Job-tree

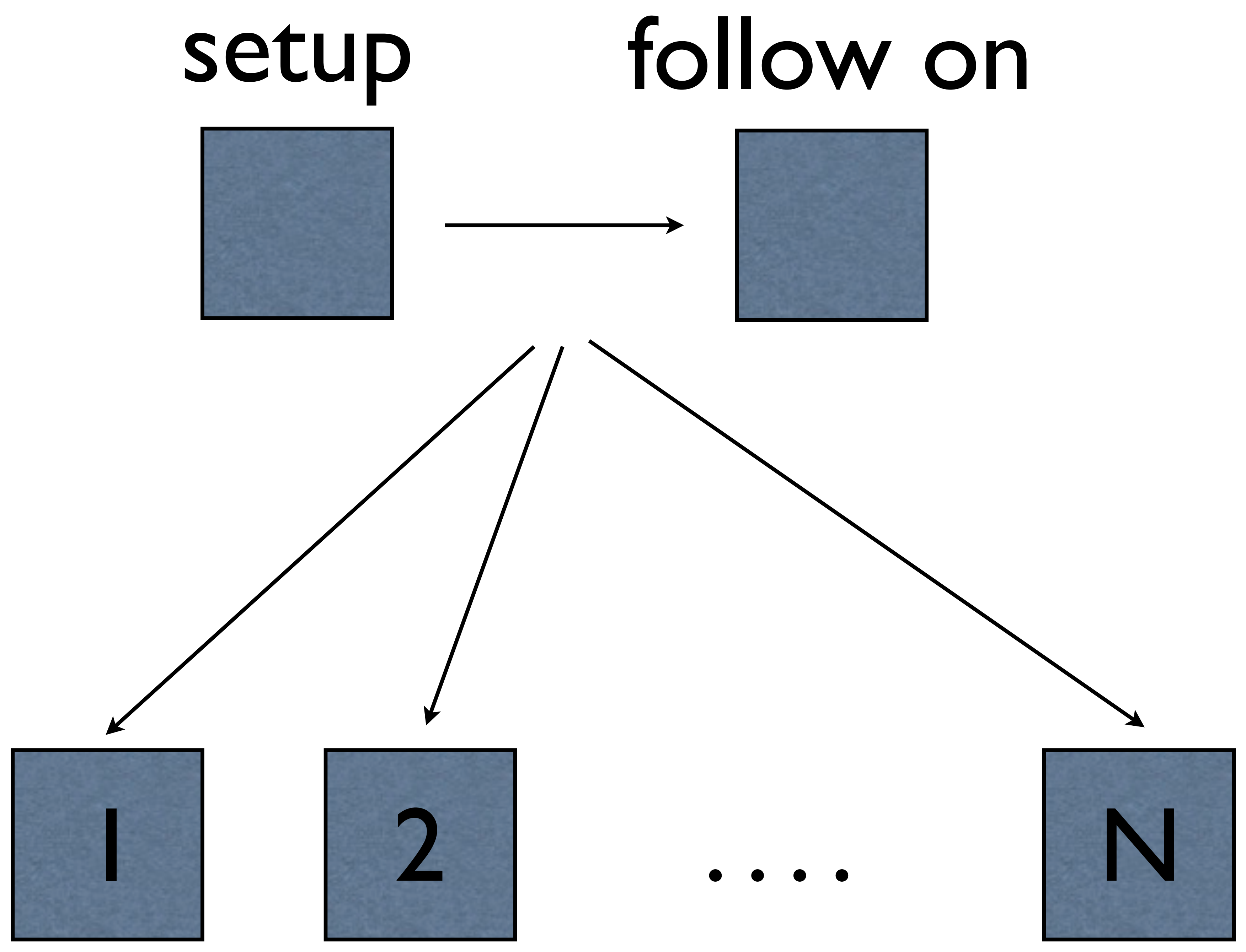
benedict@soe.ucsc.edu

First off...

- Get it at github...
  - https://benedictpaten@github.com/benedictpaten/jobTree.git
  - git@github.com:benedictpaten/jobTree.git

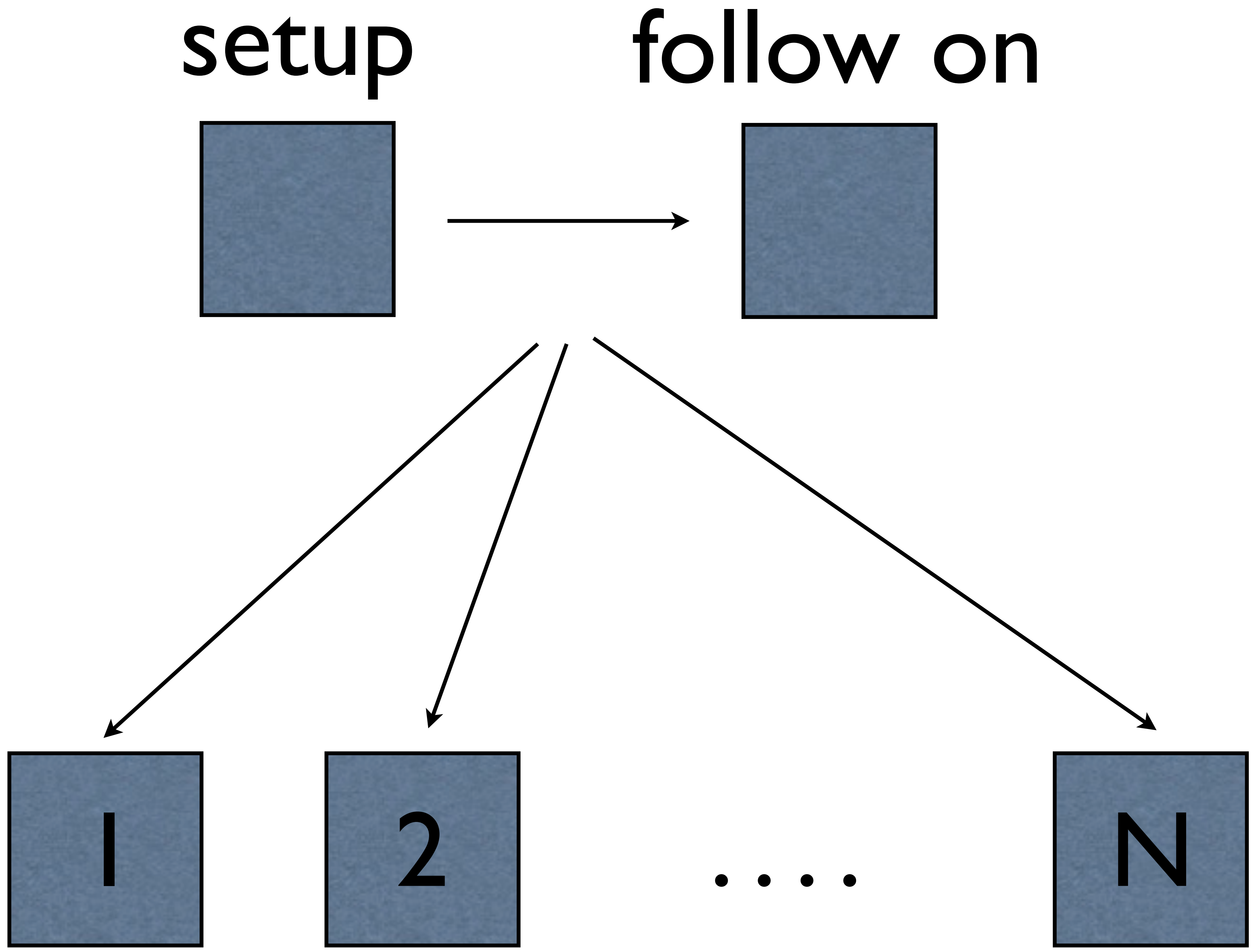
Traditional Batch System

- Composed of a series of 'jobs'
- Single 'setup' job
- Parallel 'child' job
- Single 'follow on' job



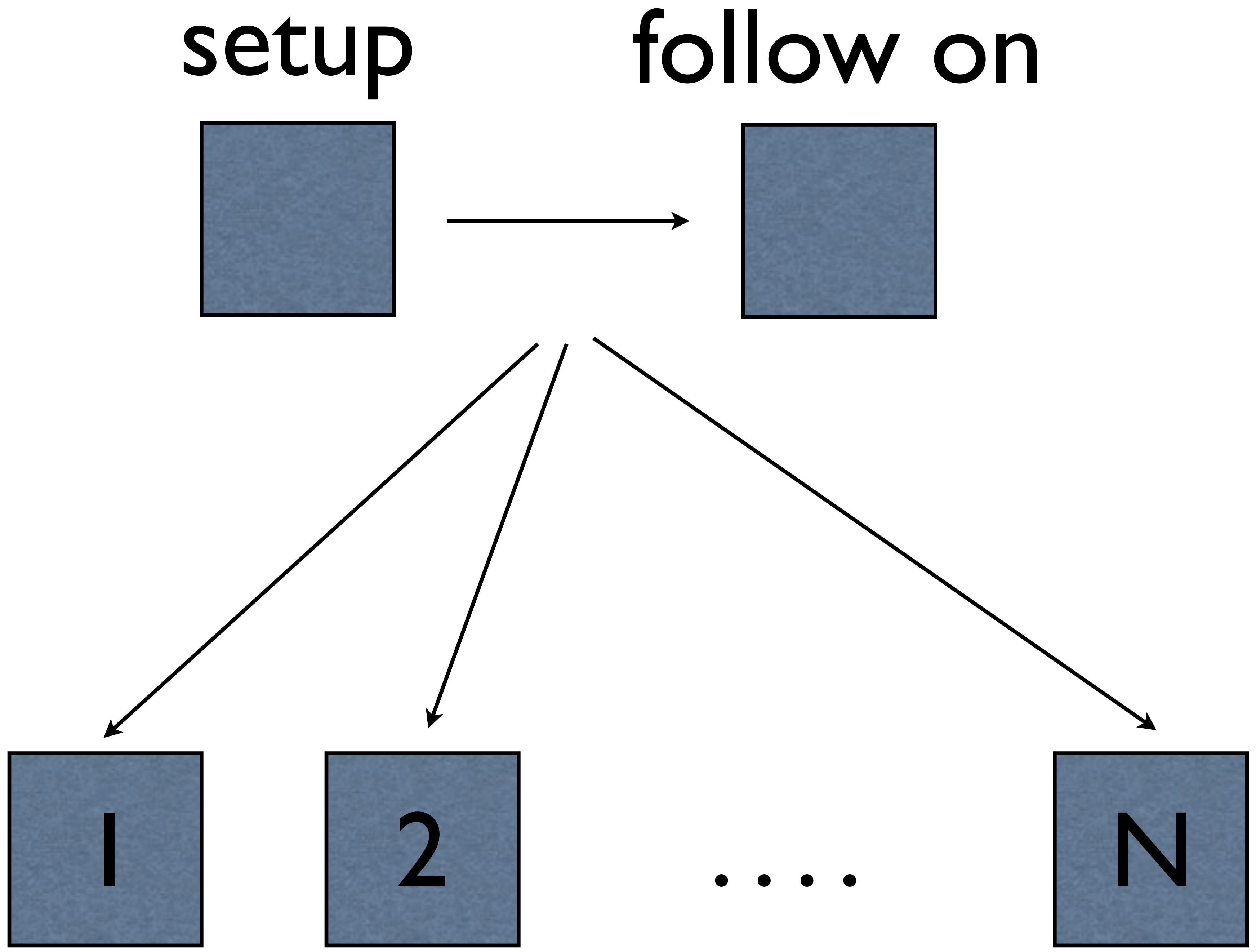
Traditional Batch System

- Setup creates inputs for children
- Children create output
- Follow on aggregates output



Traditional Batch System

- Jobs can get lost at any point during their runtime.
- To maintain 'atomicity' jobs must always be restartable, therefore:
  - No job must alter its own input.
  - The follow on 'cleans up' the setup job



Traditional Batch System Summary

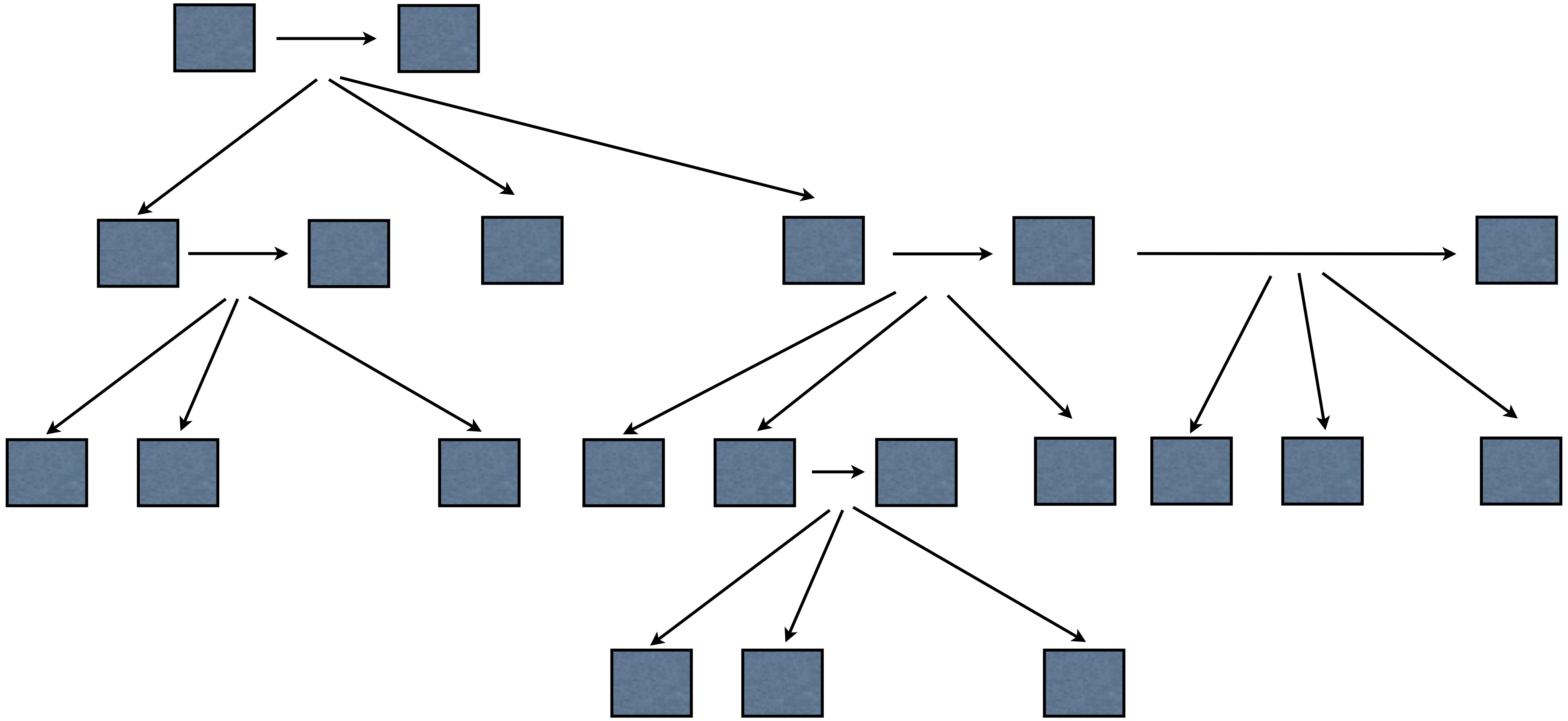
- Traditional batch system can be described, from the users point of view, as a parallel ‘for’ loop.
- Robust pipelines must maintain atomicity

Job-tree

- For loops are useful, but what if..
  - I want to further parallelise a ‘child’ job?
  - I want to do this selectively?
  - I want to do this dynamically and recursively?

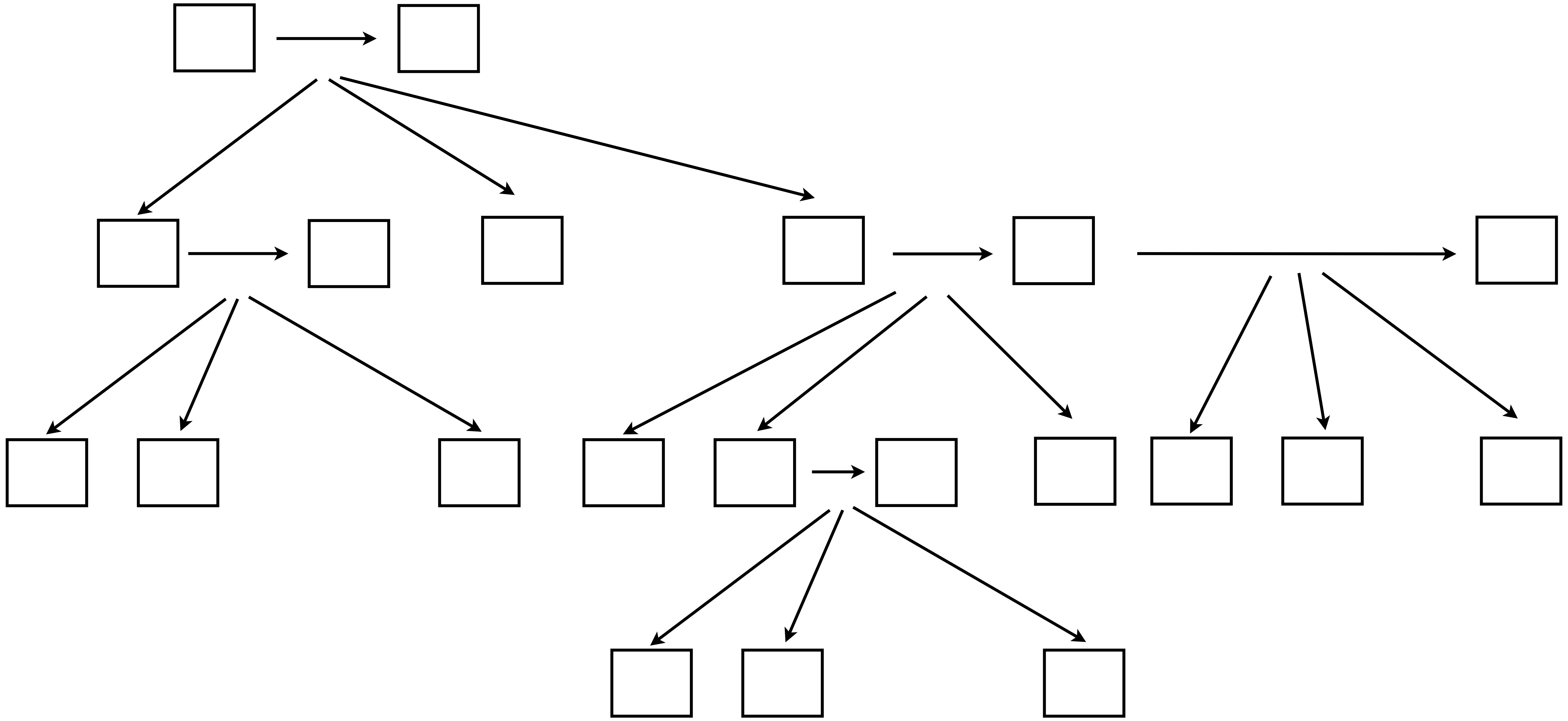
Job-tree

- Job-tree allows you to create arbitrary ‘job-trees’



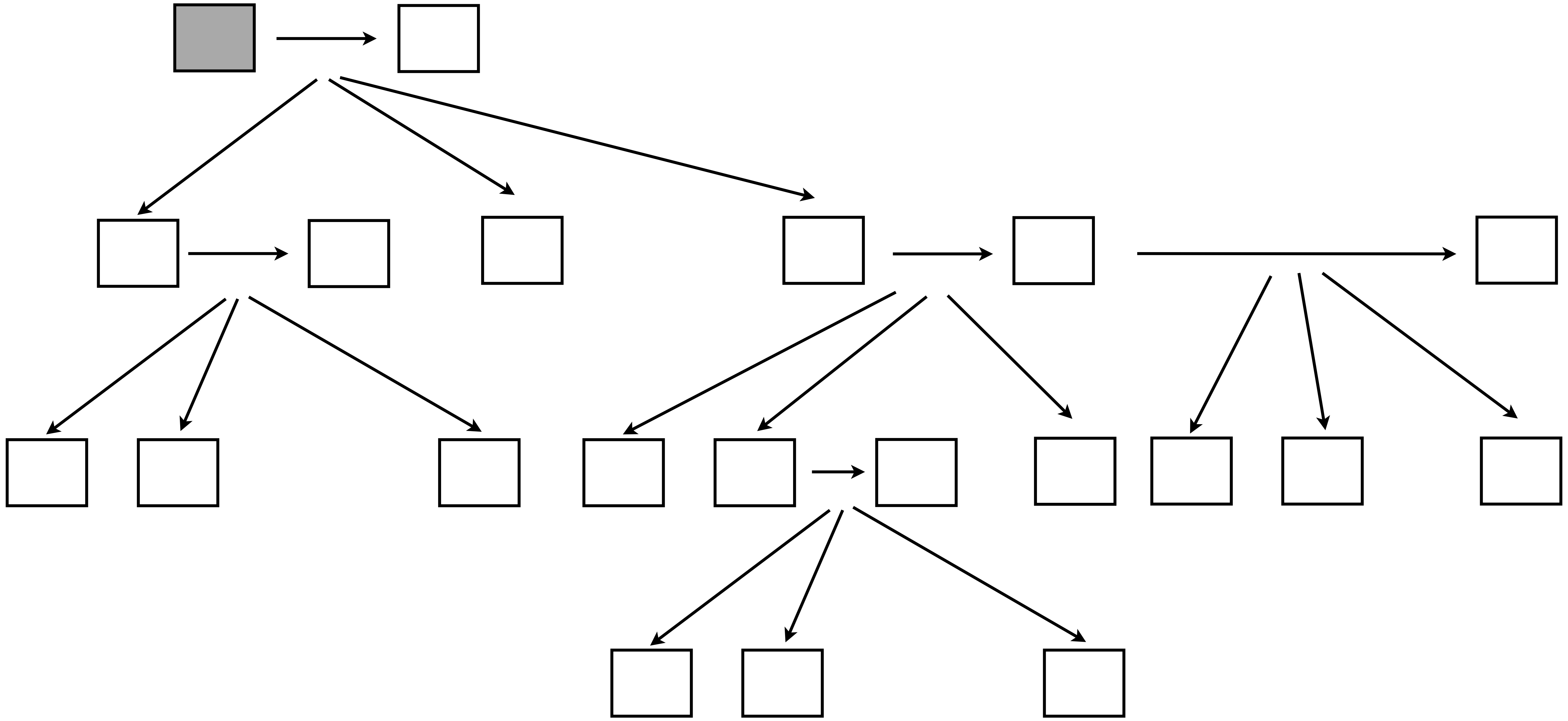
Job-tree

- Let's walk through an example.



