 8 |
| rpsblast | 100 | 1 | 1 |
| samtools_sort | 8 | 8 | 8 |
| simplify | 1 | 8 | 8 |
| spades | 1 | 8 | 8 |
| split_fasta | 1 | 1 | 1 |
| unitig_profiles | 1 | 8 | 8 |
| total | 146 | 1 | 8 |

```
Resources before job selection: {' cores': 8, ' nodes': 9223372036854775807}
Ready jobs (2)
Select jobs to execute...
Welcome to the CBC MILP Solver
Version: 2.10.10
Build Date: Apr 19 2023
command line - cbc /tmp/79e2f93dd88440b4b976d4b6c1e30548-pulp.mps max
timeMode elapsed branch printingOptions all solution
/tmp/79e2f93dd88440b4b976d4b6c1e30548-pulp.sol (default strategy 1)
At line 2 NAME
                        MODEL
At line 3 ROWS
At line 7 COLUMNS
At line 18 RHS
At line 21 BOUNDS
At line 24 ENDATA
Problem MODEL has 2 rows, 2 columns and 4 elements
Coin0008I MODEL read with 0 errors
```

Option for timeMode changed from cpu to elapsed

```
Continuous objective value is 16 - 0.00 seconds
Cg10004I processed model has 1 rows, 2 columns (2 integer (2 of which
binary)) and 2 elements
Cutoff increment increased from 1e-05 to 1.9999
Cbc0038I Initial state - 0 integers unsatisfied sum - 0
Cbc0038I Solution found of 16
Cbc0038I Before mini branch and bound, 2 integers at bound fixed and 0
continuous
Cbc0038I Mini branch and bound did not improve solution (0.00 seconds)
Cbc0038I After 0.00 seconds - Feasibility pump exiting with objective of 16 -
took 0.00 seconds
Cbc0012I Integer solution of 16 found by feasibility pump after 0 iterations
and 0 nodes (0.00 seconds)
Cbc0001I Search completed - best objective 16, took 0 iterations and 0 nodes
(0.00 seconds)
Cbc0035I Maximum depth 0, 0 variables fixed on reduced cost
Cuts at root node changed objective from 16 to 16
Probing was tried 0 times and created 0 cuts of which 0 were active after
adding rounds of cuts (0.000 seconds)
Gomory was tried 0 times and created 0 cuts of which 0 were active after
adding rounds of cuts (0.000 seconds)
Knapsack was tried 0 times and created 0 cuts of which 0 were active after
adding rounds of cuts (0.000 seconds)
Clique was tried 0 times and created 0 cuts of which 0 were active after
adding rounds of cuts (0.000 seconds)
MixedIntegerRounding2 was tried 0 times and created 0 cuts of which 0 were
active after adding rounds of cuts (0.000 seconds)
FlowCover was tried 0 times and created 0 cuts of which 0 were active after
adding rounds of cuts (0.000 seconds)
TwoMirCuts was tried 0 times and created 0 cuts of which 0 were active after
adding rounds of cuts (0.000 seconds)
ZeroHalf was tried 0 times and created 0 cuts of which 0 were active after
adding rounds of cuts (0.000 seconds)
Result - Optimal solution found
                                16.00000000
Objective value:
Enumerated nodes:
                                0
Total iterations:
                               0
                               0.00
Time (CPU seconds):
Time (Wallclock seconds):
                               0.00
Option for printingOptions changed from normal to all
Total time (CPU seconds):
                               0.01
                                     (Wallclock seconds): 0.00
Selected jobs (1)
Resources after job selection: { 'cores': 0, 'nodes': 9223372036854775806}
[Wed Jul 19 10:00:59 2023]
Job 7: Assembling with metaSPAdes
Reason: Missing output files: assembly/high res/graph pack.gfa,
assembly/spades/assembly.fasta
        /mnt/strong/tools/apps/STRONG/SPAdes/assembler/bin/spades.py --meta -