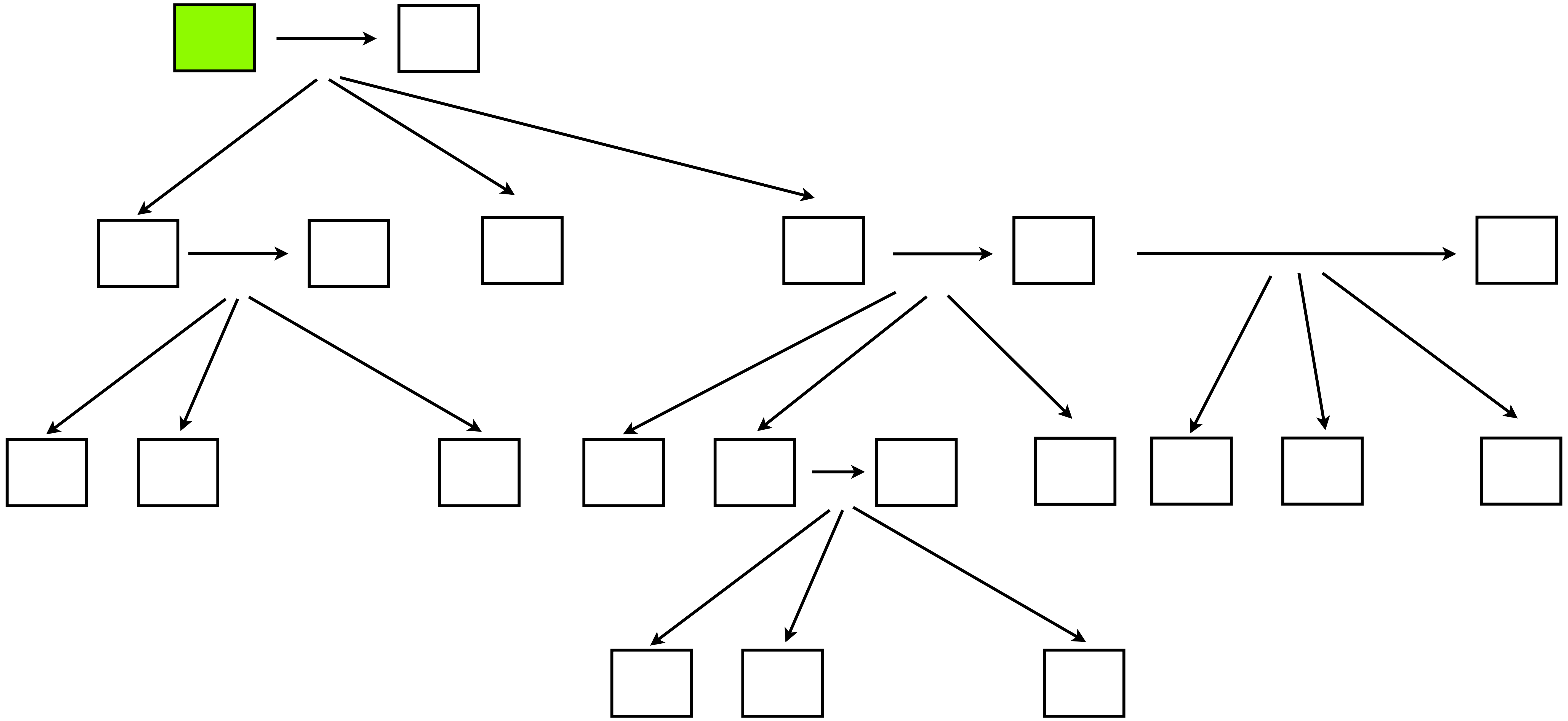
Job-tree

- The first job is issued to the system (grey)
- White boxes are jobs not yet created.



Job-tree

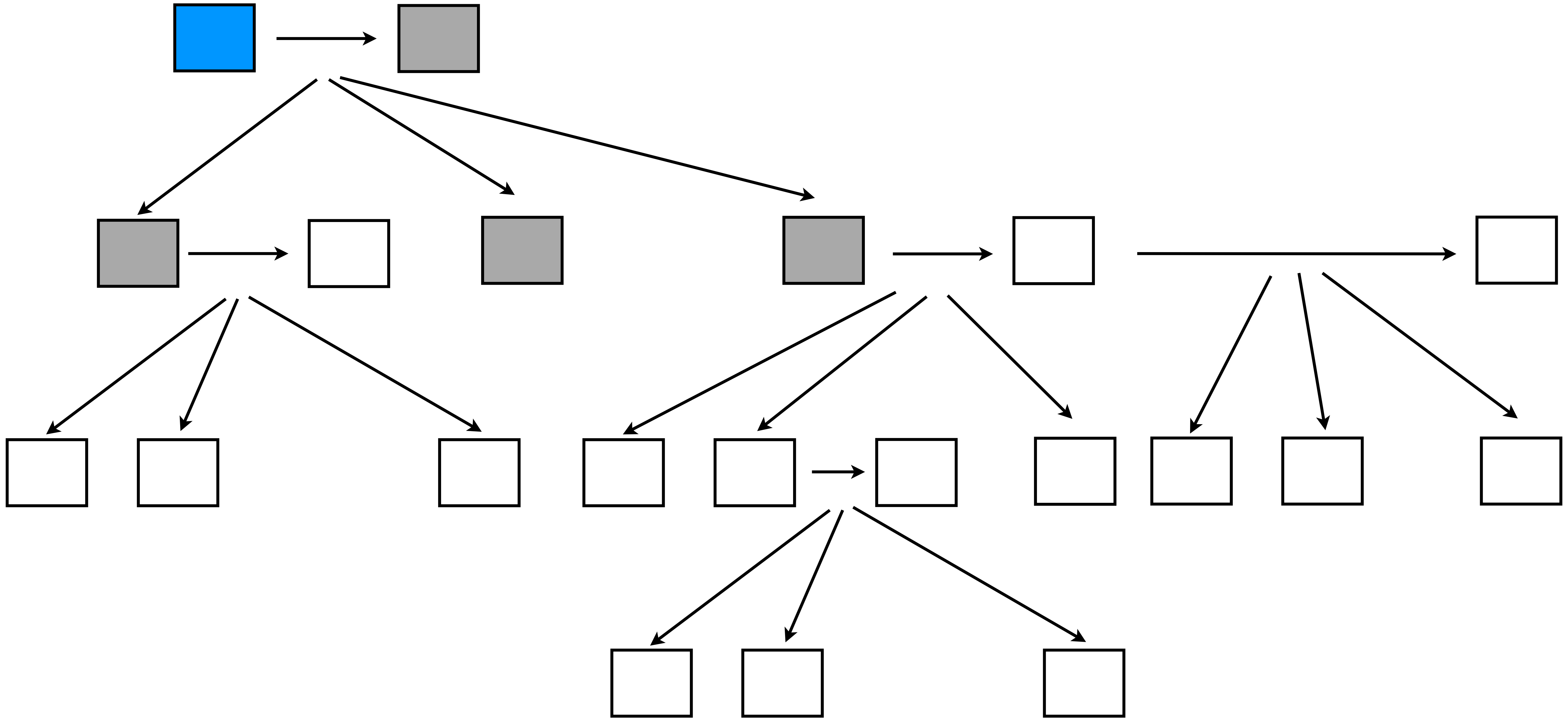
- The first job is run (green)



Job-tree

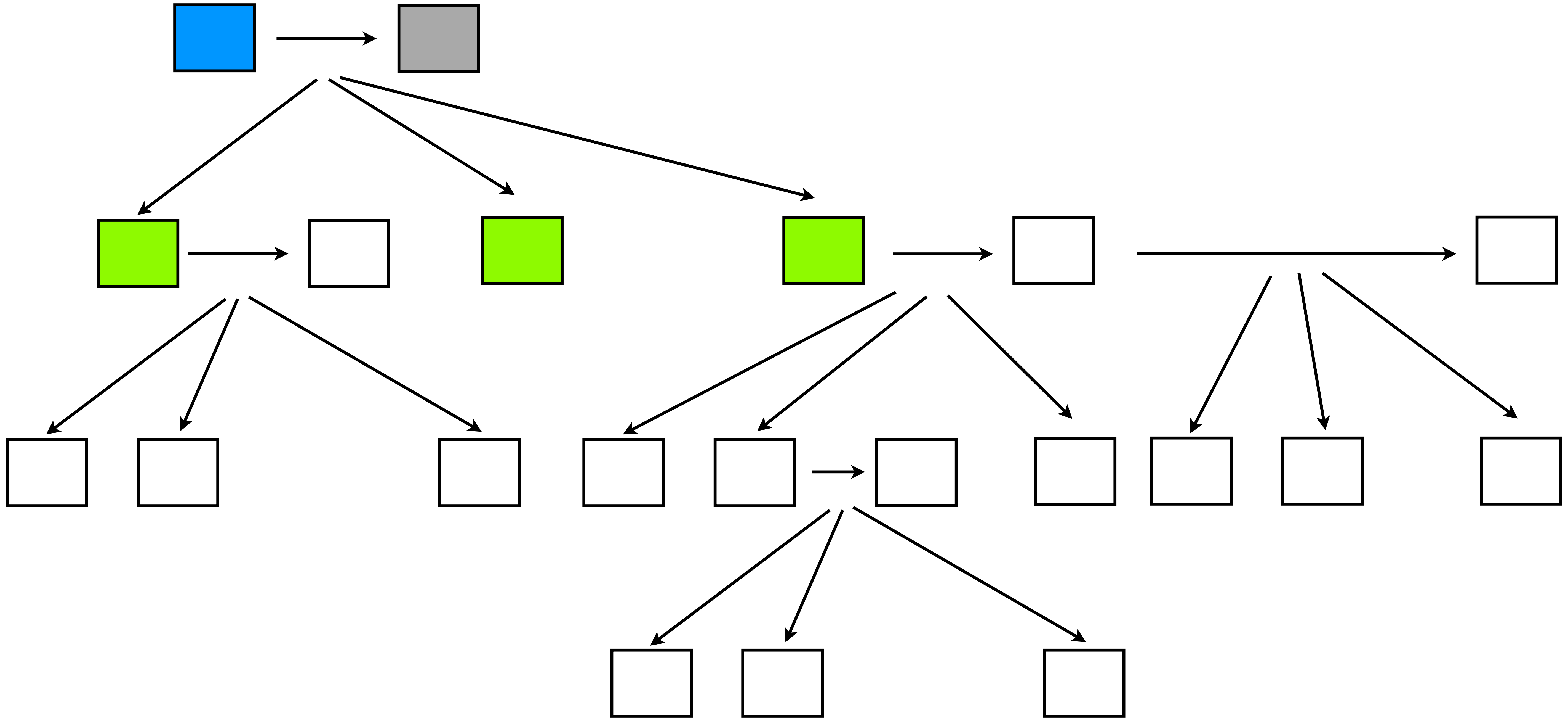
- It completes successively and creates some children and a follow on.

- It is blue, indicating it has children/follow ons not yet complete.



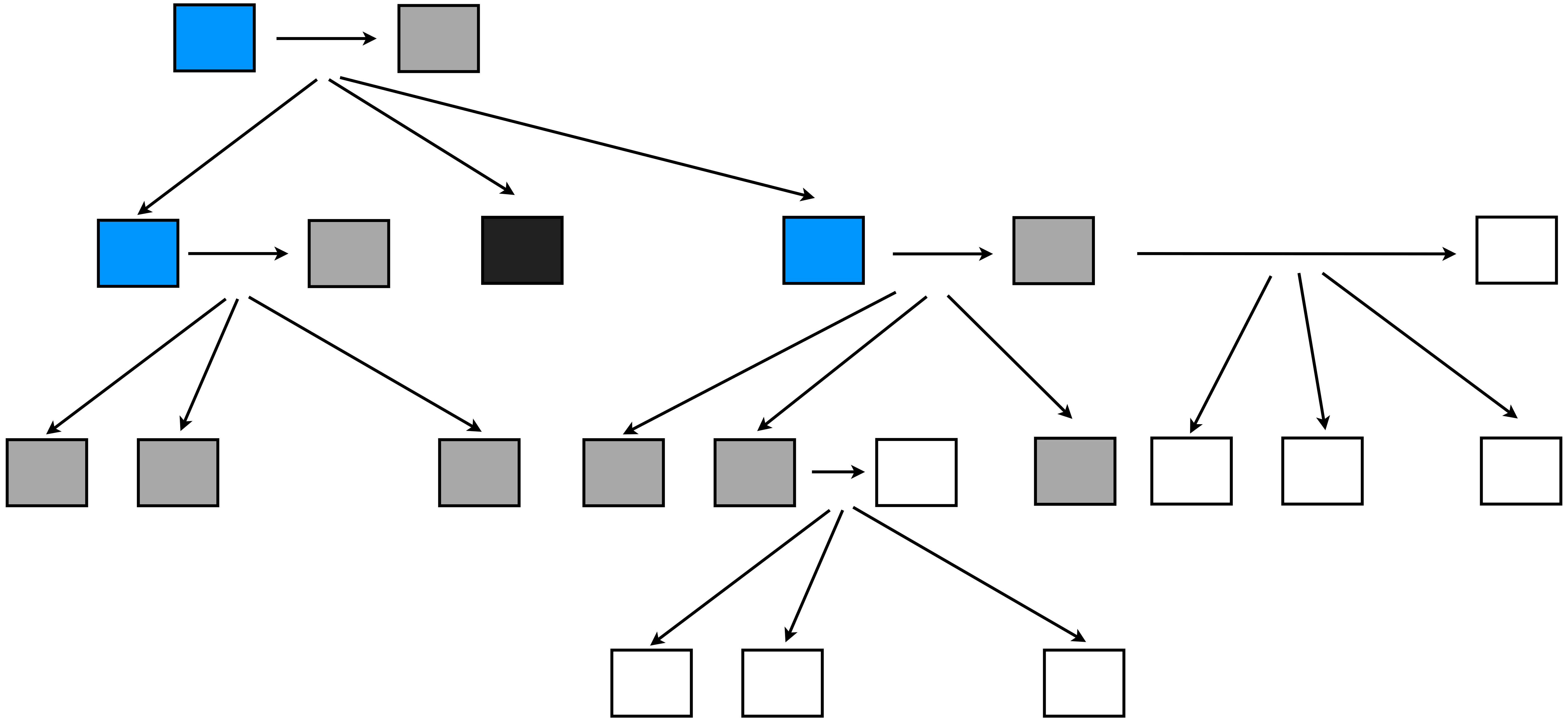
Job-tree

- The children are run



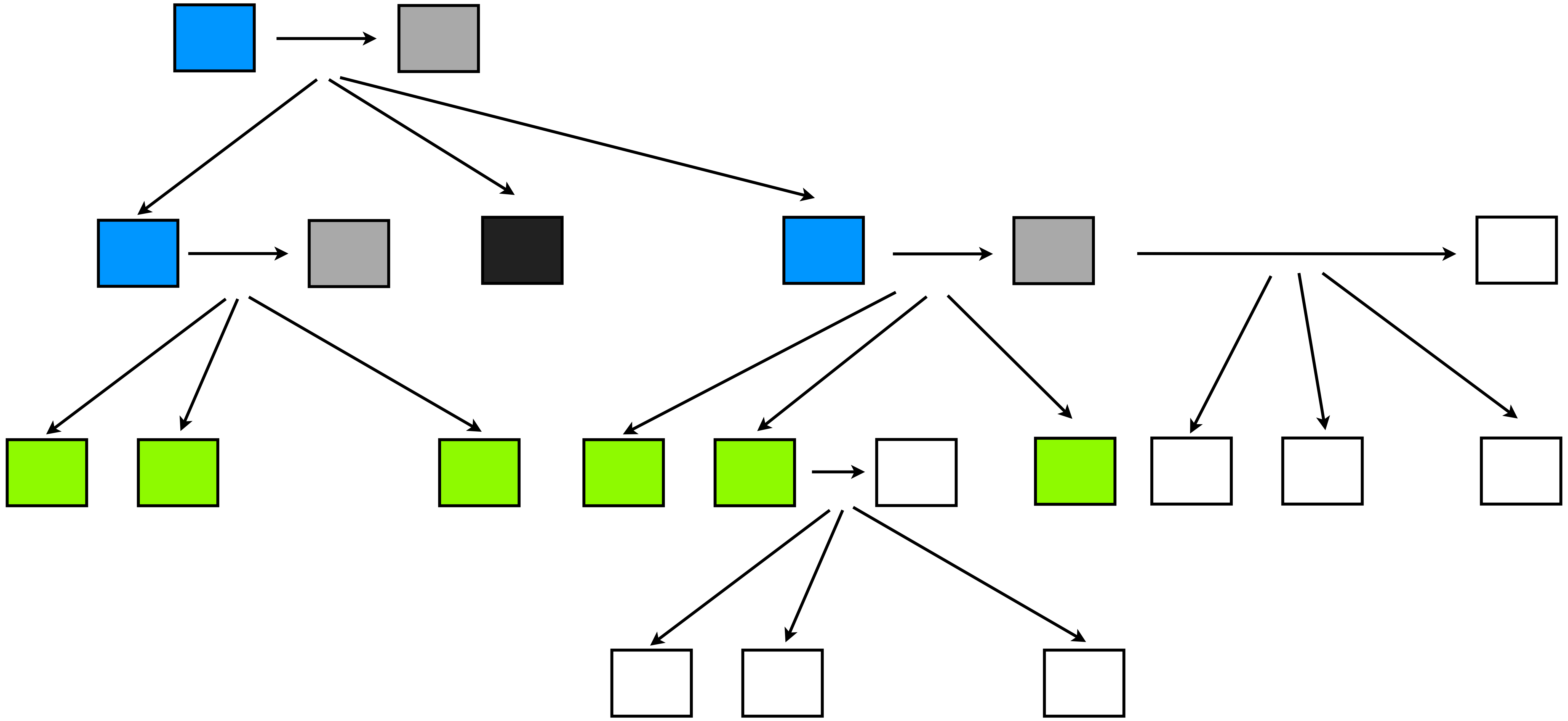
Job-tree

- Some create children and follow ons.
- Some do not, they are now complete (coloured black)