-only-assembler --save-gp -t 8 -k 77 -m 2000 -1
/mnt/strong/tools/apps/STRONG Runs/Test/sample1/sample1 R1.fq.gz -1
```

```
/mnt/strong/tools/apps/STRONG Runs/Test/sample2/sample2 R1.fq.gz -1
/mnt/strong/tools/apps/STRONG Runs/Test/sample3/sample3 R1.fq.gz -1
/mnt/strong/tools/apps/STRONG_Runs/Test/sample4/sample4_R1.fq.gz -1
/mnt/strong/tools/apps/STRONG Runs/Test/sample5/sample5 R1.fq.gz -1
/mnt/strong/tools/apps/STRONG Runs/Test/sample6/sample6 R1.fq.gz -1
/mnt/strong/tools/apps/STRONG Runs/Test/sample7/sample7 R1.fq.qz -1
/mnt/strong/tools/apps/STRONG Runs/Test/sample8/sample8 R1.fq.qz -2
/mnt/strong/tools/apps/STRONG Runs/Test/sample1/sample1 R2.fq.qz -2
/mnt/strong/tools/apps/STRONG Runs/Test/sample2/sample2 R2.fg.gz -2
/mnt/strong/tools/apps/STRONG_Runs/Test/sample3/sample3_R2.fq.gz -2
/mnt/strong/tools/apps/STRONG Runs/Test/sample4/sample4 R2.fq.gz -2
/mnt/strong/tools/apps/STRONG_Runs/Test/sample5/sample5_R2.fq.gz -2
/mnt/strong/tools/apps/STRONG Runs/Test/sample6/sample6 R2.fq.gz -2
/mnt/strong/tools/apps/STRONG Runs/Test/sample7/sample7 R2.fq.gz -2
/mnt/strong/tools/apps/STRONG Runs/Test/sample8/sample8 R2.fq.gz -o
assembly/spades/ &> assembly/spades.log
        cp assembly/spades//contigs.fasta assembly/spades/assembly.fasta
        cp assembly/spades//K77/saves/00 before simplification/graph pack*
$(dirname assembly/high res/graph pack.gfa)
Full Traceback (most recent call last):
  File "/mnt/strong/tools/apps/miniconda3.10/envs/STRONG/lib/python3.10/site-
packages/snakemake/executors/ init .py", line 2561, in run_wrapper
    run (
  File "/mnt/strong/tools/apps/STRONG/SnakeNest/Assembly.snake", line 50, in
 rule spades
  File "/mnt/strong/tools/apps/miniconda3.10/envs/STRONG/lib/python3.10/site-
packages/snakemake/shell.py", line 294, in __new__
    raise sp.CalledProcessError(retcode, cmd)
subprocess.CalledProcessError: Command 'set -euo pipefail;
        /mnt/strong/tools/apps/STRONG/SPAdes/assembler/bin/spades.py --meta -
-only-assembler --save-gp -t 8 -k 77 -m 2000 -1
/mnt/strong/tools/apps/STRONG Runs/Test/sample1/sample1 R1.fq.gz -1
/mnt/strong/tools/apps/STRONG Runs/Test/sample2/sample2 R1.fq.qz -1
/mnt/strong/tools/apps/STRONG Runs/Test/sample3/sample3 R1.fq.gz -1
/mnt/strong/tools/apps/STRONG Runs/Test/sample4/sample4 R1.fq.gz -1
/mnt/strong/tools/apps/STRONG Runs/Test/sample5/sample5 R1.fq.qz -1
/mnt/strong/tools/apps/STRONG Runs/Test/sample6/sample6 R1.fq.gz -1
/mnt/strong/tools/apps/STRONG Runs/Test/sample7/sample7 R1.fq.gz -1
/mnt/strong/tools/apps/STRONG Runs/Test/sample8/sample8 R1.fq.gz -2
/mnt/strong/tools/apps/STRONG Runs/Test/sample1/sample1 R2.fq.qz -2
/mnt/strong/tools/apps/STRONG Runs/Test/sample2/sample2 R2.fq.gz -2
/mnt/strong/tools/apps/STRONG Runs/Test/sample3/sample3 R2.fq.qz -2
/mnt/strong/tools/apps/STRONG_Runs/Test/sample4/sample4_R2.fq.gz -2
/mnt/strong/tools/apps/STRONG_Runs/Test/sample5/sample5_R2.fq.gz -2
/mnt/strong/tools/apps/STRONG Runs/Test/sample6/sample6 R2.fq.gz -2
/mnt/strong/tools/apps/STRONG Runs/Test/sample7/sample7 R2.fq.gz -2
/mnt/strong/tools/apps/STRONG Runs/Test/sample8/sample8 R2.fq.gz -o
assembly/spades/ &> assembly/spades.log
        cp assembly/spades//contigs.fasta assembly/spades/assembly.fasta
        cp assembly/spades//K77/saves/00 before simplification/graph pack*
$(dirname assembly/high res/graph pack.gfa)' returned non-zero exit status
127.