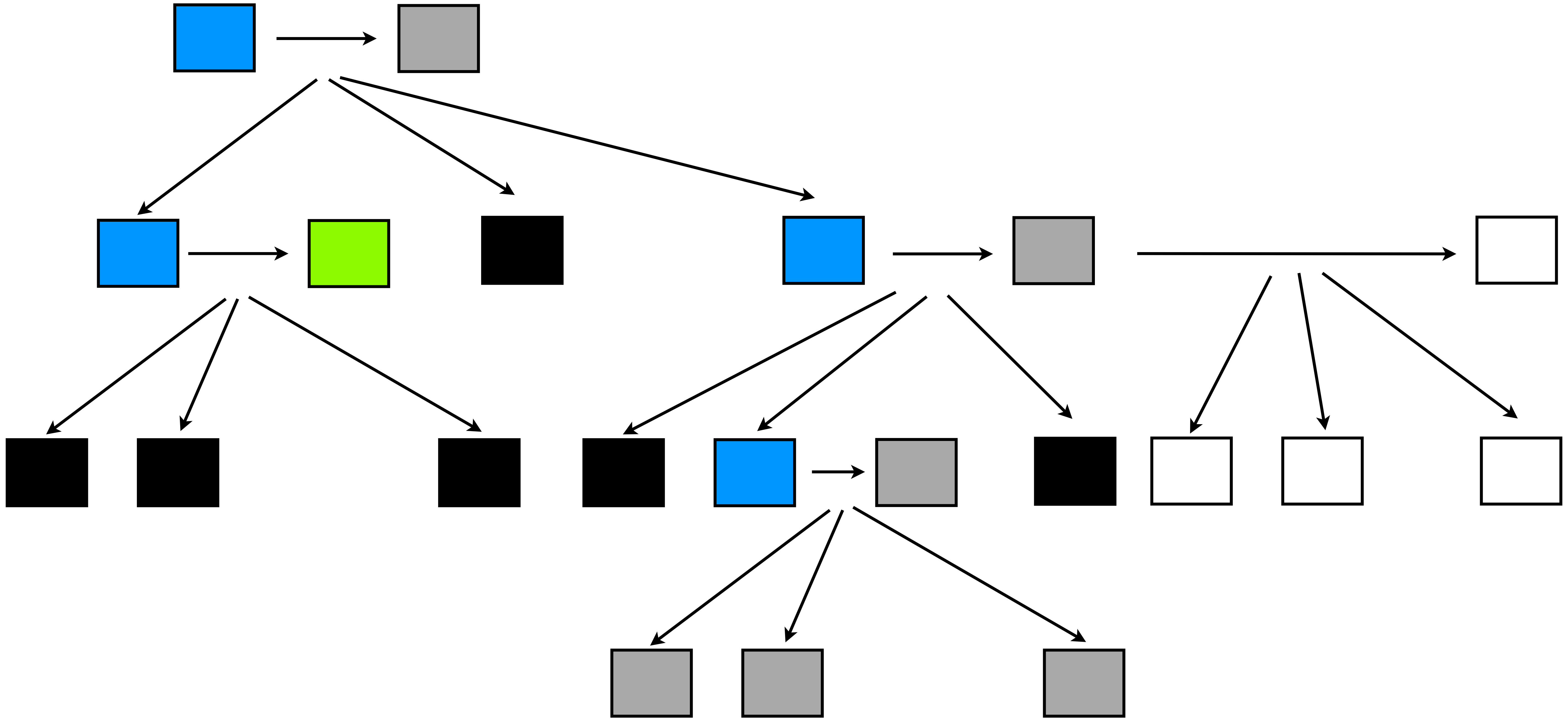
Job-tree

- More children are run



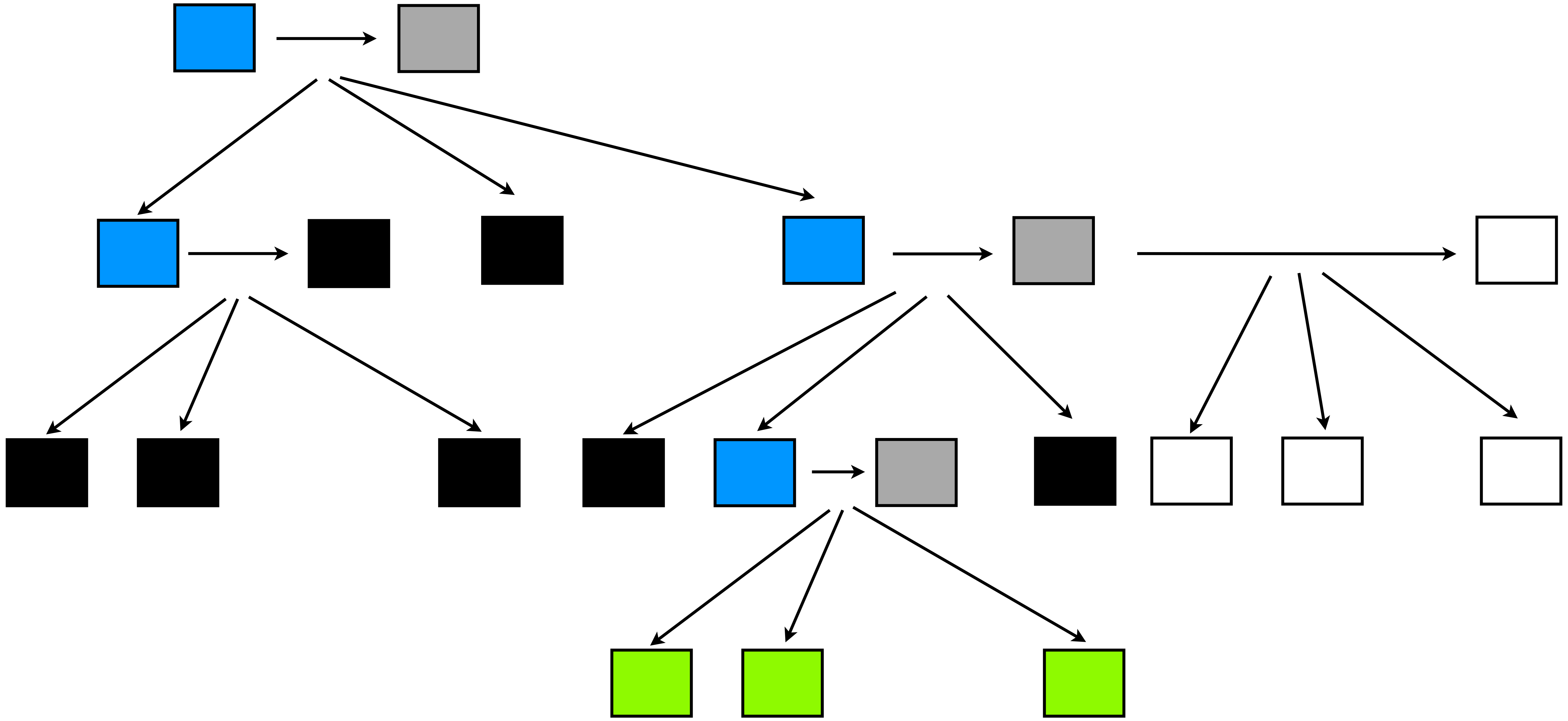
Job-tree

- Most are finished, one creates more children, and one follow can be run



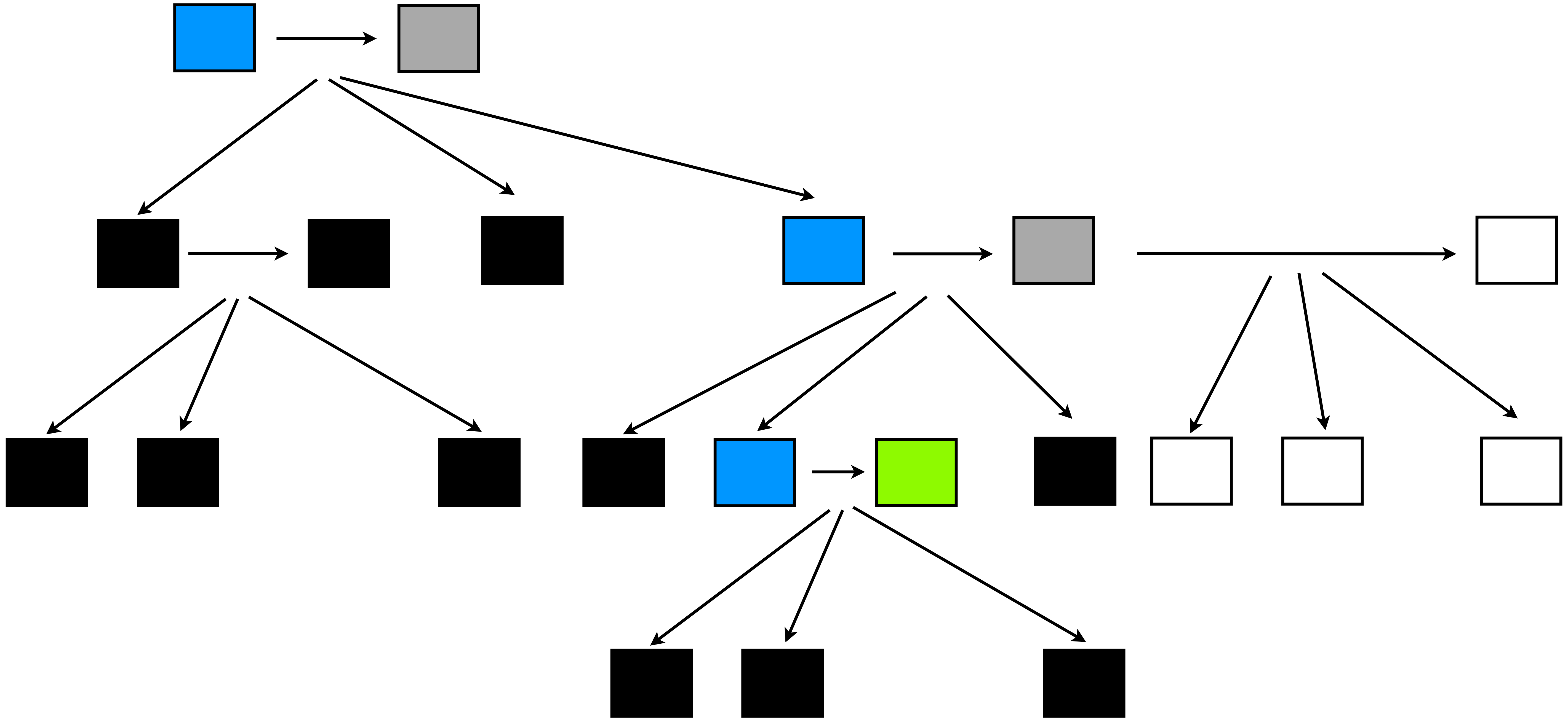
Job-tree

- etc, etc..



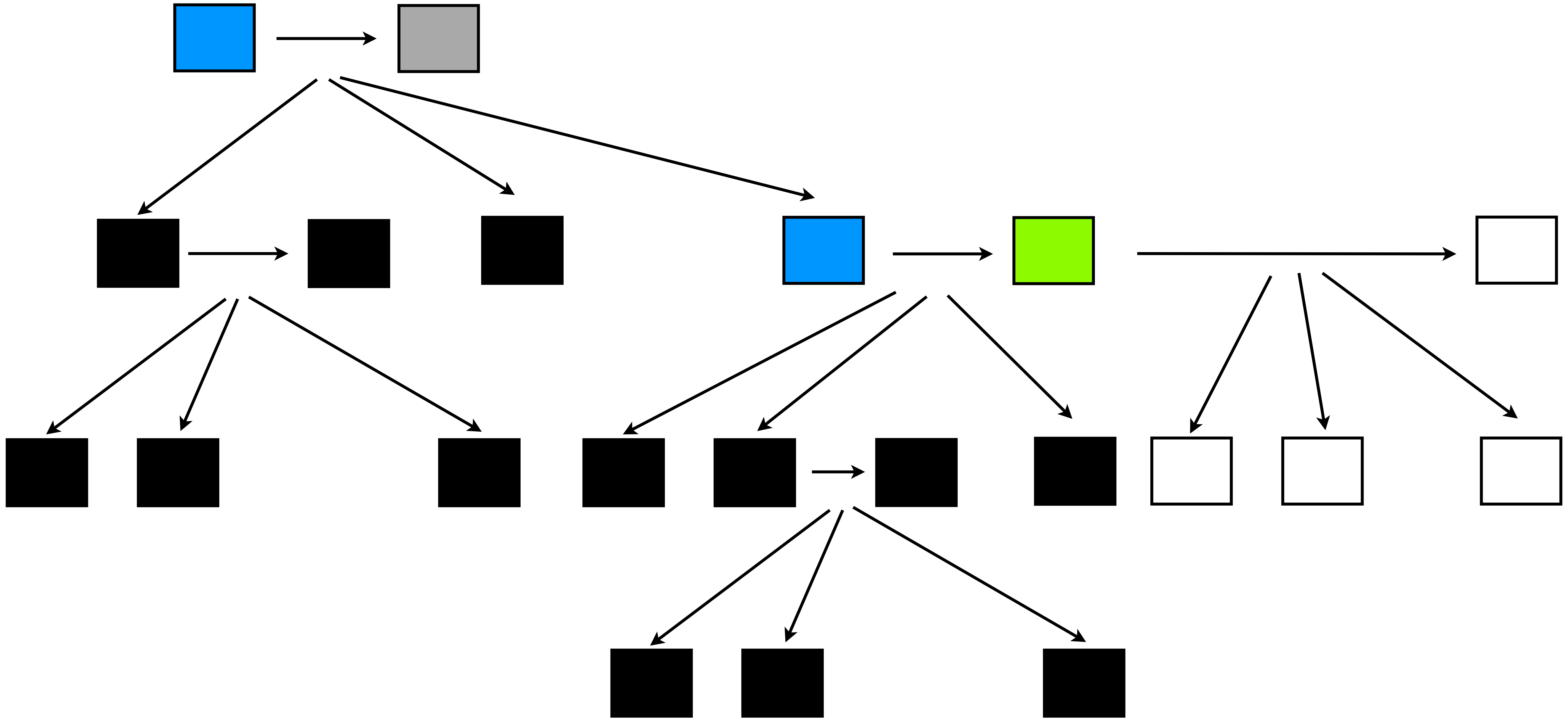
Job-tree

- etc, etc..



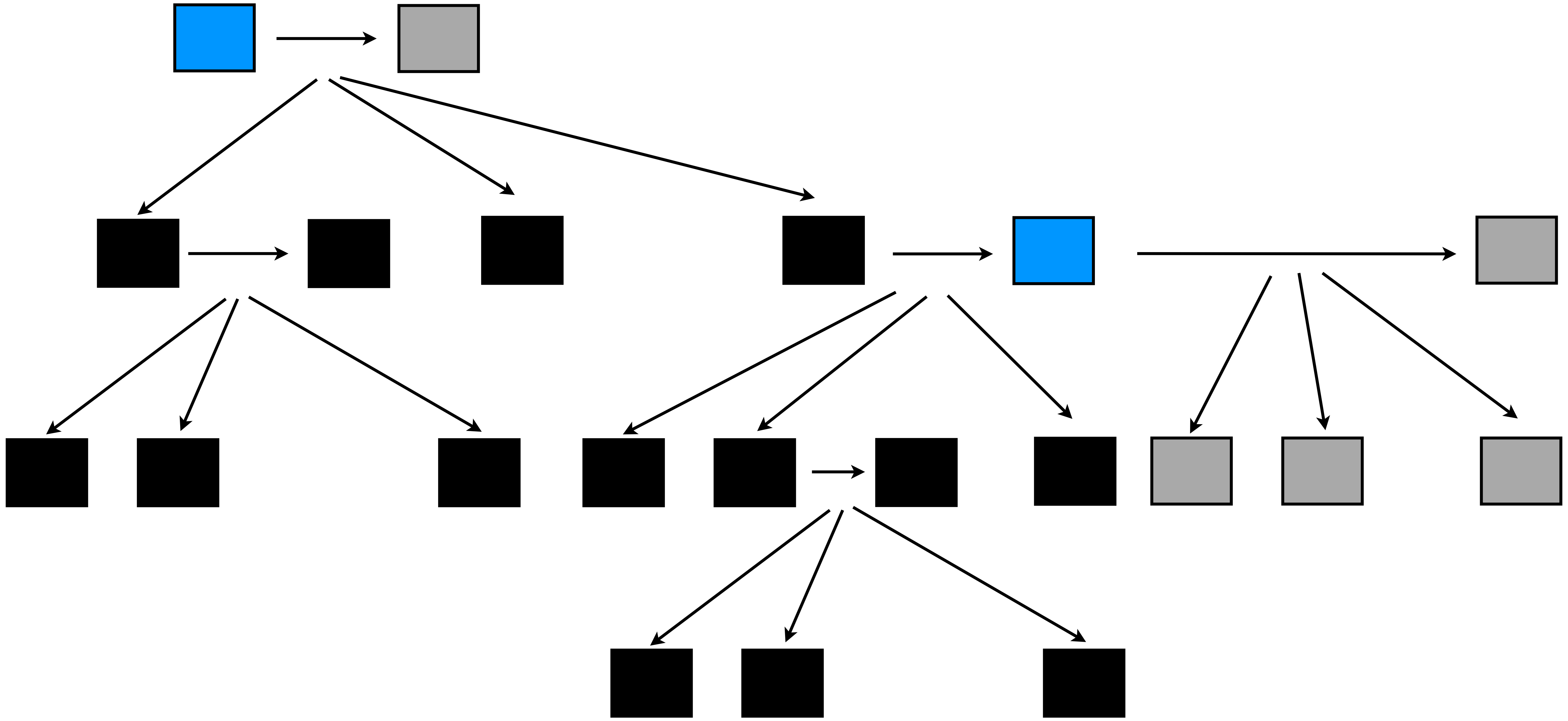
Job-tree

- etc, etc..



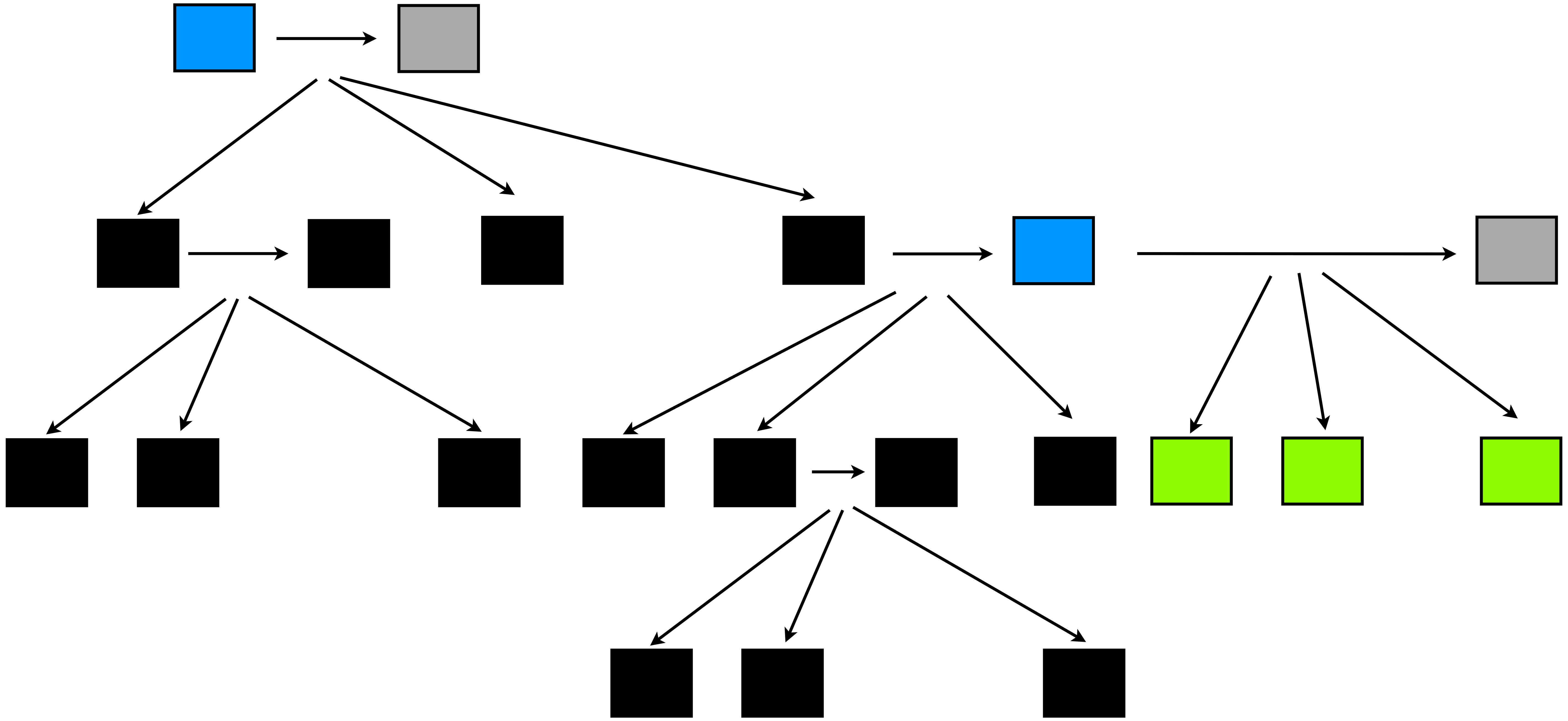
Job-tree

- etc, etc..



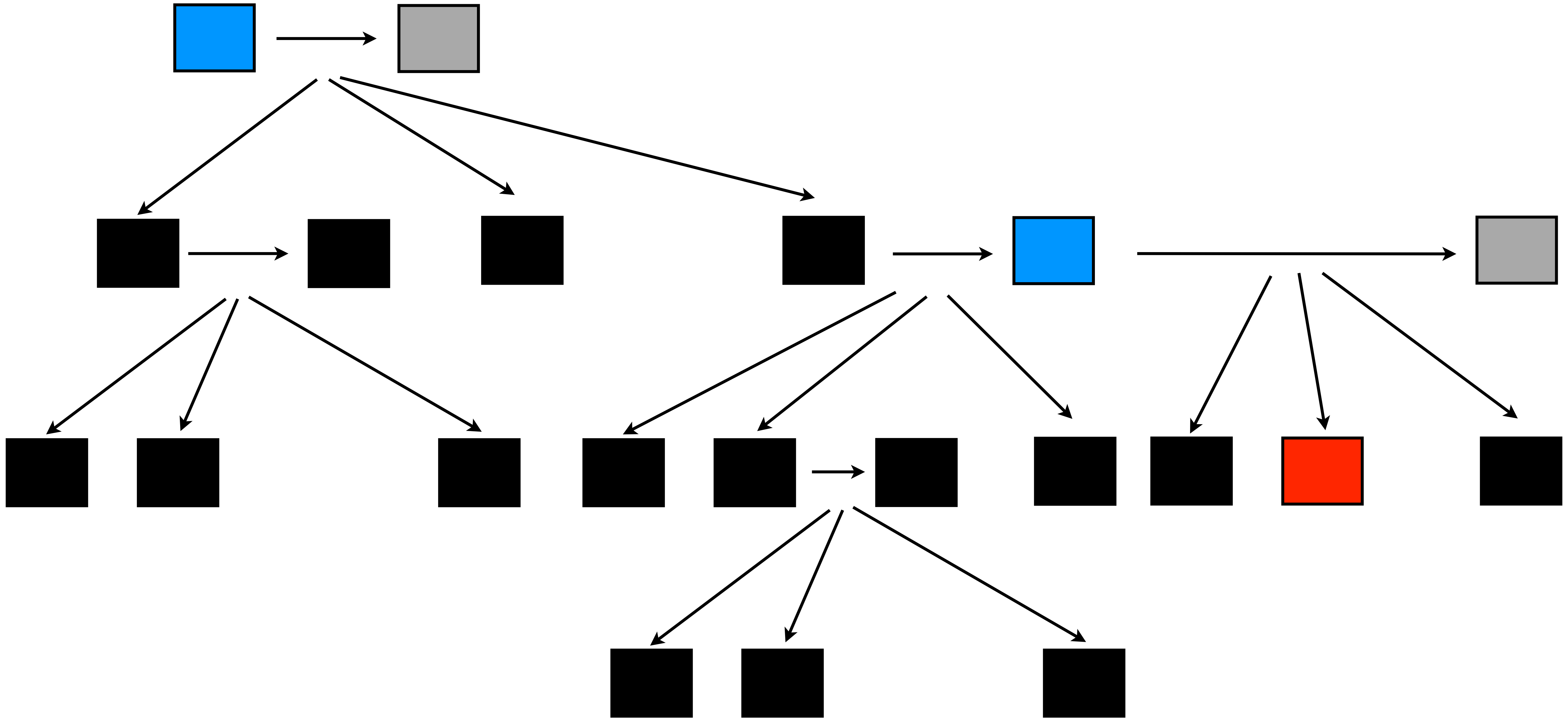
Job-tree

- etc, etc..