[Wed Jul 19 10:00:59 2023]
Error in rule spades:
    jobid: 7
```

```
input: /mnt/strong/tools/apps/STRONG Runs/Test/sample1/sample1 R1.fq.gz,
/mnt/strong/tools/apps/STRONG Runs/Test/sample2/sample2 R1.fq.gz,
/mnt/strong/tools/apps/STRONG Runs/Test/sample3/sample3 R1.fq.gz,
/mnt/strong/tools/apps/STRONG Runs/Test/sample4/sample4 R1.fq.gz,
/mnt/strong/tools/apps/STRONG Runs/Test/sample5/sample5 R1.fq.gz,
/mnt/strong/tools/apps/STRONG Runs/Test/sample6/sample6 R1.fq.qz,
/mnt/strong/tools/apps/STRONG Runs/Test/sample7/sample7 R1.fq.qz,
/mnt/strong/tools/apps/STRONG Runs/Test/sample8/sample8 R1.fq.gz,
/mnt/strong/tools/apps/STRONG Runs/Test/sample1/sample1 R2.fq.gz,
/mnt/strong/tools/apps/STRONG_Runs/Test/sample2/sample2_R2.fq.gz,
/mnt/strong/tools/apps/STRONG Runs/Test/sample3/sample3 R2.fq.gz,
/mnt/strong/tools/apps/STRONG Runs/Test/sample4/sample4 R2.fq.gz,
/mnt/strong/tools/apps/STRONG Runs/Test/sample5/sample5 R2.fq.qz,
/mnt/strong/tools/apps/STRONG Runs/Test/sample6/sample6 R2.fq.qz,
/mnt/strong/tools/apps/STRONG Runs/Test/sample7/sample7 R2.fq.gz,
/mnt/strong/tools/apps/STRONG Runs/Test/sample8/sample8 R2.fq.gz
    output: assembly/spades/assembly.fasta, assembly/high res/graph pack.gfa
    log: assembly/spades.log (check log file(s) for error details)
    shell:
        /mnt/strong/tools/apps/STRONG/SPAdes/assembler/bin/spades.py --meta -
-only-assembler --save-gp -t 8 - k 77 -m 2000 -1
/mnt/strong/tools/apps/STRONG Runs/Test/sample1/sample1 R1.fq.qz -1
/mnt/strong/tools/apps/STRONG_Runs/Test/sample2/sample2_R1.fq.gz -1
/mnt/strong/tools/apps/STRONG Runs/Test/sample3/sample3 R1.fq.gz -1
/mnt/strong/tools/apps/STRONG Runs/Test/sample4/sample4 R1.fq.gz -1
/mnt/strong/tools/apps/STRONG Runs/Test/sample5/sample5 R1.fg.qz -1
/mnt/strong/tools/apps/STRONG Runs/Test/sample6/sample6 R1.fq.qz -1
/mnt/strong/tools/apps/STRONG Runs/Test/sample7/sample7 R1.fq.gz -1
/mnt/strong/tools/apps/STRONG Runs/Test/sample8/sample8 R1.fq.gz -2
/mnt/strong/tools/apps/STRONG_Runs/Test/sample1/sample1_R2.fq.gz -2
/mnt/strong/tools/apps/STRONG Runs/Test/sample2/sample2 R2.fq.gz -2
/mnt/strong/tools/apps/STRONG Runs/Test/sample3/sample3 R2.fq.gz -2
/mnt/strong/tools/apps/STRONG Runs/Test/sample4/sample4 R2.fq.gz -2
/mnt/strong/tools/apps/STRONG Runs/Test/sample5/sample5 R2.fq.gz -2
/mnt/strong/tools/apps/STRONG Runs/Test/sample6/sample6 R2.fq.gz -2
/mnt/strong/tools/apps/STRONG Runs/Test/sample7/sample7 R2.fq.qz -2
/mnt/strong/tools/apps/STRONG Runs/Test/sample8/sample8 R2.fq.gz -o
assembly/spades/ &> assembly/spades.log
        cp assembly/spades//contigs.fasta assembly/spades/assembly.fasta
        cp assembly/spades//K77/saves/00 before simplification/graph pack*
$(dirname assembly/high res/graph pack.gfa)
        (one of the commands exited with non-zero exit code; note that
snakemake uses bash strict mode!)