Job-tree

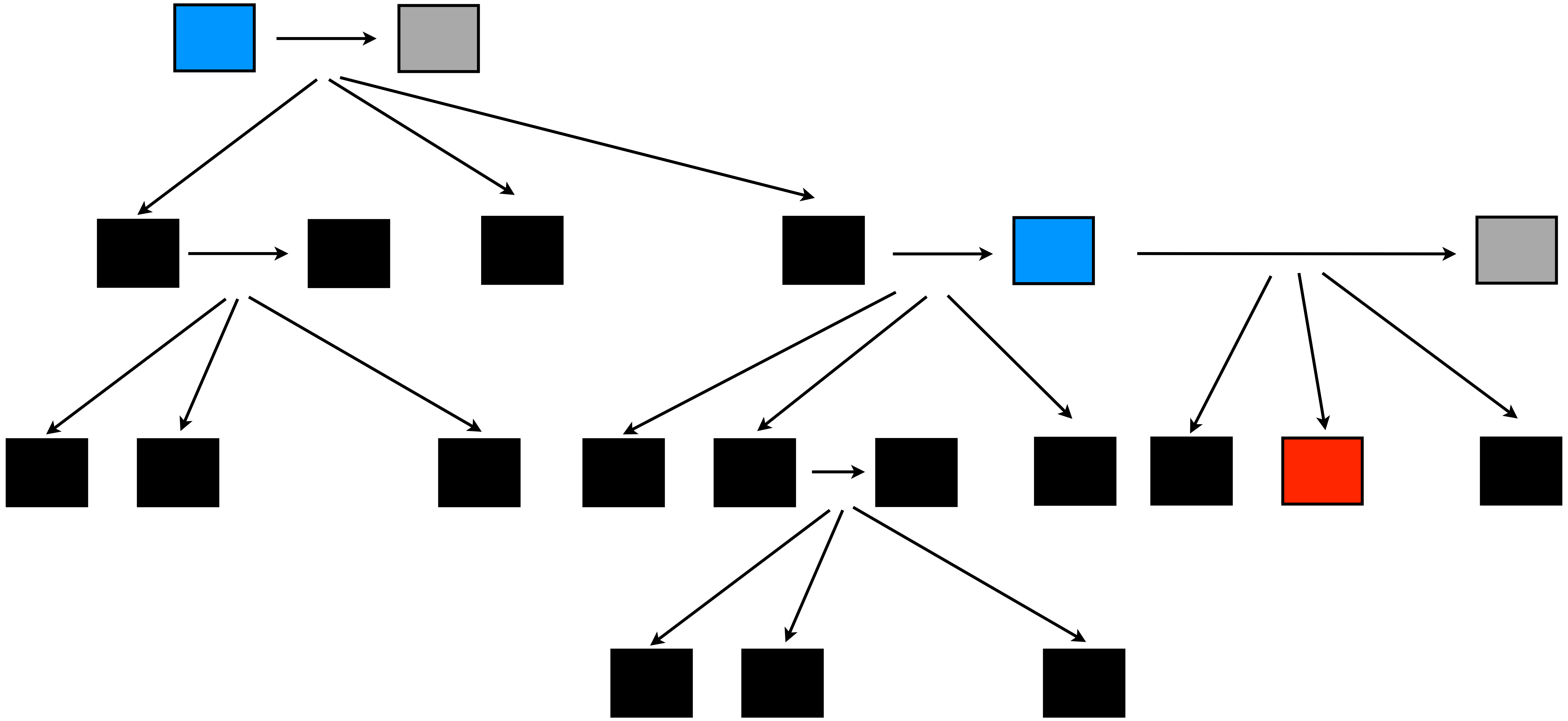
- Oh no! A job failed (coloured red)
    - It will be restarted a preset number of times.



Job-tree

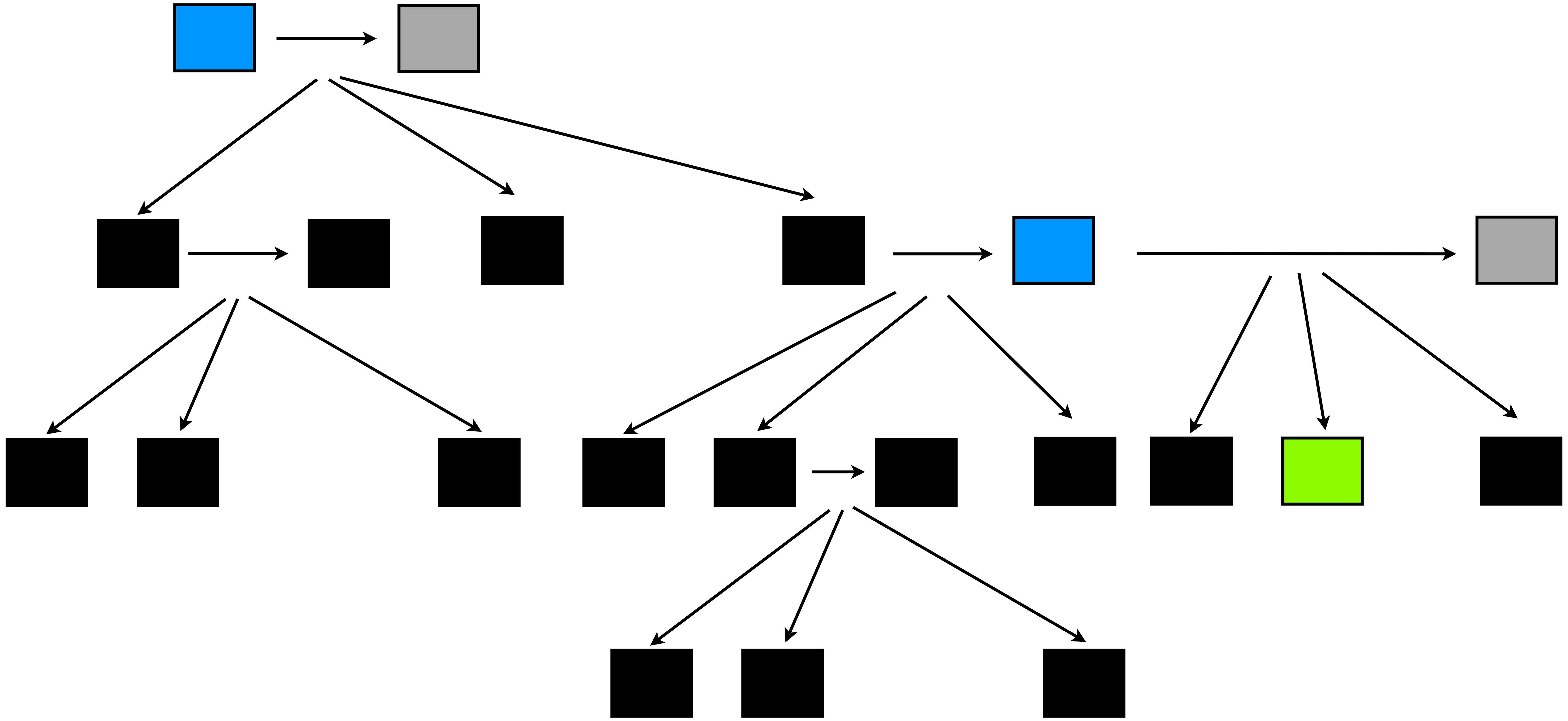
- If it still fails Job-tree will continue as far as it can, then return, so you can fix the job.

- Job-tree will then re-start from that point.



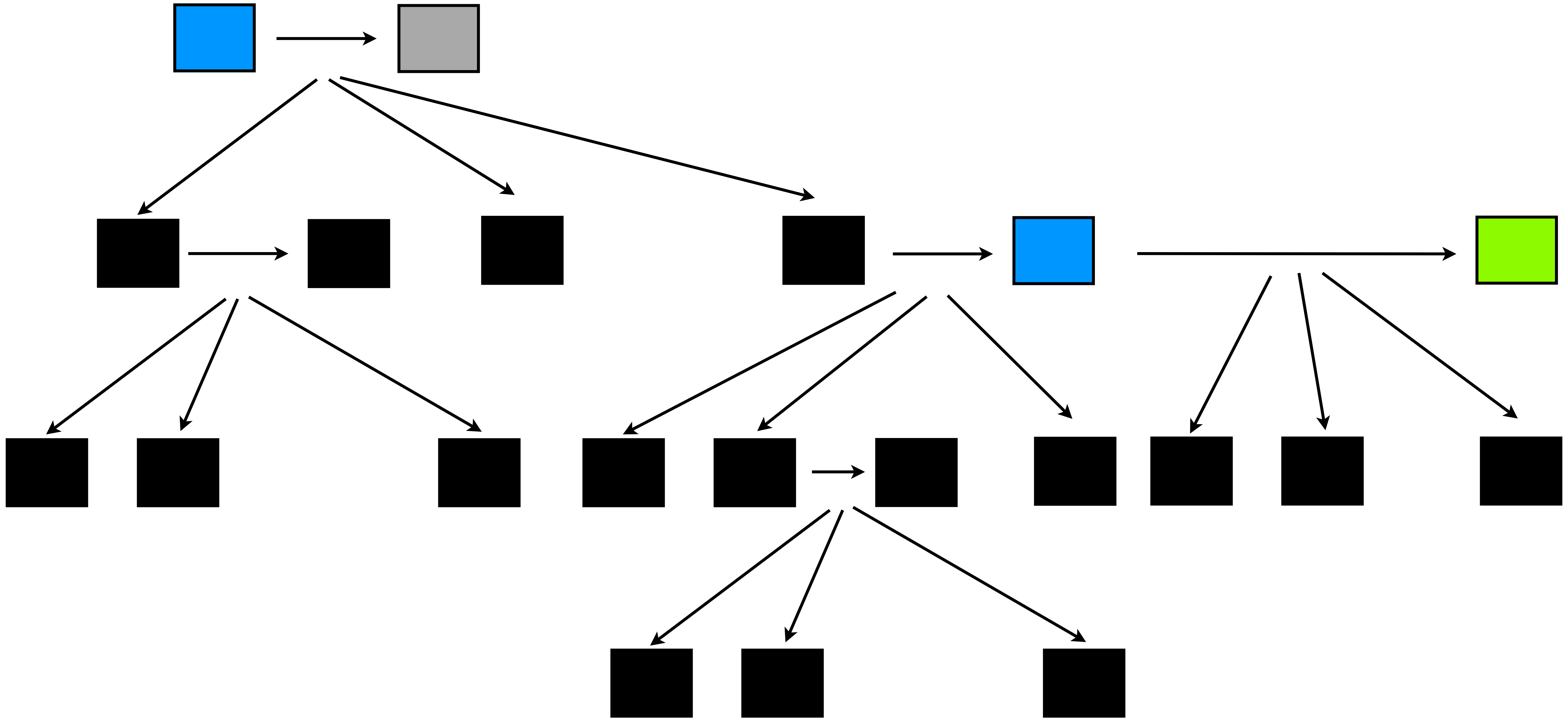
Job-tree

- So now we're running again..

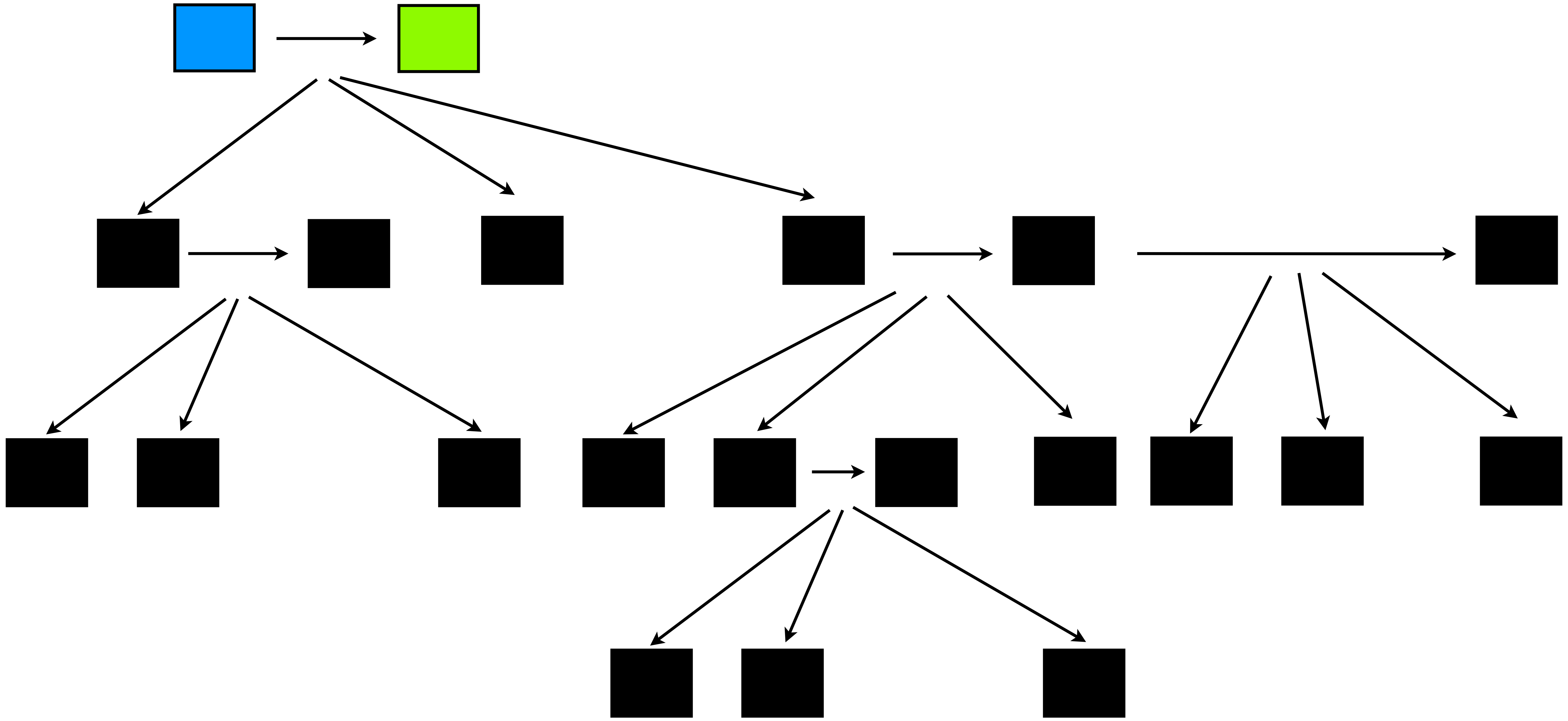


Job-tree

- etc, etc..



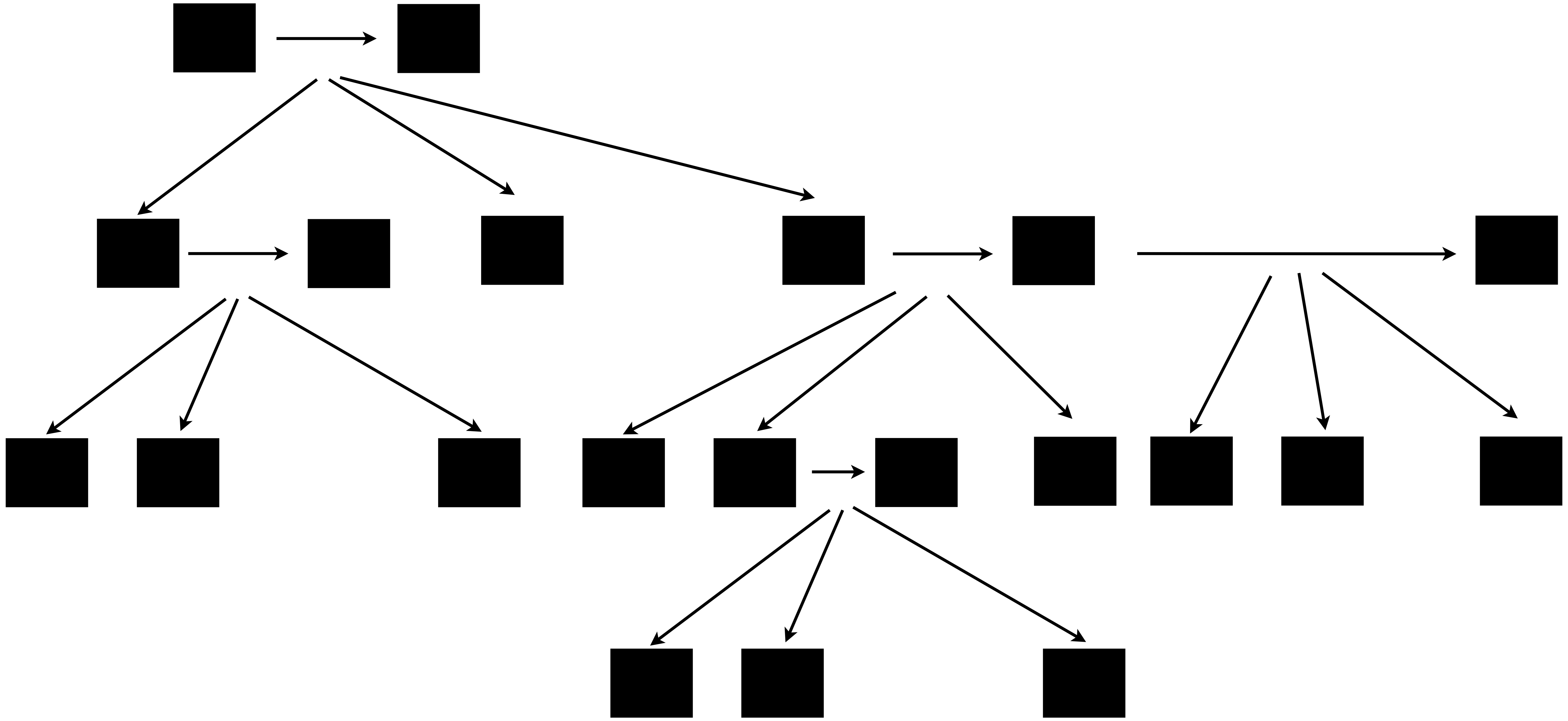
Job-tree



- etc, etc..

Job-tree

- And we're done.



Job-tree/Script-tree

- jobTree communicates by clunky XML files. Each job is passed a an xml file, which it edits and when the job is complete this file is processed.
- scriptTree removes this pain, you just inherit a ‘Target’ python class, as follows (we’ll look at example for doing parallel merge sort).

Job-tree/Script-tree

```
import os
from workflow.jobTree.scriptTree.target import Target

class Setup(Target):
    """Sets up the sort.
    """
    def __init__(self, inputFile, N):
        Target.__init__(self, time=1, memory=1000000, cpu=1)
        self.inputFile = inputFile
        self.N = N

    def run(self):
        tempOutputFile = getTempFile(rootDir=self.getGlobalTempDir())
        self.addChildTarget(Down(self.inputFile, 0, os.path.getsize(self.inputFile),
self.N, tempOutputFile))
        self.setFollowOnTarget(Cleanup(tempOutputFile, self.inputFile))
```

Job-tree/Script-tree

```
import os
from workflow.jobTree.scriptTree.target import Target

class Setup(Target):
    """Sets up the sort.
    """
    def __init__(self, inputFile, N):
        Target.__init__(self, time=1, memory=1000000, cpu=1)
        self.inputFile = inputFile
        self.N = N

    def run(self):
        tempOutputFile = getTempFile(rootDir=self.getGlobalTempDir())
        self.addChildTarget(Down(self.inputFile, 0, os.path.getsize(self.inputFile), 
self.N, tempOutputFile))
        self.setFollowOnTarget(Cleanup(tempOutputFile, self.inputFile))
```

Estimated runtime lets the meta-scheduler be more efficient

Job-tree/Script-tree

Memory (bytes) and cpu requirements can be specified

```
import os
from workflow.jobTree.scriptTree.target import Target

class Setup(Target):
    """Sets up the sort.
    """
    def __init__(self, inputFile, N):
        Target.__init__(self, time=1, memory=1000000, cpu=1)
        self.inputFile = inputFile
        self.N = N

    def run(self):
        tempOutputFile = getTempFile(rootDir=self.getGlobalTempDir())
        self.addChildTarget(Down(self.inputFile, 0, os.path.getsize(self.inputFile),
self.N, tempOutputFile))
        self.setFollowOnTarget(Cleanup(tempOutputFile, self.inputFile))
```

Job-tree/Script-tree

```
import os
from workflow.jobTree.scriptTree.target import Target

class Setup(Target):
    """Sets up the sort.
    """
    def __init__(self, inputFile, N):
        Target.__init__(self, time=1, memory=1000000, cpu=1)
        self.inputFile = inputFile
        self.N = N

    def run(self):
        tempOutputFile = getTempFile(rootDir=self.getGlobalTempDir())
        self.addChildTarget(Down(self.inputFile, 0, os.path.getsize(self.inputFile), 
self.N, tempOutputFile))
        self.setFollowOnTarget(Cleanup(tempOutputFile, self.inputFile))
```

Run, where you create children, a follow on and do work

Job-tree/Script-tree

```
import os
from workflow.jobTree.scriptTree.target import Target

class Setup(Target):
    """Sets up the sort.
    """
    def __init__(self, inputFile, N):
        Target.__init__(self, time=1, memory=1000000, cpu=1)
        self.inputFile = inputFile
        self.N = N

    def run(self):
        tempOutputFile = getTempFile(rootDir=self.getGlobalTempDir())
        self.addChildTarget(Down(self.inputFile, 0, os.path.getsize(self.inputFile), 
self.N, tempOutputFile))
        self.setFollowOnTarget(Cleanup(tempOutputFile, self.inputFile))
```

Creating a child

Job-tree/Script-tree

```
import os
from workflow.jobTree.scriptTree.target import Target

class Setup(Target):
    """Sets up the sort.
    """
    def __init__(self, inputFile, N):
        Target.__init__(self, time=1, memory=1000000, cpu=1)
        self.inputFile = inputFile
        self.N = N

    def run(self):
        tempOutputFile = getTempFile(rootDir=self.getGlobalTempDir())
        self.addChildTarget(Down(self.inputFile, 0, os.path.getsize(self.inputFile),
self.N, tempOutputFile))
        self.setFollowOnTarget(Cleanup(tempOutputFile, self.inputFile))
```