Full Traceback (most recent call last):
  File "/mnt/strong/tools/apps/miniconda3.10/envs/STRONG/lib/python3.10/site-
packages/snakemake/executors/ init .py", line 2561, in run wrapper
    run (
  File "/mnt/strong/tools/apps/STRONG/SnakeNest/Assembly.snake", line 50, in
 rule spades
  File "/mnt/strong/tools/apps/miniconda3.10/envs/STRONG/lib/python3.10/site-
packages/snakemake/shell.py", line 294, in new
    raise sp.CalledProcessError(retcode, cmd)
subprocess.CalledProcessError: Command 'set -euo pipefail;
```

```
/mnt/strong/tools/apps/STRONG/SPAdes/assembler/bin/spades.py --meta -
-only-assembler --save-gp -t 8 -k 77 -m 2000 -1
/mnt/strong/tools/apps/STRONG Runs/Test/sample1/sample1 R1.fq.qz -1
/mnt/strong/tools/apps/STRONG Runs/Test/sample2/sample2 R1.fq.qz -1
/mnt/strong/tools/apps/STRONG Runs/Test/sample3/sample3 R1.fq.qz -1
/mnt/strong/tools/apps/STRONG Runs/Test/sample4/sample4 R1.fq.qz -1
/mnt/strong/tools/apps/STRONG Runs/Test/sample5/sample5 R1.fg.gz -1
/mnt/strong/tools/apps/STRONG Runs/Test/sample6/sample6 R1.fg.gz -1
/mnt/strong/tools/apps/STRONG Runs/Test/sample7/sample7 R1.fq.qz -1
/mnt/strong/tools/apps/STRONG_Runs/Test/sample8/sample8_R1.fq.gz -2
/mnt/strong/tools/apps/STRONG Runs/Test/sample1/sample1 R2.fq.gz -2
/mnt/strong/tools/apps/STRONG Runs/Test/sample2/sample2 R2.fq.gz -2
/mnt/strong/tools/apps/STRONG Runs/Test/sample3/sample3 R2.fq.qz -2
/mnt/strong/tools/apps/STRONG Runs/Test/sample4/sample4 R2.fq.gz -2
/mnt/strong/tools/apps/STRONG Runs/Test/sample5/sample5 R2.fq.gz -2
/mnt/strong/tools/apps/STRONG Runs/Test/sample6/sample6 R2.fq.gz -2
/mnt/strong/tools/apps/STRONG_Runs/Test/sample7/sample7_R2.fq.gz -2
/mnt/strong/tools/apps/STRONG Runs/Test/sample8/sample8 R2.fq.gz -o
assembly/spades/ &> assembly/spades.log
        cp assembly/spades//contigs.fasta assembly/spades/assembly.fasta
        cp assembly/spades//K77/saves/00 before simplification/graph pack*
$(dirname assembly/high res/graph pack.gfa)' returned non-zero exit status
127.
During handling of the above exception, another exception occurred:
Traceback (most recent call last):
  File "/mnt/strong/tools/apps/miniconda3.10/envs/STRONG/lib/python3.10/site-
packages/snakemake/executors/ init .py", line 656, in callback
    raise ex
  File
"/mnt/strong/tools/apps/miniconda3.10/envs/STRONG/lib/python3.10/concurrent/f
utures/thread.py", line 58, in run
    result = self.fn(*self.args, **self.kwargs)
  File "/mnt/strong/tools/apps/miniconda3.10/envs/STRONG/lib/python3.10/site-
packages/snakemake/executors/ init .py", line 642, in cached or run
    run func(*args)
  File "/mnt/strong/tools/apps/miniconda3.10/envs/STRONG/lib/python3.10/site-
packages/snakemake/executors/ init .py", line 2597, in run wrapper
    raise RuleException(
snakemake.exceptions.RuleException: CalledProcessError in file
/mnt/strong/tools/apps/STRONG/SnakeNest/Assembly.snake, line 22:
Command 'set -euo pipefail;
        /mnt/strong/tools/apps/STRONG/SPAdes/assembler/bin/spades.py --meta -
-only-assembler --save-gp -t 8 - k 77 -m 2000 -1
/mnt/strong/tools/apps/STRONG Runs/Test/sample1/sample1 R1.fq.gz -1
/mnt/strong/tools/apps/STRONG Runs/Test/sample2/sample2 R1.fq.gz -1
/mnt/strong/tools/apps/STRONG Runs/Test/sample3/sample3 R1.fg.gz -1
/mnt/strong/tools/apps/STRONG Runs/Test/sample4/sample4 R1.fq.gz -1
/mnt/strong/tools/apps/STRONG Runs/Test/sample5/sample5 R1.fq.gz -1
/mnt/strong/tools/apps/STRONG Runs/Test/sample6/sample6 R1.fq.gz -1
/mnt/strong/tools/apps/STRONG Runs/Test/sample7/sample7 R1.fq.gz -1
/mnt/strong/tools/apps/STRONG Runs/Test/sample8/sample8 R1.fq.gz -2
/mnt/strong/tools/apps/STRONG Runs/Test/sample1/sample1 R2.fq.qz -2
/mnt/strong/tools/apps/STRONG Runs/Test/sample2/sample2 R2.fg.gz -2
/mnt/strong/tools/apps/STRONG Runs/Test/sample3/sample3 R2.fq.gz -2
/mnt/strong/tools/apps/STRONG Runs/Test/sample4/sample4 R2.fq.gz -2
```

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/mnt/strong/tools/apps/STRONG Runs/Test/sample5/sample5 R2.fq.gz -2
/mnt/strong/tools/apps/STRONG Runs/Test/sample6/sample6 R2.fq.gz -2
/mnt/strong/tools/apps/STRONG Runs/Test/sample7/sample7_R2.fq.gz -2
/mnt/strong/tools/apps/STRONG Runs/Test/sample8/sample8 R2.fq.qz -o
assembly/spades/ &> assembly/spades.log
        cp assembly/spades//contigs.fasta assembly/spades/assembly.fasta
        cp assembly/spades//K77/saves/00 before simplification/graph pack*
$(dirname assembly/high res/graph pack.gfa)' returned non-zero exit status
127.