Creating the follow on

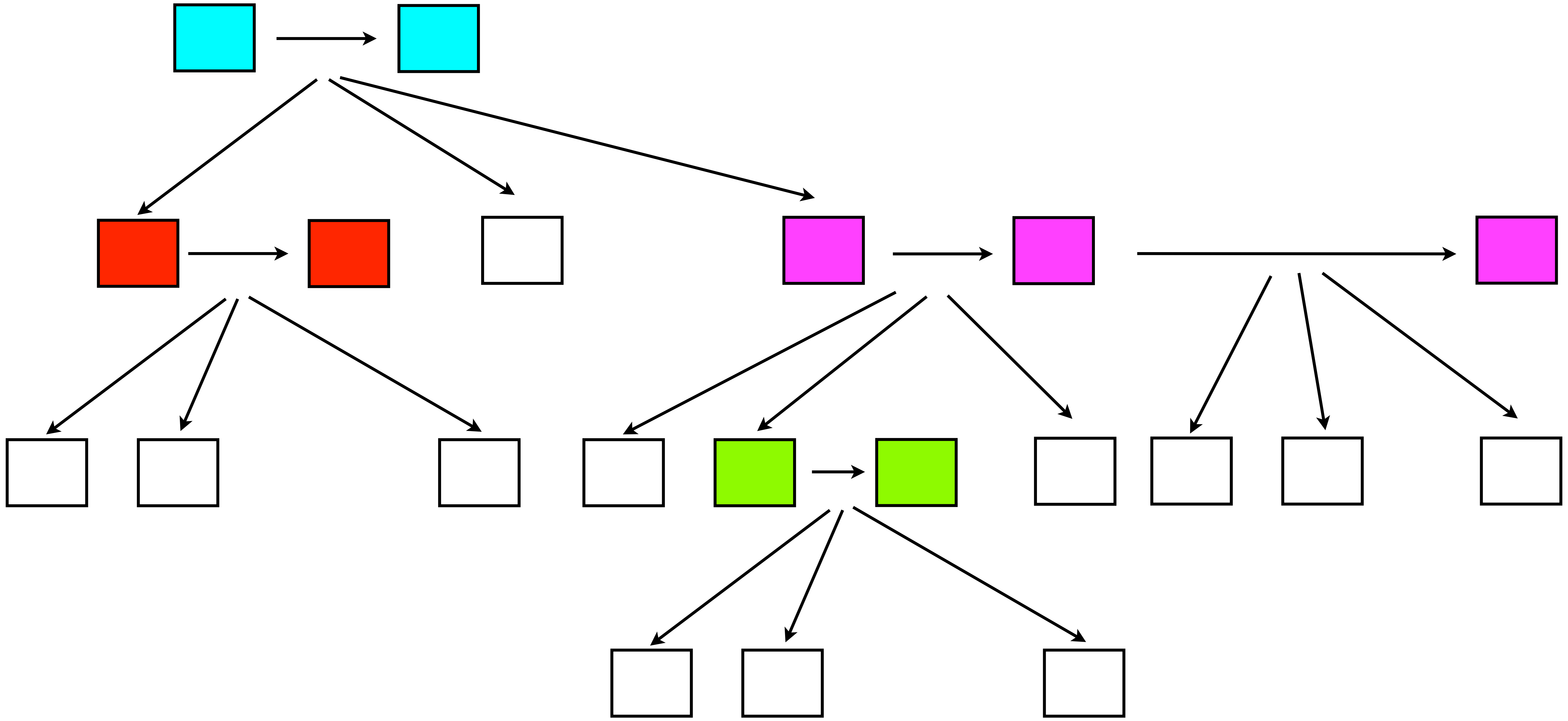
Job-tree/Script-tree

```
import os
from workflow.jobTree.scriptTree.target import Target

class Setup(Target):
    """Sets up the sort.
    """
    def __init__(self, inputFile, N):
        Target.__init__(self, time=1, memory=1000000, cpu=1)
        self.inputFile = inputFile
        self.N = N

    def run(self):
        tempOutputFile = getTempFile(rootDir=self.getGlobalTempDir())
        self.addChildTarget(Down(self.inputFile, 0, os.path.getsize(self.inputFile), 
self.N, tempOutputFile))
        self.setFollowOnTarget(Cleanup(tempOutputFile, self.inputFile))
```

A global (visible to all machines on the cluster) temporary directory that exists for the life of the job, its setup jobs and its follow ons.

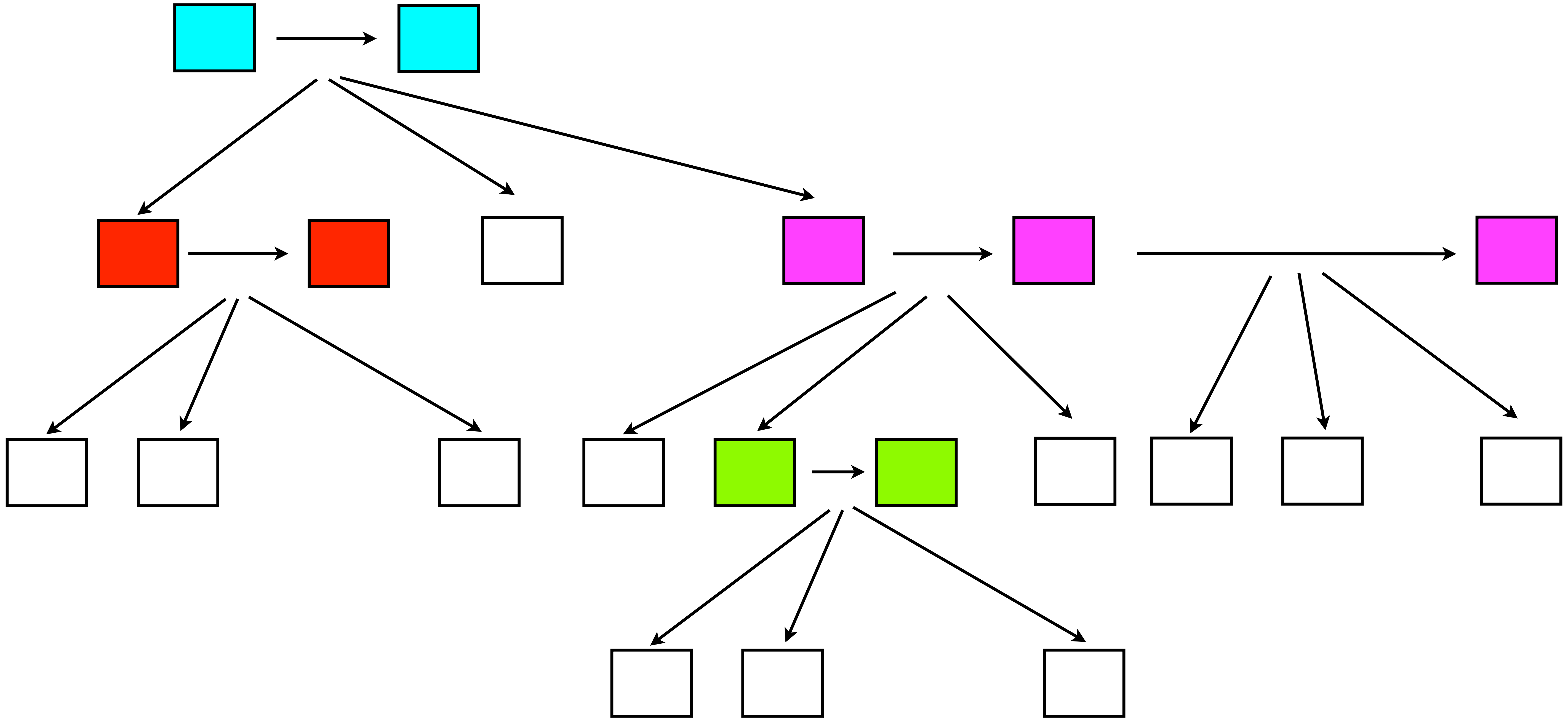
GlobalTempDir

- A chain consists of a founder, a sequence of successive follow ons and a closer.
- Non-trivial chains are coloured in example



GlobalTempDir

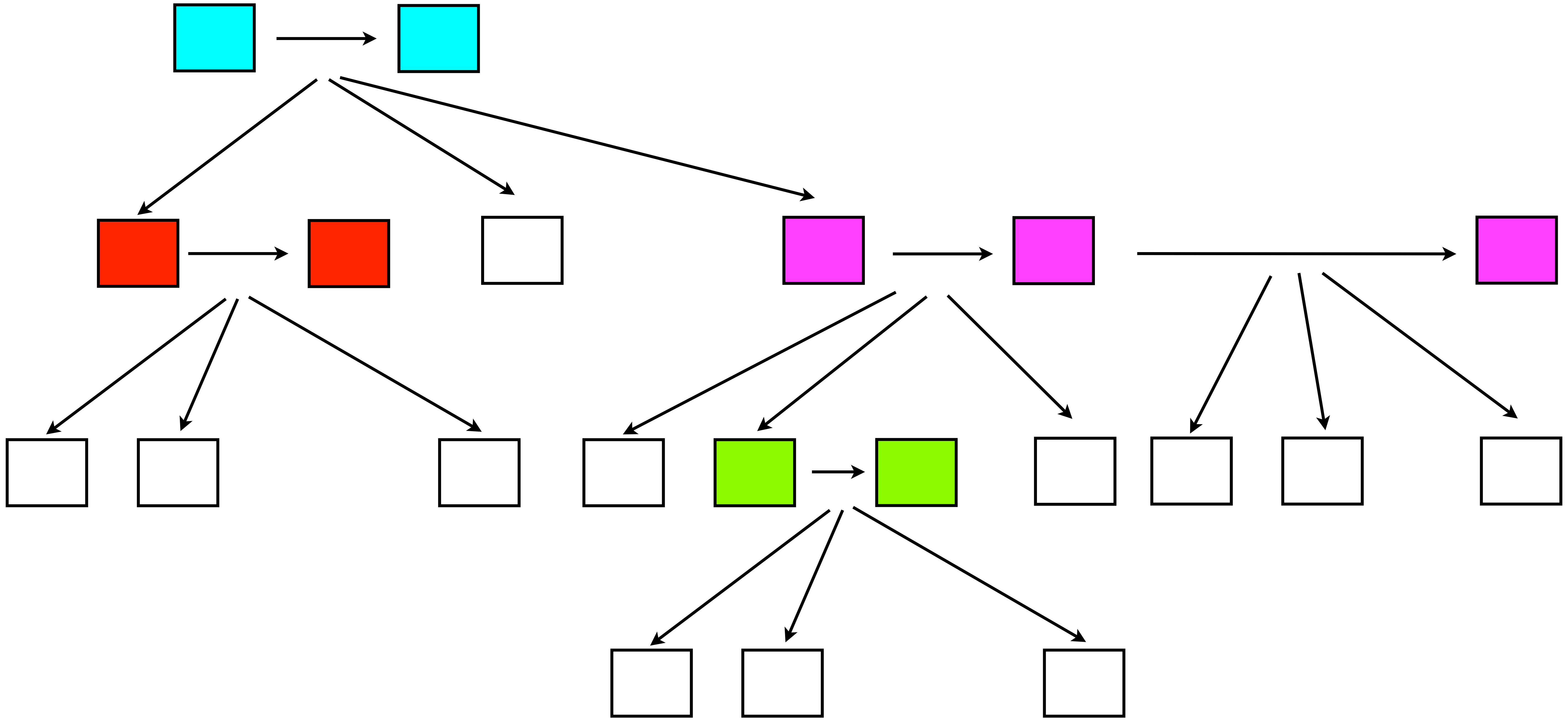
- A 'globalTempDir' temporary directory is created for each chain.



GlobalTempDir

- It is created just before the founder and deleted just after the closer.

- It allows files to be passed around between follow ons and their children.



Job-tree/Script-tree

```python
#!/usr/bin/env python

"""A demonstration of jobTree. Sorts the lines of a file into ascending order by doing a parallel merge
sort.
"""
from optparse import OptionParser
import os
import shutil
from sonLib.bioio import getTempFile
from workflow.jobTree.scriptTree.target import Target
from workflow.jobTree.scriptTree.stack import Stack
from workflow.jobTree.test.sort.lib import merge, sort, copySubRangeOfFile, getMidPoint

class Setup(Target):
    """Sets up the sort.
    """
    def __init__(self, inputFile, N):
        Target.__init__(self, time=1, memory=1000000, cpu=1)
        self.inputFile = inputFile
        self.N = N

    def run(self):
        tempOutputFile = getTempFile(rootDir=self.getGlobalTempDir())
        self.addChildTarget(Down(self.inputFile, 0, os.path.getsize(self.inputFile), self.N,
tempOutputFile))
        self.setFollowOnTarget(Cleanup(tempOutputFile, self.inputFile))

class Cleanup(Target):
    """Copies back the temporary file to input once we've successfully sorted the temporary file.
    """
    def __init__(self, tempOutputFile, outputFile):
        Target.__init__(self)
        self.tempOutputFile = tempOutputFile
        self.outputFile = outputFile

    def run(self):
        shutil.copyfile(self.tempOutputFile, self.outputFile)
```

```python
class Down(Target):
    """Input is a file and a range into that file to sort and an output location in which
    to write the sorted file.
    If the range is larger than a threshold N the range is divided recursively and
    a follow on job is then created which merges back the results else
    the file is sorted and placed in the output.
    """
    def __init__(self, inputFile, fileStart, fileEnd, N, outputFile):
        assert fileStart >= 0
        assert fileStart <= fileEnd
        Target.__init__(self, time=0.05)
        self.inputFile = inputFile
        self.fileStart = fileStart
        self.fileEnd = fileEnd
        self.N = N
        self.outputFile = outputFile

    def run(self):
        length = self.fileEnd - self.fileStart
        assert length >= 0
        if length > self.N:
            midPoint = getMidPoint(self.inputFile, self.fileStart, self.fileEnd)
            assert midPoint >= self.fileStart
            assert midPoint+1 < self.fileEnd
            #We will subdivide the file
            tempFile1 = getTempFile(rootDir=self.getGlobalTempDir())
            tempFile2 = getTempFile(rootDir=self.getGlobalTempDir())
            self.addChildTarget(Down(self.inputFile, self.fileStart, midPoint+1, self.N, tempFile1))
            self.addChildTarget(Down(self.inputFile, midPoint+1, self.fileEnd, self.N, tempFile2)) #Add
one to avoid the newline
            self.setFollowOnTarget(Up(tempFile1, tempFile2, self.outputFile))
        else:
            #We can sort this bit of the file
            copySubRangeOfFile(self.inputFile, self.fileStart, self.fileEnd, self.outputFile)
            sort(self.outputFile)

class Up(Target):
    """Merges the two files and places them in the output.
    """
    def __init__(self, inputFile1, inputFile2, outputFile):
        Target.__init__(self, time=0.05)
        self.inputFile1 = inputFile1
        self.inputFile2 = inputFile2
        self.outputFile = outputFile

    def run(self):
        merge(self.inputFile1, self.inputFile2, self.outputFile)
```

Running Job-tree/Script-tree

```
def main():
    parser = OptionParser()
    Stack.addJobTreeOptions(parser)

    parser.add_option("--fileToSort", dest="fileToSort",
                      help="The file you wish to sort")

    options, args = parser.parse_args()

    if options.fileToSort == None:
        raise RuntimeError("No file to sort given")

    #Now we are ready to run
    i = Stack(Setup(options.fileToSort, int(options.N))).startJobTree(options)

    if i:
        raise RuntimeError("The jobtree contained %i failed jobs" % i)

if __name__ == '__main__':
    from workflow.jobTree.test.sort.Script-treeTest_Sort import *
    main()
```

```
benedict$ Script-treeTest_Sort.py --jobTree foo/Job-tree --logDebug --fileToSort bar.txt
```

Running Job-tree/Script-tree

```
def main():
    parser = OptionParser()
    Stack.addJobTreeOptions(parser)

    parser.add_option("--fileToSort", dest="fileToSort",
                      help="The file you wish to sort")

    options, args = parser.parse_args()

    if options.fileToSort == None:
        raise RuntimeError("No file to sort given")

    #Now we are ready to run
    i = Stack(Setup(options.fileToSort, int(options.N))).startJobTree(options)

    if i:
        raise RuntimeError("The jobtree contained %i failed jobs" % i)

if __name__ == '__main__':
    from workflow.jobTree.test.sort.Script-treeTest_Sort import *
    main()
```

Create a parser for the script and add the Job-tree options to it.

```
benedict$ Script-treeTest_Sort.py --jobTree foo/Job-tree --logDebug --fileToSort bar.txt
```

Running Job-tree/Script-tree

```
def main():
    parser = OptionParser()
    Stack.addJobTreeOptions(parser)

    parser.add_option("--fileToSort", dest="fileToSort",
                      help="The file you wish to sort")

    options, args = parser.parse_args()

    if options.fileToSort == None:
        raise RuntimeError("No file to sort given")

    #Now we are ready to run
    i = Stack(Setup(options.fileToSort, int(options.N))).startJobTree(options)

    if i:
        raise RuntimeError("The jobtree contained %i failed jobs" % i)

if __name__ == '__main__':
    from workflow.jobTree.test.sort.Script-treeTest_Sort import *
    main()
```

Parse the options and args

```
benedict$ Script-treeTest_Sort.py --jobTree foo/Job-tree --logDebug --fileToSort bar.txt
```

Running Job-tree/Script-tree

```python
def main():
    parser = OptionParser()
    Stack.addJobTreeOptions(parser)

    parser.add_option("--fileToSort", dest="fileToSort",
                      help="The file you wish to sort")

    options, args = parser.parse_args()

    if options.fileToSort == None:
        raise RuntimeError("No file to sort given")

    #Now we are ready to run
    i = Stack(Setup(options.fileToSort, int(options.N))).startJobTree(options)

    if i:
        raise RuntimeError("The jobtree contained %i failed jobs" % i)

if __name__ == '__main__':
    from workflow.jobTree.test.sort.Script-treeTest_Sort import *
    main()
```

Run Job-tree (alternatively
you can pass in the options to jobtre
manually and use your own options/args
parser)

```
benedict$ Script-treeTest_Sort.py --jobTree foo/Job-tree --logDebug --fileToSort bar.txt
```

Running Job-tree/Script-tree

```
def main():
    parser = OptionParser()
    Stack.addJobTreeOptions(parser)

    parser.add_option("--fileToSort", dest="fileToSort",
                      help="The file you wish to sort")

    options, args = parser.parse_args()

    if options.fileToSort == None:
        raise RuntimeError("No file to sort given")

    #Now we are ready to run
    i = Stack(Setup(options.fileToSort, int(options.N))).startJobTree(options)

    if i:
        raise RuntimeError("The jobtree contained %i failed jobs" % i)

if __name__ == '__main__':
    from workflow.jobTree.test.sort.Script-treeTest_Sort import *
    main()
```

The command line

```
benedict$ Script-treeTest_Sort.py --jobTree foo/Job-tree --logDebug --fileToSort bar.txt
```

Running Job-tree/Script-tree

```
def main():
    parser = OptionParser()
    Stack.addJobTreeOptions(parser)

    parser.add_option("--fileToSort", dest="fileToSort",
                      help="The file you wish to sort")

    options, args = parser.parse_args()

    if options.fileToSort == None:
        raise RuntimeError("No file to sort given")

    #Now we are ready to run
    i = Stack(Setup(options.fileToSort, int(options.N))).startJobTree(options)

    if i:
        raise RuntimeError("The jobtree contained %i failed jobs" % i)

if __name__ == '__main__':
    from workflow.jobTree.test.sort.Script-treeTest_Sort import *
    main()
```

Oh, and a little voodoo
required by
the pickler

```
benedict$ Script-treeTest_Sort.py --jobTree foo/Job-tree --logDebug --fileToSort bar.txt
```

Restarting a job-tree

- A job-tree is run initially by executing the script.
- If it fails call:
  - jobTree --jobTree FOO
  - Where foo is the location of the jobTree
- The job-tree will restart from where it failed.

Cleaning up

- Once a job-tree finishes up you can check it completed okay by running:
  - jobTreeStatus --jobTree FOO
  - Where FOO is the jobTree
  - Adding the --verbose flag will print out any error log files associated with failed jobs
  - To finish up, simply delete the job-tree.

Job-tree/Script-tree Misc.

- Your environment variables are inherited from the executing shell, so you can use relative path names and program names without stressing.

- Can run on a parasol cluster, a grid engine cluster, or in single machine mode (using multiple threads), so you can test on a workstation before you push your pipeline to the cluster.

- Is (theoretically) easily extended to work on another batch system - just inherit the abstract batch system class.

Job-tree Summary

- Allows you to dynamically create arbitrarily parallelised batches of jobs.
- Provides other nice features.
- Is stable and used by me, Dent, Krish, Charlie, Daniel, Ngan and run by others, including Wendy, Ted, Bernard, etc.
- Unfortunately, the code is pretty dense and prototype-y, and there are some clunky edges.

Utilities

- These next slides detail the utilities for job-tree

jobTreeStats

- Run as jobTreeStats --jobTree foo
- Reports status of tree, importantly telling you how many jobs are failed etc.
- Verbose flag will report log files of failed jobs
- Output could be improved!

jobTreeKill

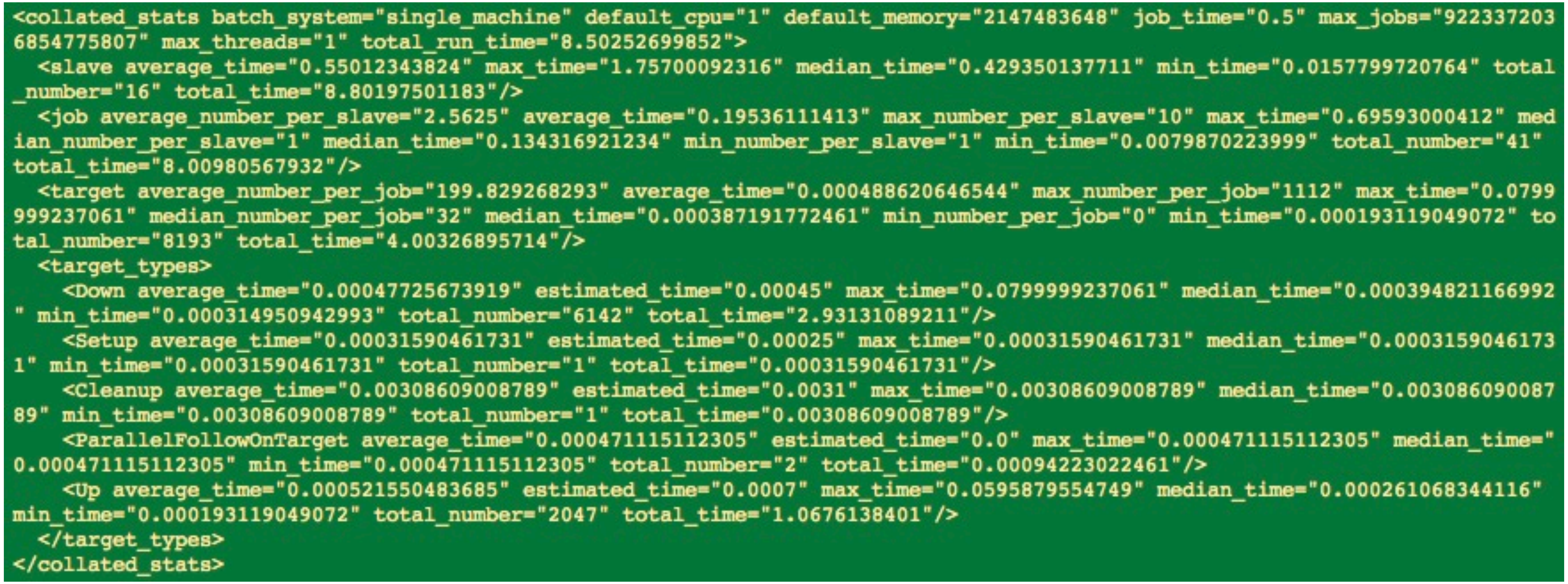
- To kill a jobtree, first kill the master process, then run:
- jobTreeKill --jobTree foo
- Kills all queued and running jobs associated with the job-tree on the batch system (only works with parasol currently, not grid engine).
- Does not remove the batch (can be restarted again)

jobTreeStats: Balancing job-trees

- Your jobs on the cluster should run for some ‘ideal’ time in order to efficient.
- Job-tree will attempt to agglomerate your short running jobs to avoid paying scheduling costs (which may be a few seconds of latency per job!)
- Running job-tree with --stats option allows you to run jobTreeStats

```
benedict$ Script-treeTest_Sort.py --jobTree foo/Job-tree --logDebug --fileToSort bar.txt --stats
benedict$ jobTreeStats --jobTree foo/Job-tree
```

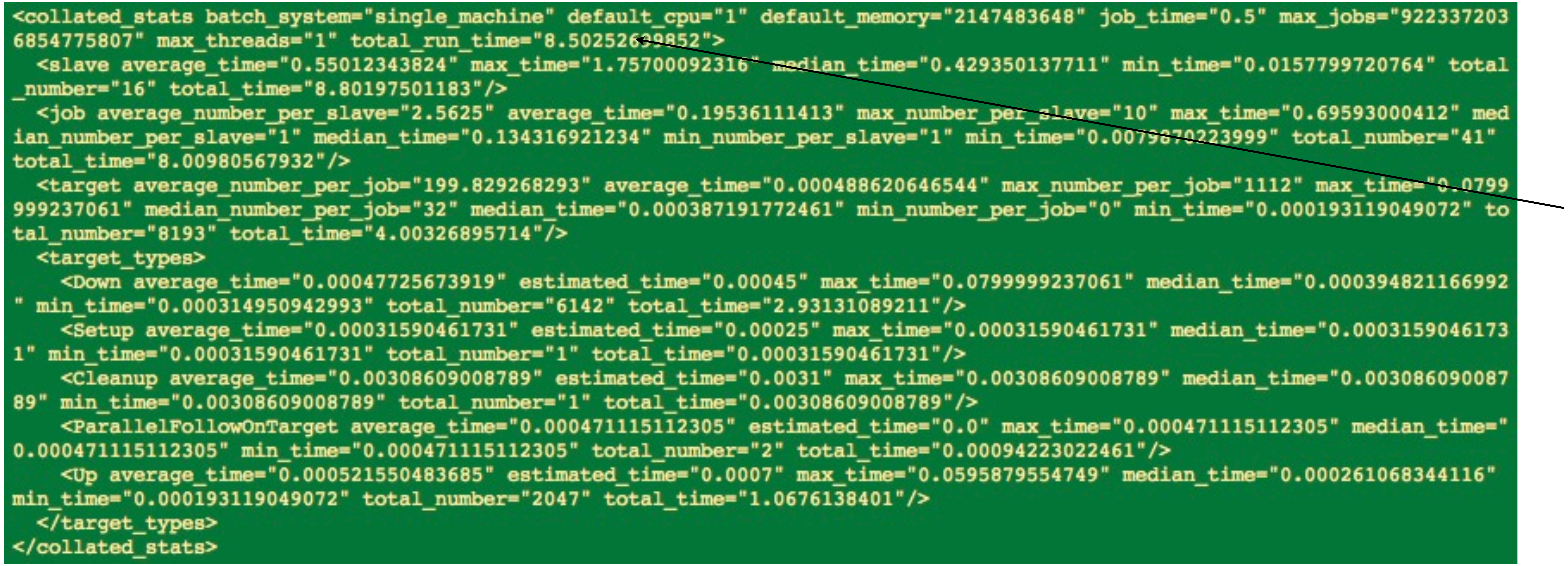
jobTreeStats: Balancing job-trees



```
<collated_stats batch_system="single_machine" default_cpu="1" default_memory="2147483648" job_time="0.5" max_jobs="922337203
6854775807" max_threads="1" total_run_time="8.50252699852">
  <slave average_time="0.55012343824" max_time="1.75700092316" median_time="0.429350137711" min_time="0.0157799720764" total
_number="16" total_time="8.80197501183"/>
  <job average_number_per_slave="2.5625" average_time="0.19536111413" max_number_per_slave="10" max_time="0.69593000412" med
ian_number_per_slave="1" median_time="0.134316921234" min_number_per_slave="1" min_time="0.0079870223999" total_number="41"
total_time="8.00980567932"/>
  <target average_number_per_job="199.829268293" average_time="0.000488620646544" max_number_per_job="1112" max_time="0.0799
999237061" median_number_per_job="32" median_time="0.000387191772461" min_number_per_job="0" min_time="0.000193119049072" to
tal_number="8193" total_time="4.00326895714"/>
  <target_types>
    <Down average_time="0.00047725673919" estimated_time="0.00045" max_time="0.0799999237061" median_time="0.000394821166992
" min_time="0.000314950942993" total_number="6142" total_time="2.93131089211"/>
    <Setup average_time="0.00031590461731" estimated_time="0.00025" max_time="0.00031590461731" median_time="0.0003159046173
1" min_time="0.00031590461731" total_number="1" total_time="0.00031590461731"/>
    <Cleanup average_time="0.00308609008789" estimated_time="0.0031" max_time="0.00308609008789" median_time="0.003086090087
89" min_time="0.00308609008789" total_number="1" total_time="0.00308609008789"/>
    <ParallelFollowOnTarget average_time="0.000471115112305" estimated_time="0.0" max_time="0.000471115112305" median_time="
0.000471115112305" min_time="0.000471115112305" total_number="2" total_time="0.00094223022461"/>
    <Up average_time="0.000521550483685" estimated_time="0.0007" max_time="0.0595879554749" median_time="0.000261068344116"
min_time="0.000193119049072" total_number="2047" total_time="1.0676138401"/>
  </target_types>
</collated_stats>
```

Example from script-treeTest_Sort.py

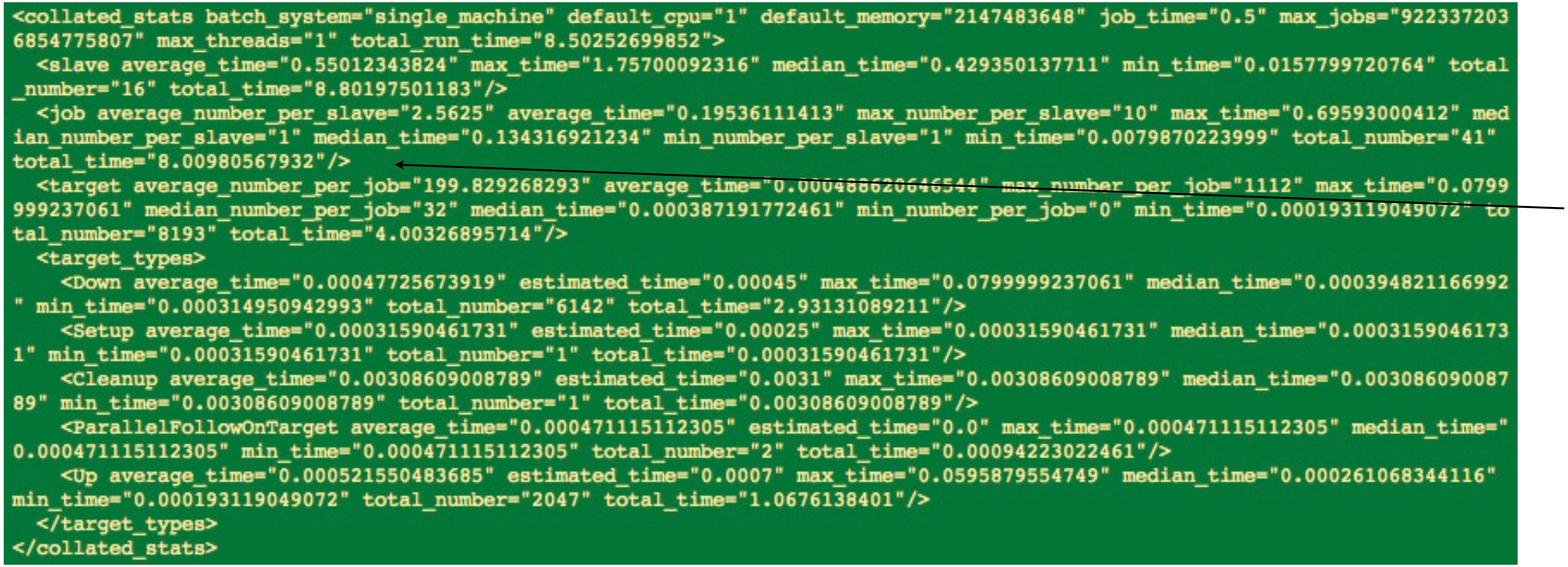
jobTreeStats: Balancing job-trees



```
<collated_stats batch_system="single_machine" default_cpu="1" default_memory="2147483648" job_time="0.5" max_jobs="922337203
6854775807" max_threads="1" total_run_time="8.50252699852">
  <slave average_time="0.55012343824" max_time="1.75700092316" median_time="0.429350137711" min_time="0.0157799720764" total
_number="16" total_time="8.80197501183"/>
  <job average_number_per_slave="2.5625" average_time="0.19536111413" max_number_per_slave="10" max_time="0.69593000412" med
ian_number_per_slave="1" median_time="0.134316921234" min_number_per_slave="1" min_time="0.0079870223999" total_number="41"
total_time="8.00980567932"/>
  <target average_number_per_job="199.829268293" average_time="0.000488620646544" max_number_per_job="1112" max_time="0.0799
999237061" median_number_per_job="32" median_time="0.000387191772461" min_number_per_job="0" min_time="0.000193119049072" to
tal_number="8193" total_time="4.00326895714"/>
  <target_types>
    <Down average_time="0.00047725673919" estimated_time="0.00045" max_time="0.0799999237061" median_time="0.000394821166992
" min_time="0.000314950942993" total_number="6142" total_time="2.93131089211"/>
    <Setup average_time="0.00031590461731" estimated_time="0.00025" max_time="0.00031590461731" median_time="0.0003159046173
1" min_time="0.00031590461731" total_number="1" total_time="0.00031590461731"/>
    <Cleanup average_time="0.00308609008789" estimated_time="0.0031" max_time="0.00308609008789" median_time="0.003086090087
89" min_time="0.00308609008789" total_number="1" total_time="0.00308609008789"/>
    <ParallelFollowOnTarget average_time="0.000471115112305" estimated_time="0.0" max_time="0.000471115112305" median_time="
0.000471115112305" min_time="0.000471115112305" total_number="2" total_time="0.00094223022461"/>
    <Up average_time="0.000521550483685" estimated_time="0.0007" max_time="0.0595879554749" median_time="0.000261068344116"
min_time="0.000193119049072" total_number="2047" total_time="1.0676138401"/>
  </target_types>
</collated_stats>
```

Total runtime and stats about job tree.

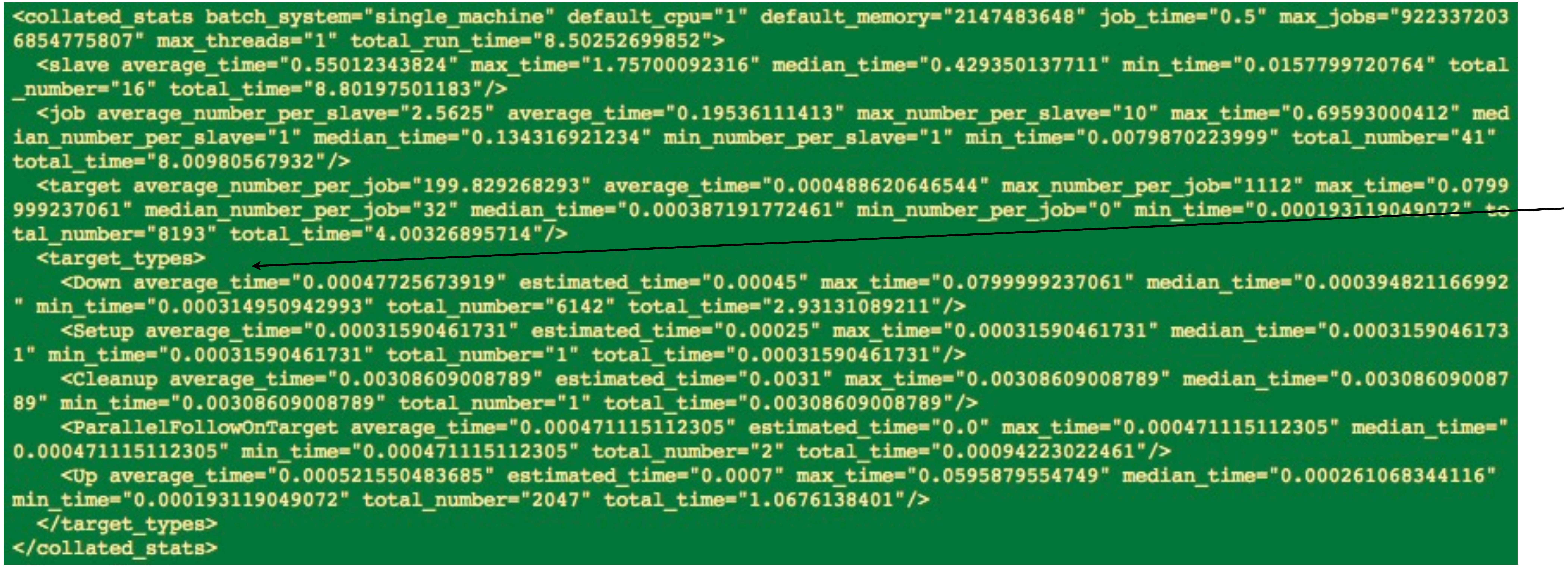
jobTreeStats: Balancing job-trees



```
<collated_stats batch_system="single_machine" default_cpu="1" default_memory="2147483648" job_time="0.5" max_jobs="922337203
6854775807" max_threads="1" total_run_time="8.50252699852">
  <slave average_time="0.55012343824" max_time="1.75700092316" median_time="0.429350137711" min_time="0.0157799720764" total
_number="16" total_time="8.80197501183"/>
  <job average_number_per_slave="2.5625" average_time="0.19536111413" max_number_per_slave="10" max_time="0.69593000412" med
ian_number_per_slave="1" median_time="0.134316921234" min_number_per_slave="1" min_time="0.0079870223999" total_number="41"
total_time="8.00980567932"/>
  <target average_number_per_job="199.829268293" average_time="0.000488620646544" max_number_per_job="1112" max_time="0.0799
999237061" median_number_per_job="32" median_time="0.000387191772461" min_number_per_job="0" min_time="0.000193119049072" to
tal_number="8193" total_time="4.00326895714"/>
  <target_types>
    <Down average_time="0.00047725673919" estimated_time="0.00045" max_time="0.0799999237061" median_time="0.000394821166992
" min_time="0.000314950942993" total_number="6142" total_time="2.93131089211"/>
    <Setup average_time="0.00031590461731" estimated_time="0.00025" max_time="0.00031590461731" median_time="0.0003159046173
1" min_time="0.00031590461731" total_number="1" total_time="0.00031590461731"/>
    <Cleanup average_time="0.00308609008789" estimated_time="0.0031" max_time="0.00308609008789" median_time="0.003086090087
89" min_time="0.00308609008789" total_number="1" total_time="0.00308609008789"/>
    <ParallelFollowOnTarget average_time="0.000471115112305" estimated_time="0.0" max_time="0.000471115112305" median_time="
0.000471115112305" min_time="0.000471115112305" total_number="2" total_time="0.00094223022461"/>
    <Up average_time="0.000521550483685" estimated_time="0.0007" max_time="0.0595879554749" median_time="0.000261068344116"
min_time="0.000193119049072" total_number="2047" total_time="1.0676138401"/>
  </target_types>
</collated_stats>
```

Times on targets, which are agglomerated into jobs

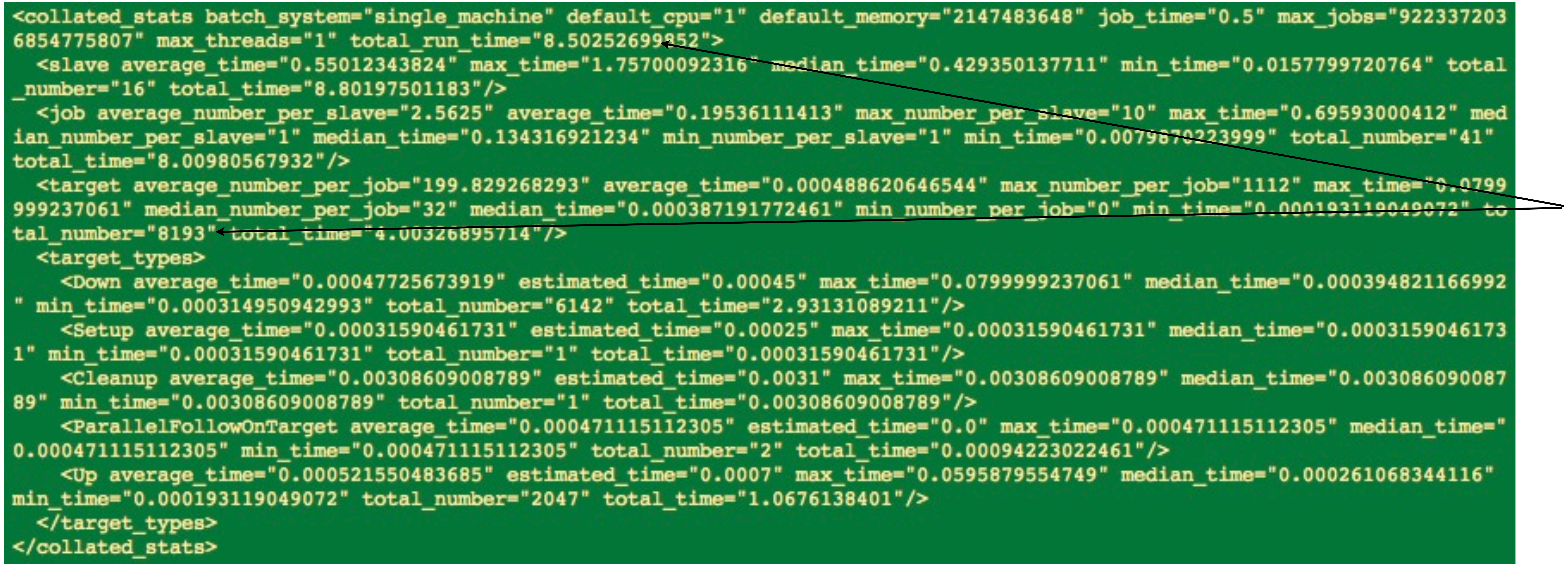
jobTreeStats: Balancing job-trees



```
<collated_stats batch_system="single_machine" default_cpu="1" default_memory="2147483648" job_time="0.5" max_jobs="922337203
6854775807" max_threads="1" total_run_time="8.50252699852">
  <slave average_time="0.55012343824" max_time="1.75700092316" median_time="0.429350137711" min_time="0.0157799720764" total
_number="16" total_time="8.80197501183"/>
  <job average_number_per_slave="2.5625" average_time="0.19536111413" max_number_per_slave="10" max_time="0.69593000412" med
ian_number_per_slave="1" median_time="0.134316921234" min_number_per_slave="1" min_time="0.0079870223999" total_number="41"
total_time="8.00980567932"/>
  <target average_number_per_job="199.829268293" average_time="0.000488620646544" max_number_per_job="1112" max_time="0.0799
999237061" median_number_per_job="32" median_time="0.000387191772461" min_number_per_job="0" min_time="0.000193119049072" to
tal_number="8193" total_time="4.00326895714"/>
  <target_types>
    <Down average_time="0.00047725673919" estimated_time="0.00045" max_time="0.0799999237061" median_time="0.000394821166992
" min_time="0.000314950942993" total_number="6142" total_time="2.93131089211"/>
    <Setup average_time="0.00031590461731" estimated_time="0.00025" max_time="0.00031590461731" median_time="0.0003159046173
1" min_time="0.00031590461731" total_number="1" total_time="0.00031590461731"/>
    <Cleanup average_time="0.00308609008789" estimated_time="0.0031" max_time="0.00308609008789" median_time="0.003086090087
89" min_time="0.00308609008789" total_number="1" total_time="0.00308609008789"/>
    <ParallelFollowOnTarget average_time="0.000471115112305" estimated_time="0.0" max_time="0.000471115112305" median_time="
0.000471115112305" min_time="0.000471115112305" total_number="2" total_time="0.00094223022461"/>
    <Up average_time="0.000521550483685" estimated_time="0.0007" max_time="0.0595879554749" median_time="0.000261068344116"
min_time="0.000193119049072" total_number="2047" total_time="1.0676138401"/>
  </target_types>
</collated_stats>
```

Times on individual targets, showing how close your estimated jobs came to the actual run-times