 File "/mnt/strong/tools/apps/STRONG/SnakeNest/Assembly.snake", line 22, in
rule spades
RuleException:
CalledProcessError in file
/mnt/strong/tools/apps/STRONG/SnakeNest/Assembly.snake, line 22:
Command 'set -euo pipefail;
        /mnt/strong/tools/apps/STRONG/SPAdes/assembler/bin/spades.py --meta -
-only-assembler --save-gp -t 8 - k 77 -m 2000 -1
/mnt/strong/tools/apps/STRONG Runs/Test/sample1/sample1 R1.fq.gz -1
/mnt/strong/tools/apps/STRONG Runs/Test/sample2/sample2 R1.fq.gz -1
/mnt/strong/tools/apps/STRONG Runs/Test/sample3/sample3 R1.fq.qz -1
/mnt/strong/tools/apps/STRONG Runs/Test/sample4/sample4 R1.fq.gz -1
/mnt/strong/tools/apps/STRONG Runs/Test/sample5/sample5 R1.fq.qz -1
/mnt/strong/tools/apps/STRONG_Runs/Test/sample6/sample6_R1.fq.gz -1
/mnt/strong/tools/apps/STRONG Runs/Test/sample7/sample7 R1.fq.gz -1
/mnt/strong/tools/apps/STRONG Runs/Test/sample8/sample8 R1.fq.gz -2
/mnt/strong/tools/apps/STRONG Runs/Test/sample1/sample1 R2.fq.qz -2
/mnt/strong/tools/apps/STRONG Runs/Test/sample2/sample2 R2.fq.qz -2
/mnt/strong/tools/apps/STRONG Runs/Test/sample3/sample3 R2.fq.gz -2
/mnt/strong/tools/apps/STRONG Runs/Test/sample4/sample4 R2.fq.gz -2
/mnt/strong/tools/apps/STRONG_Runs/Test/sample5/sample5_R2.fq.gz -2
/mnt/strong/tools/apps/STRONG Runs/Test/sample6/sample6 R2.fq.gz -2
/mnt/strong/tools/apps/STRONG Runs/Test/sample7/sample7 R2.fq.gz -2
/mnt/strong/tools/apps/STRONG Runs/Test/sample8/sample8 R2.fg.gz -o
assembly/spades/ &> assembly/spades.log
        cp assembly/spades//contigs.fasta assembly/spades/assembly.fasta
        cp assembly/spades//K77/saves/00 before simplification/graph pack*
$(dirname assembly/high res/graph pack.gfa)' returned non-zero exit status
127.
 File "/mnt/strong/tools/apps/STRONG/SnakeNest/Assembly.snake", line 22, in
__rule spades
"/mnt/strong/tools/apps/miniconda3.10/envs/STRONG/lib/python3.10/concurrent/f
utures/thread.py", line 58, in run
Resources before job selection: {' cores': 8, ' nodes': 9223372036854775807}
Ready jobs (1)
Select jobs to execute...
Using greedy selector because only single job has to be scheduled.
Selected jobs (1)
Resources after job selection: { 'cores': 7, 'nodes': 9223372036854775806}
[Wed Jul 19 10:00:59 2023]
rule reads yaml:
   output: samples.yaml
   jobid: 33
    reason: Missing output files: samples.yaml
    resources: tmpdir=/tmp
```

```
Config file config.yaml is extended by additional config specified via the
command line.
Building DAG of jobs...
Using shell: /usr/bin/bash
Provided cores: 8
Rules claiming more threads will be scaled down.
Select jobs to execute...
[Wed Jul 19 10:00:59 2023]
Finished job 33.
1 of 146 steps (1%) done
Exiting because a job execution failed. Look above for error message
Complete log: .snakemake/log/2023-07-19T100058.643637.snakemake.log
unlocking
removing lock
removing lock
removed all locks
Traceback (most recent call last):
  File "/mnt/strong/tools/apps/STRONG/./bin/STRONG", line 94, in <module>
    call snake(["--snakefile", "SnakeNest/SCogSubGraph.snake"])
  File "/mnt/strong/tools/apps/STRONG/./bin/STRONG", line 83, in call snake
    subprocess.check call(base params + extra params, stdout=sys.stdout,
stderr=sys.stderr)
 File
"/mnt/strong/tools/apps/miniconda3.10/envs/STRONG/lib/python3.10/subprocess.p
y", line 369, in check call
    raise CalledProcessError(retcode, cmd)
subprocess.CalledProcessError: Command '['snakemake', '--directory',
'/mnt/strong/tools/apps/STRONG Runs/TestResults', '--cores', '8', '--config',
'LOCAL DIR=/mnt/strong/tools/apps/STRONG', '--
configfile=/mnt/strong/tools/apps/STRONG Runs/TestResults/config.yaml', '--
latency-wait', '120', '-k', '-p', '-r', '--verbose', '--snakefile',
'SnakeNest/SCogSubGraph.snake']' returned non-zero exit status 1.
```