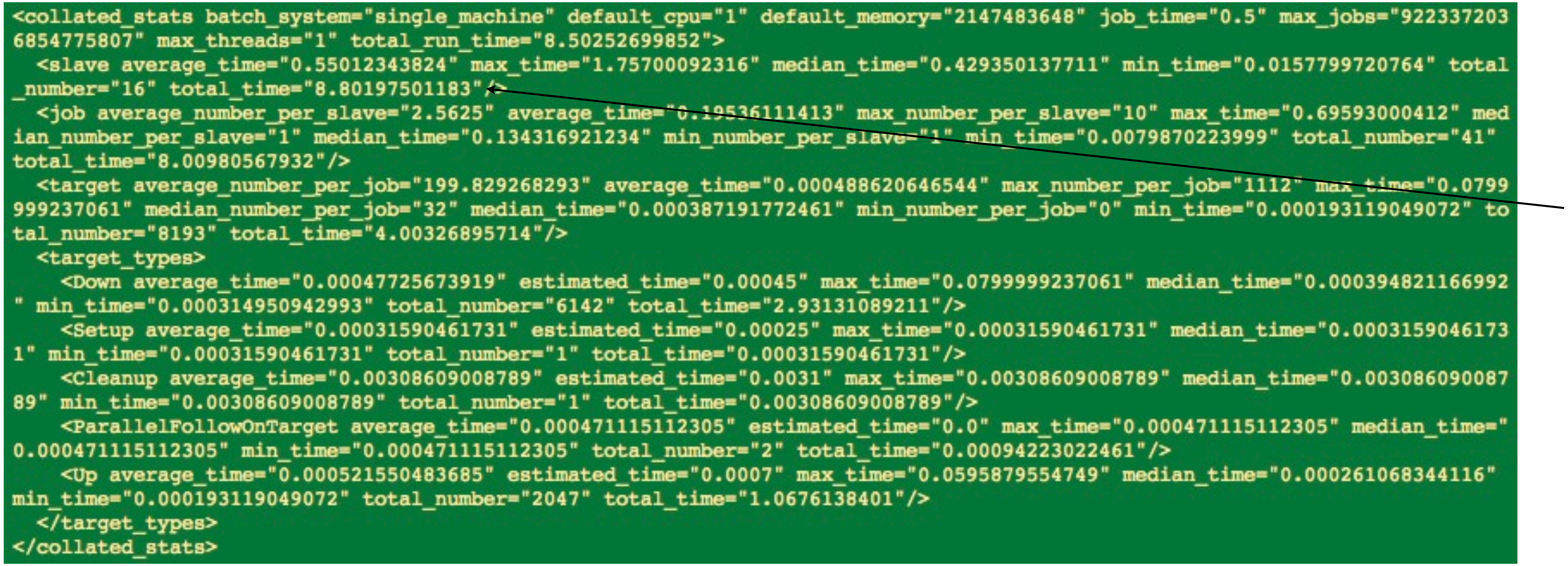
jobTreeStats: Balancing job-trees



```
<collated_stats batch_system="single_machine" default_cpu="1" default_memory="2147483648" job_time="0.5" max_jobs="922337203
6854775807" max_threads="1" total_run_time="8.50252699852">
  <slave average_time="0.55012343824" max_time="1.75700092316" median_time="0.429350137711" min_time="0.0157799720764" total
_number="16" total_time="8.80197501183"/>
  <job average_number_per_slave="2.5625" average_time="0.19536111413" max_number_per_slave="10" max_time="0.69593000412" med
ian_number_per_slave="1" median_time="0.134316921234" min_number_per_slave="1" min_time="0.00798070223999" total_number="41"
total_time="8.00980567932"/>
  <target average_number_per_job="199.829268293" average_time="0.000488620646544" max_number_per_job="1112" max_time="0.0799
999237061" median_number_per_job="32" median_time="0.000387191772461" min_number_per_job="0" min_time="0.000193119049072" to
tal_number="8193" total_time="4.00326895714"/>
  <target_types>
    <Down average_time="0.00047725673919" estimated_time="0.00045" max_time="0.0799999237061" median_time="0.000394821166992
" min_time="0.000314950942993" total_number="6142" total_time="2.93131089211"/>
    <Setup average_time="0.00031590461731" estimated_time="0.00025" max_time="0.00031590461731" median_time="0.0003159046173
1" min_time="0.00031590461731" total_number="1" total_time="0.00031590461731"/>
    <Cleanup average_time="0.00308609008789" estimated_time="0.0031" max_time="0.00308609008789" median_time="0.003086090087
89" min_time="0.00308609008789" total_number="1" total_time="0.00308609008789"/>
    <ParallelFollowOnTarget average_time="0.000471115112305" estimated_time="0.0" max_time="0.000471115112305" median_time="
0.000471115112305" min_time="0.000471115112305" total_number="2" total_time="0.00094223022461"/>
    <Up average_time="0.000521550483685" estimated_time="0.0007" max_time="0.0595879554749" median_time="0.000261068344116"
min_time="0.000193119049072" total_number="2047" total_time="1.0676138401"/>
  </target_types>
</collated_stats>
```

This example ran
8193 targets, in a
single thread in
8.5 seconds!

jobTreeStats: Balancing job-trees



```
<collated_stats batch_system="single_machine" default_cpu="1" default_memory="2147483648" job_time="0.5" max_jobs="922337203
6854775807" max_threads="1" total_run_time="8.50252699852">
  <slave average_time="0.55012343824" max_time="1.75700092316" median_time="0.429350137711" min_time="0.0157799720764" total
_number="16" total_time="8.80197501183"/>
  <job average_number_per_slave="2.5625" average_time="0.19536111413" max_number_per_slave="10" max_time="0.69593000412" med
ian_number_per_slave="1" median_time="0.134316921234" min_number_per_slave="1" min_time="0.0079870223999" total_number="41"
total_time="8.00980567932"/>
  <target average_number_per_job="199.829268293" average_time="0.000488620646544" max_number_per_job="1112" max_time="0.0799
999237061" median_number_per_job="32" median_time="0.000387191772461" min_number_per_job="0" min_time="0.000193119049072" to
tal_number="8193" total_time="4.00326895714"/>
  <target_types>
    <Down average_time="0.00047725673919" estimated_time="0.00045" max_time="0.0799999237061" median_time="0.000394821166992
" min_time="0.000314950942993" total_number="6142" total_time="2.93131089211"/>
    <Setup average_time="0.00031590461731" estimated_time="0.00025" max_time="0.00031590461731" median_time="0.0003159046173
1" min_time="0.00031590461731" total_number="1" total_time="0.00031590461731"/>
    <Cleanup average_time="0.00308609008789" estimated_time="0.0031" max_time="0.00308609008789" median_time="0.003086090087
89" min_time="0.00308609008789" total_number="1" total_time="0.00308609008789"/>
    <ParallelFollowOnTarget average_time="0.000471115112305" estimated_time="0.0" max_time="0.000471115112305" median_time="
0.000471115112305" min_time="0.000471115112305" total_number="2" total_time="0.00094223022461"/>
    <Up average_time="0.000521550483685" estimated_time="0.0007" max_time="0.0595879554749" median_time="0.000261068344116"
min_time="0.000193119049072" total_number="2047" total_time="1.0676138401"/>
  </target_types>
</collated_stats>
```

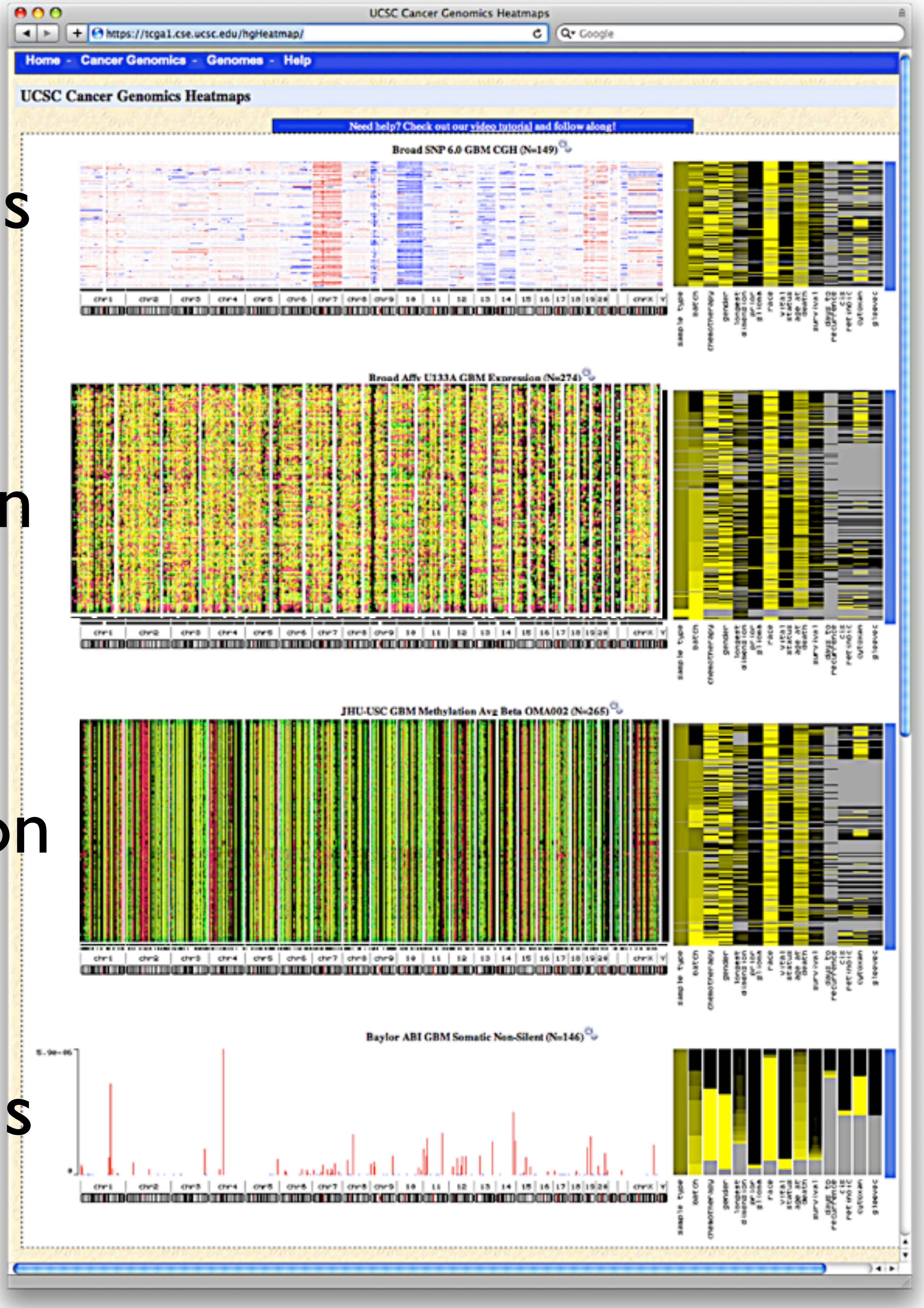
Times that the slaves ran 'jobs', in this case we've asked for a job-runtime of 0.5 seconds, the actual average was 0.55 seconds

Grid-engine cluster

- PK cluster + memk + (shortly) kolossus
  - Heterogenous cluster, with machines:
    - from 2 to 64 cpus.
    - from 4 to 1024 gigs of memory
    - ~400 nodes
- Within the cancer firewall, still working out the kinks.

Charlie

Cancer Functional Genomics



UCSC Cancer Genomics Heatmaps

https://tcga1.cse.ucsc.edu/hgHeatmap/

UCSC Cancer Genomics Heatmaps

Need help? Check out our video tutorial and follow along!

Broad SNP 6.0 GBM CGH (N=149)

Broad Affy U133A GBM Expression (N=274)

JHU-USC GBM Methylation Avg Beta OMA002 (N=265)

Baylor ABI GBM Somatic Non-Silent (N=146)

Copy Number Aberrations

Gene Expression

DNA Methylation

Genomic Mutations

Data on the horizon:

Chromatin Structure

Histone Marks

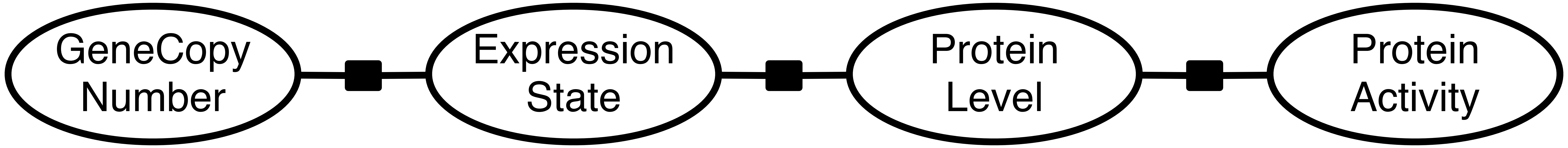
Proteomics

Metabolomics

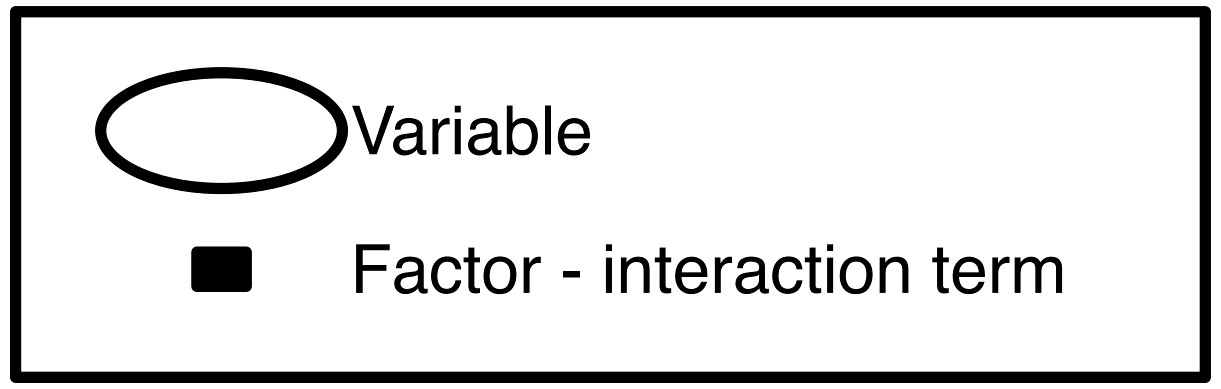
Zhu J, *Nature Methods*, 2009

http://genome-cancer.ucsc.edu

Gene Model



GeneCopy Number
Expression State
Protein Level
Protein Activity

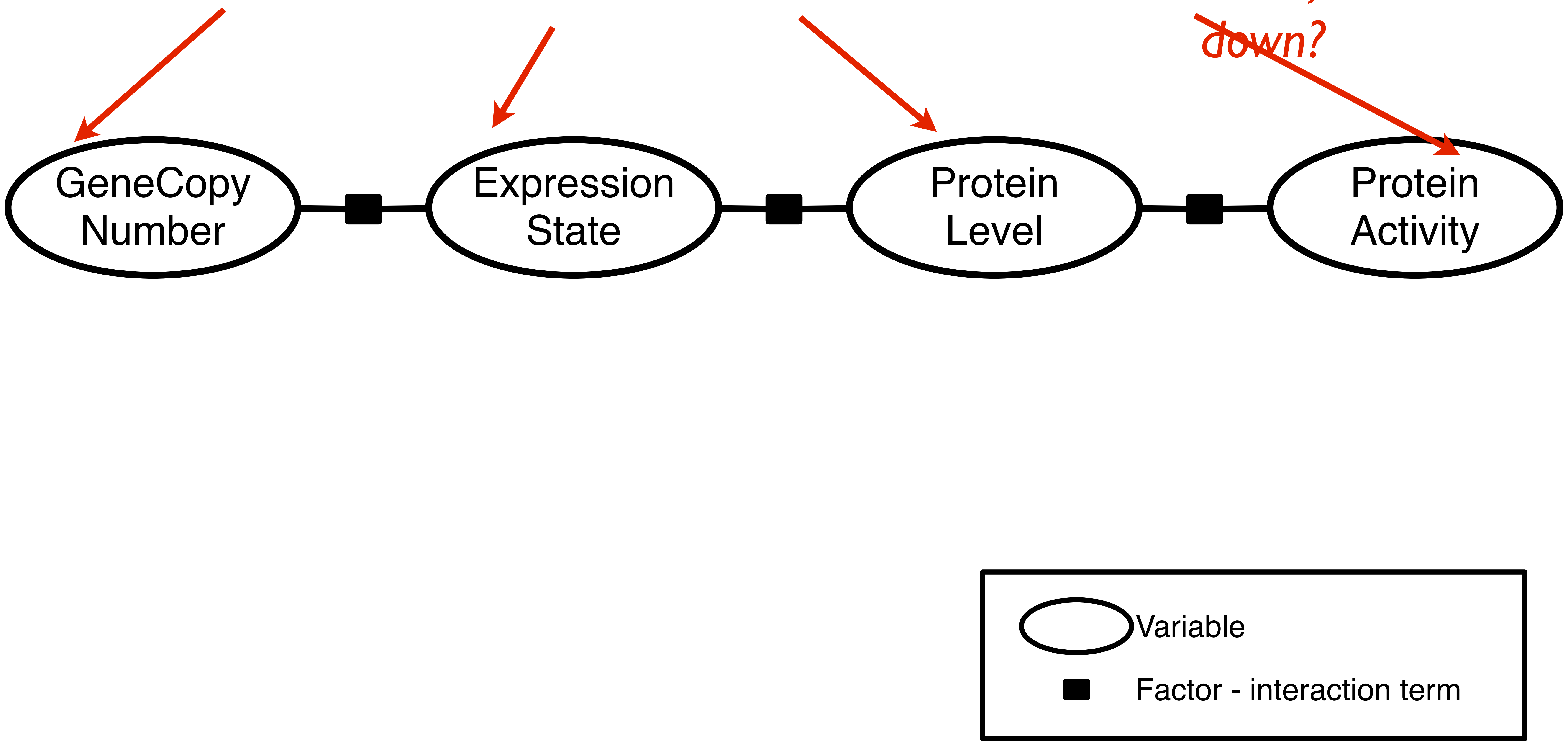


Variable
Factor - interaction term

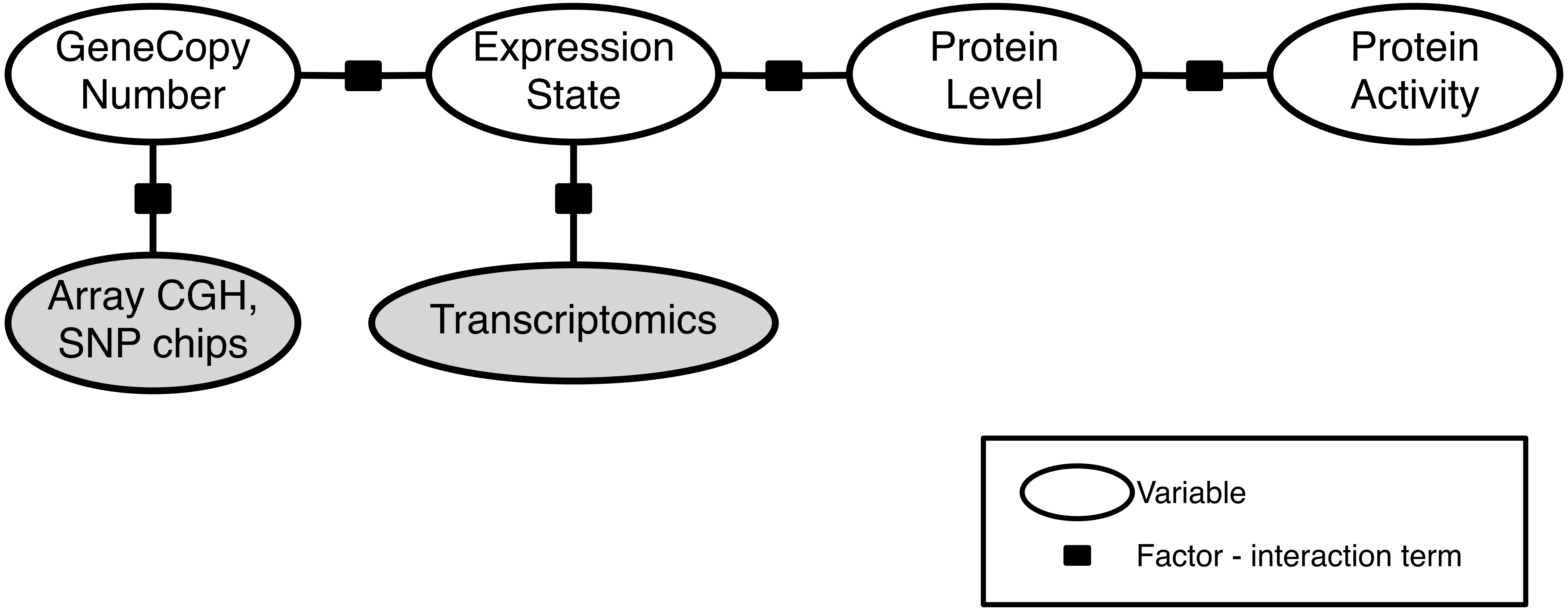
Gene Model

relative to non-cancer,
is this sample:
up,
same,
down?

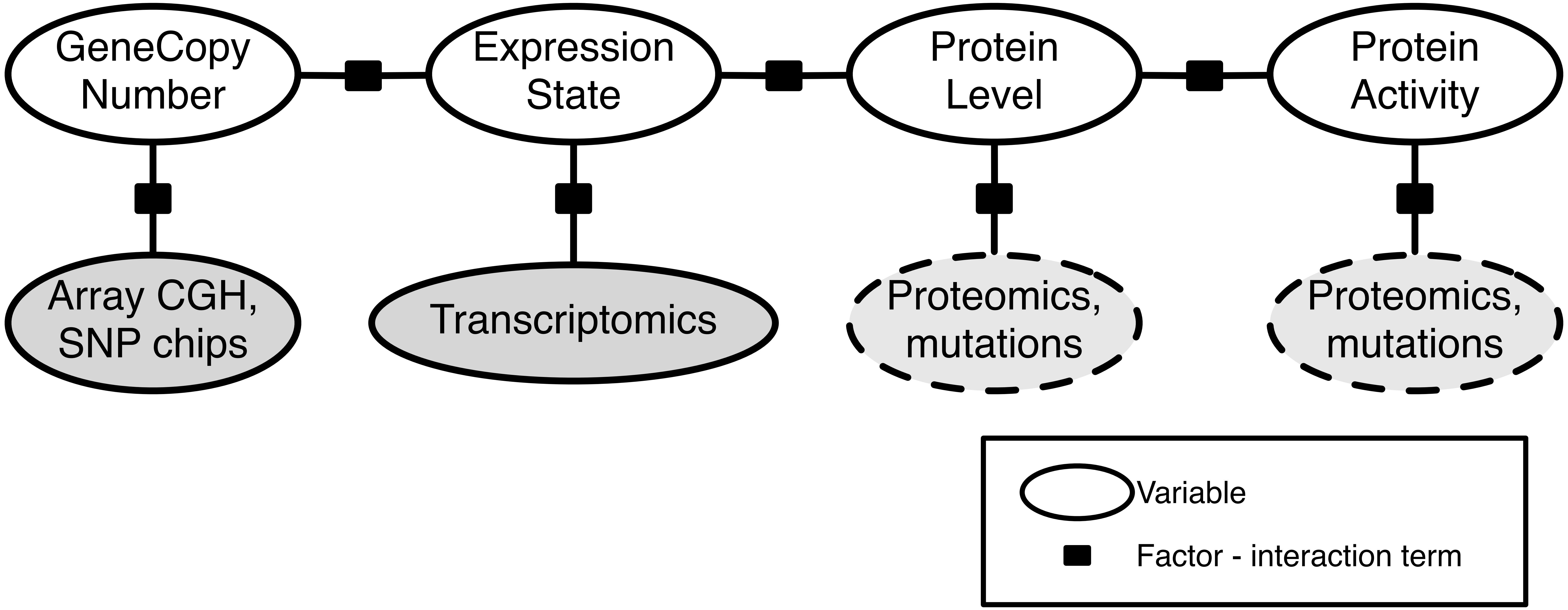
3-state discrete variables



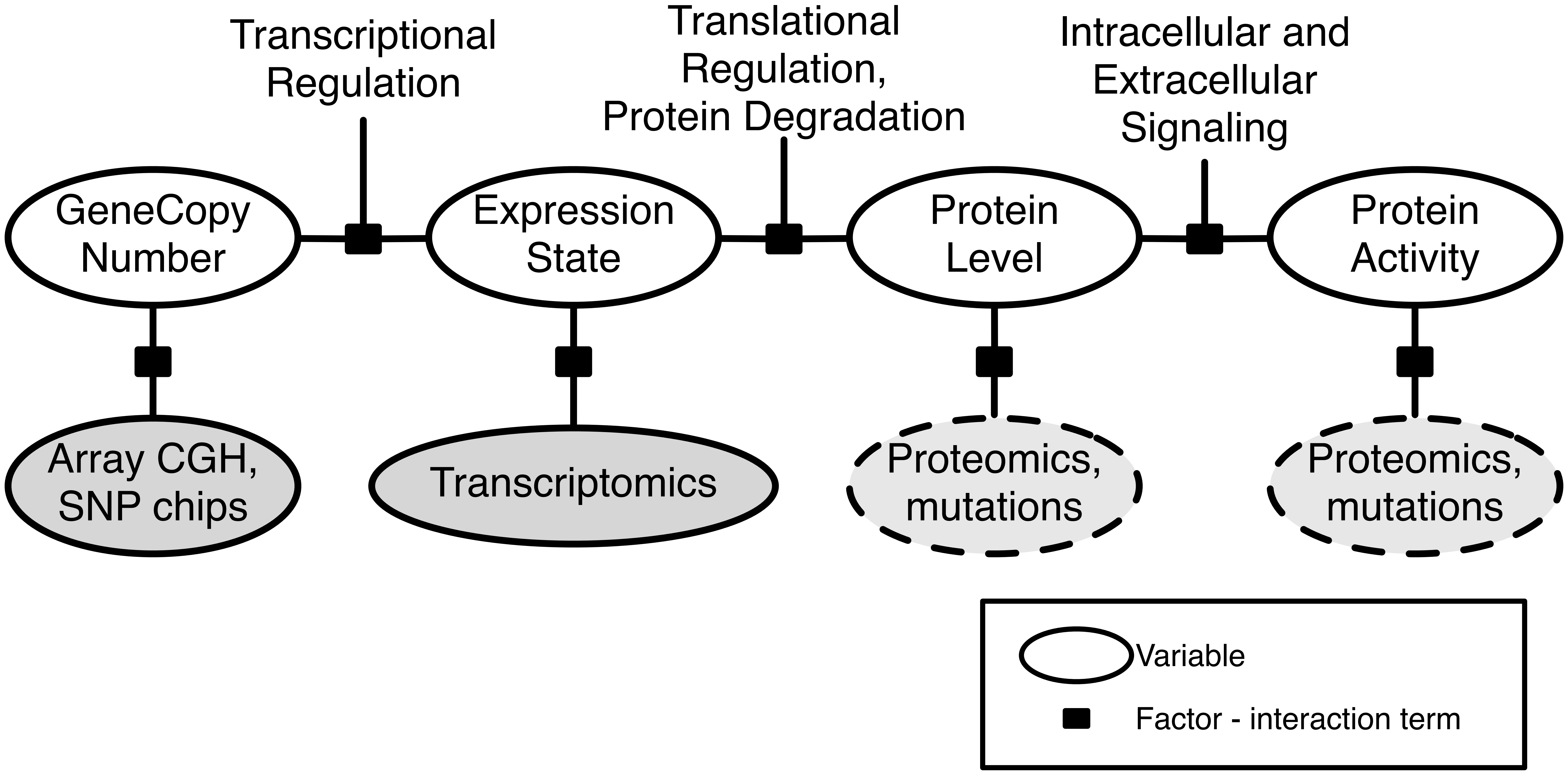
Gene Model


GeneCopy Number
Expression State
Protein Level
Protein Activity
Array CGH, SNP chips
Transcriptomics
Variable
Factor - interaction term

Gene Model

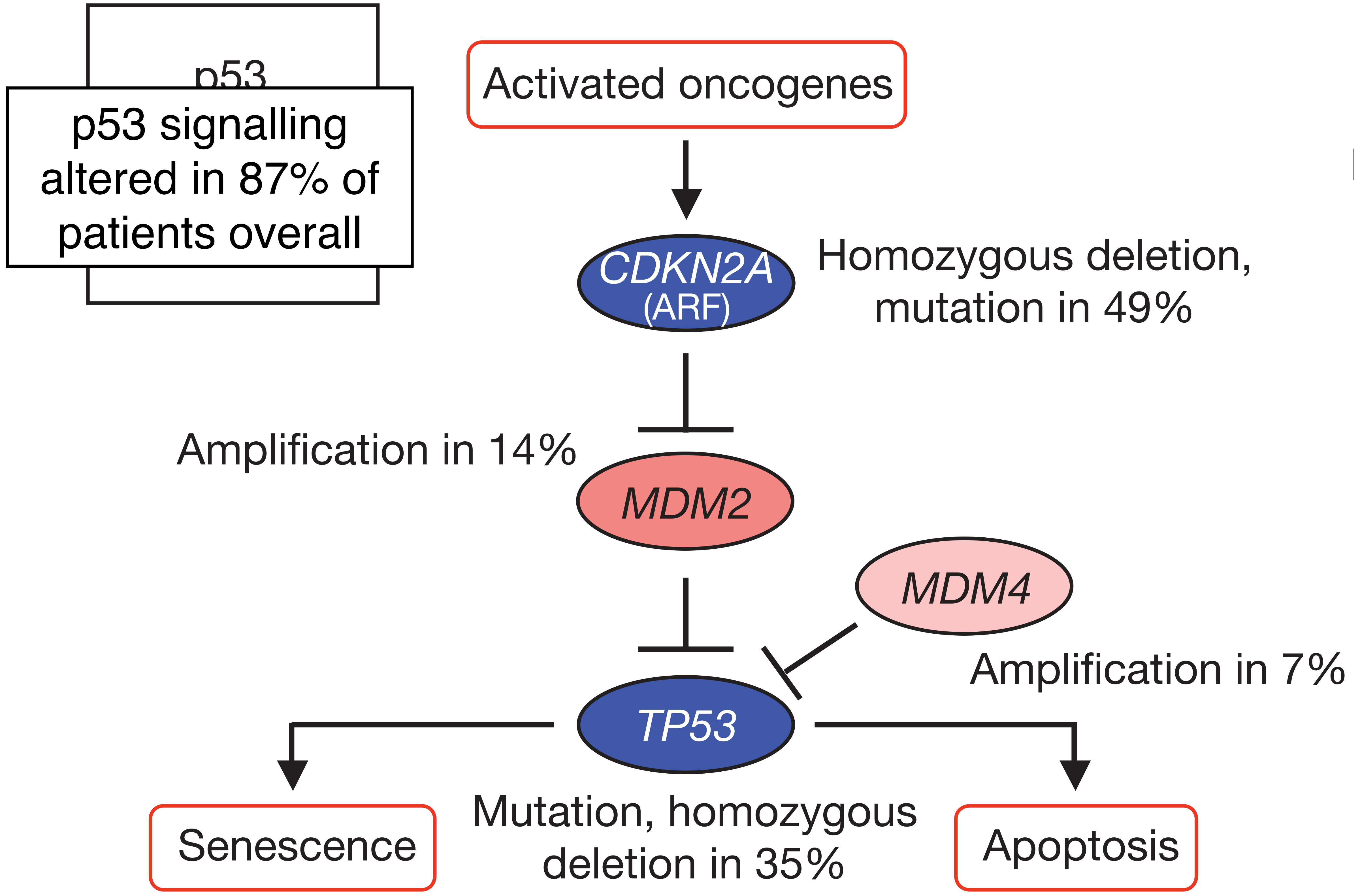

GeneCopy Number
Expression State
Protein Level
Protein Activity
Array CGH, SNP chips
Transcriptomics
Proteomics, mutations
Proteomics, mutations
Variable
Factor - interaction term

Gene Model


Transcriptional Regulation
Translational Regulation, Protein Degradation
Intracellular and Extracellular Signaling
GeneCopy Number
Expression State
Protein Level
Protein Activity
Array CGH, SNP chips
Transcriptomics
Proteomics, mutations
Proteomics, mutations
Variable
Factor - interaction term

Pathway as genetic unit

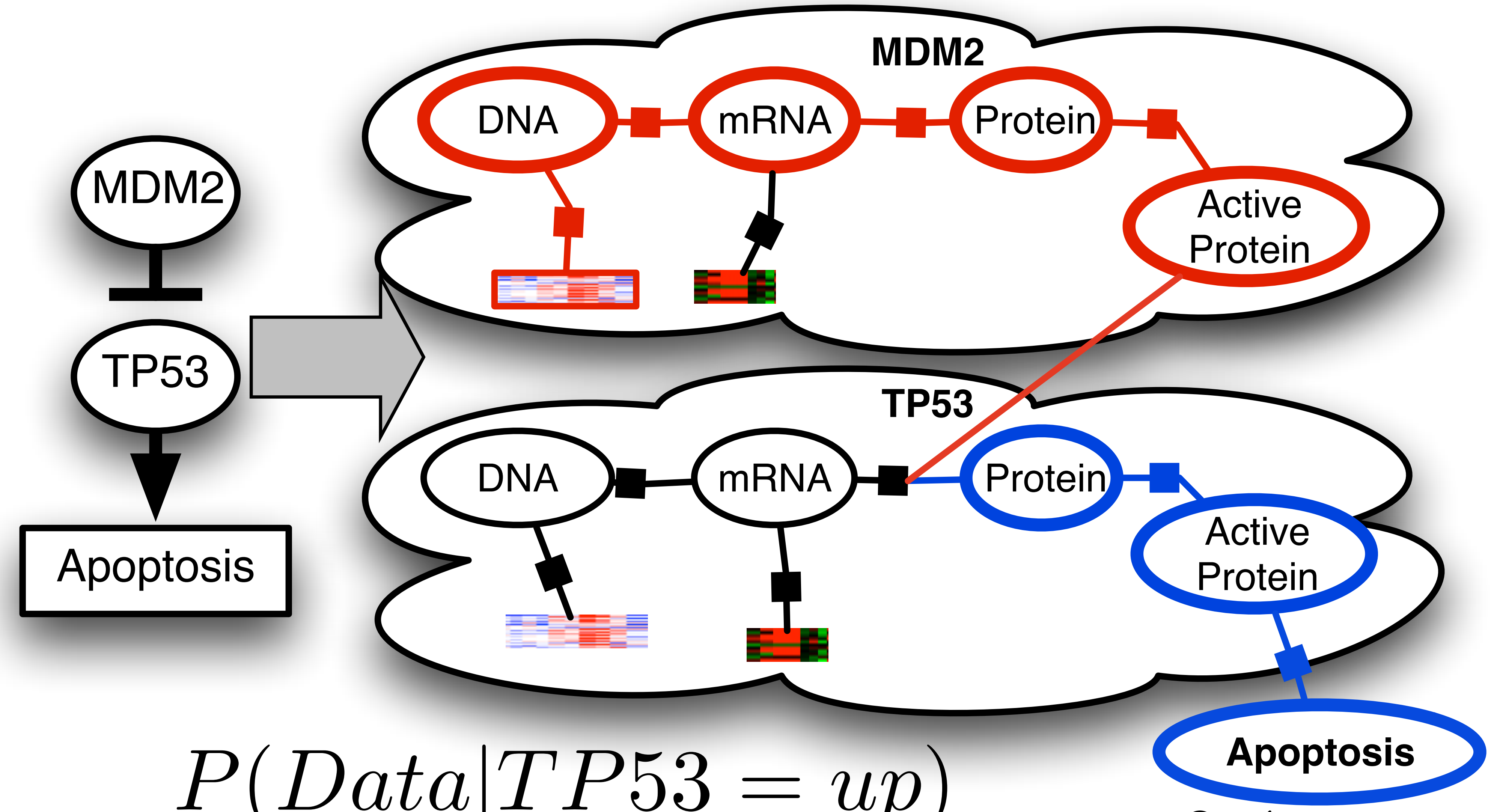
- No single gene is universally recurrent
- Subsets of cellular network (pathways) are much more recurrent
- Interaction sign matters
- Need many data types to find lesions


p53
p53 signalling altered in 87% of patients overall
Activated oncogenes
CDKN2A (ARF)
Homozygous deletion, mutation in 49%
Amplification in 14%
MDM2
MDM4
Amplification in 7%
TP53
Senescence
Mutation, homozygous deletion in 35%
Apoptosis

Glioblastoma Multiforme

The Cancer Genome Atlas, *Nature*, 2008

Integrated Pathway Activity (IPA)



$$\log_{10}\frac{P(Data|TP53 = up)}{P(Data|TP53 \neq up)} \approx \quad 0.1$$

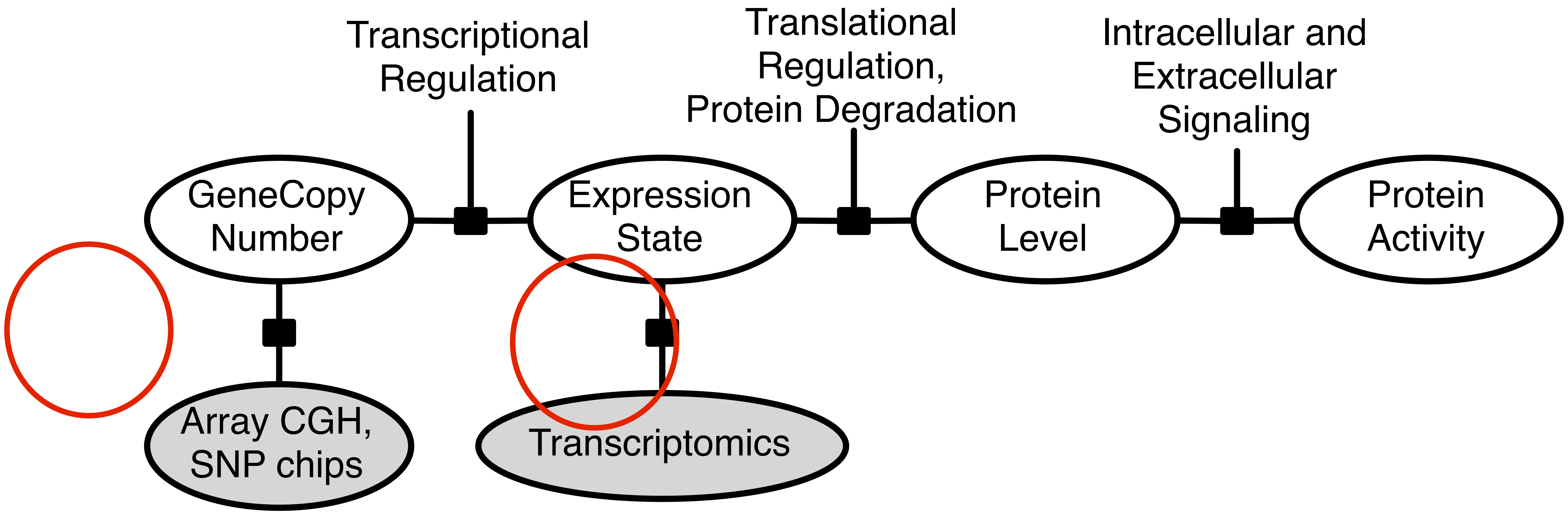
$$\log_{10}\frac{P(Data|TP53 = same)}{P(Data|TP53 \neq same)} \approx \quad -0.5$$

$$\log_{10}\frac{P(Data|TP53 = down)}{P(Data|TP53 \neq down)} \approx \quad 1.5 \quad \times -1$$

$$IPA(TP53) \approx -1.5$$

- Abstract notion of a biological entity's activity within a pathway context
- Calculate log-likelihood ratio of *up*, *same*, and *down* states
- IPA is the max of the three states, multiplied by the sign of the state

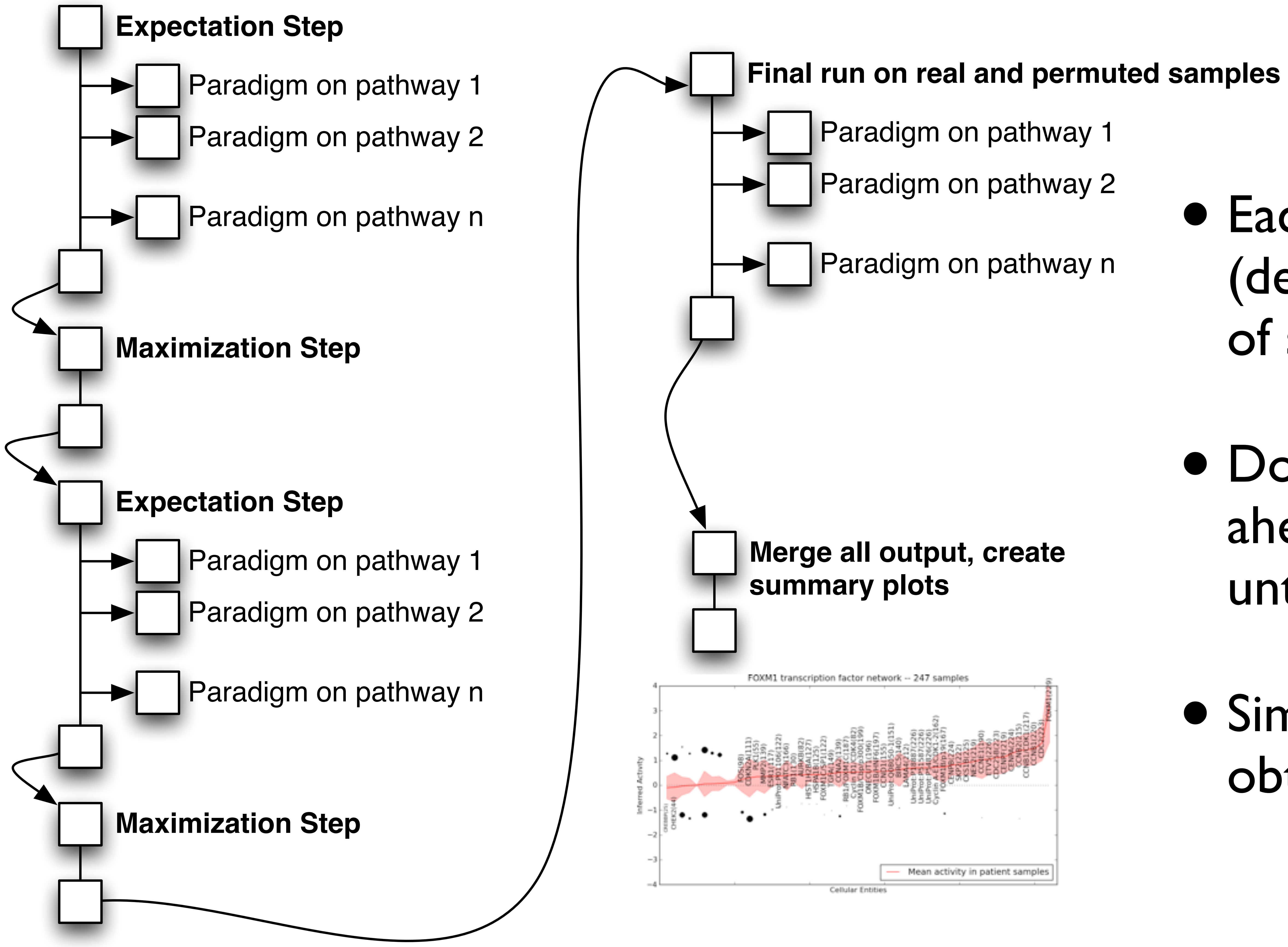
Observation Parameters



Learn via Expectation-Maximization

Wednesday, February 2, 2011

jtParadigm.py



Expectation Step

Paradigm on pathway 1

Paradigm on pathway 2

Paradigm on pathway n

Maximization Step

Expectation Step

Paradigm on pathway 1

Paradigm on pathway 2

Paradigm on pathway n

Maximization Step

Final run on real and permuted samples

Paradigm on pathway 1

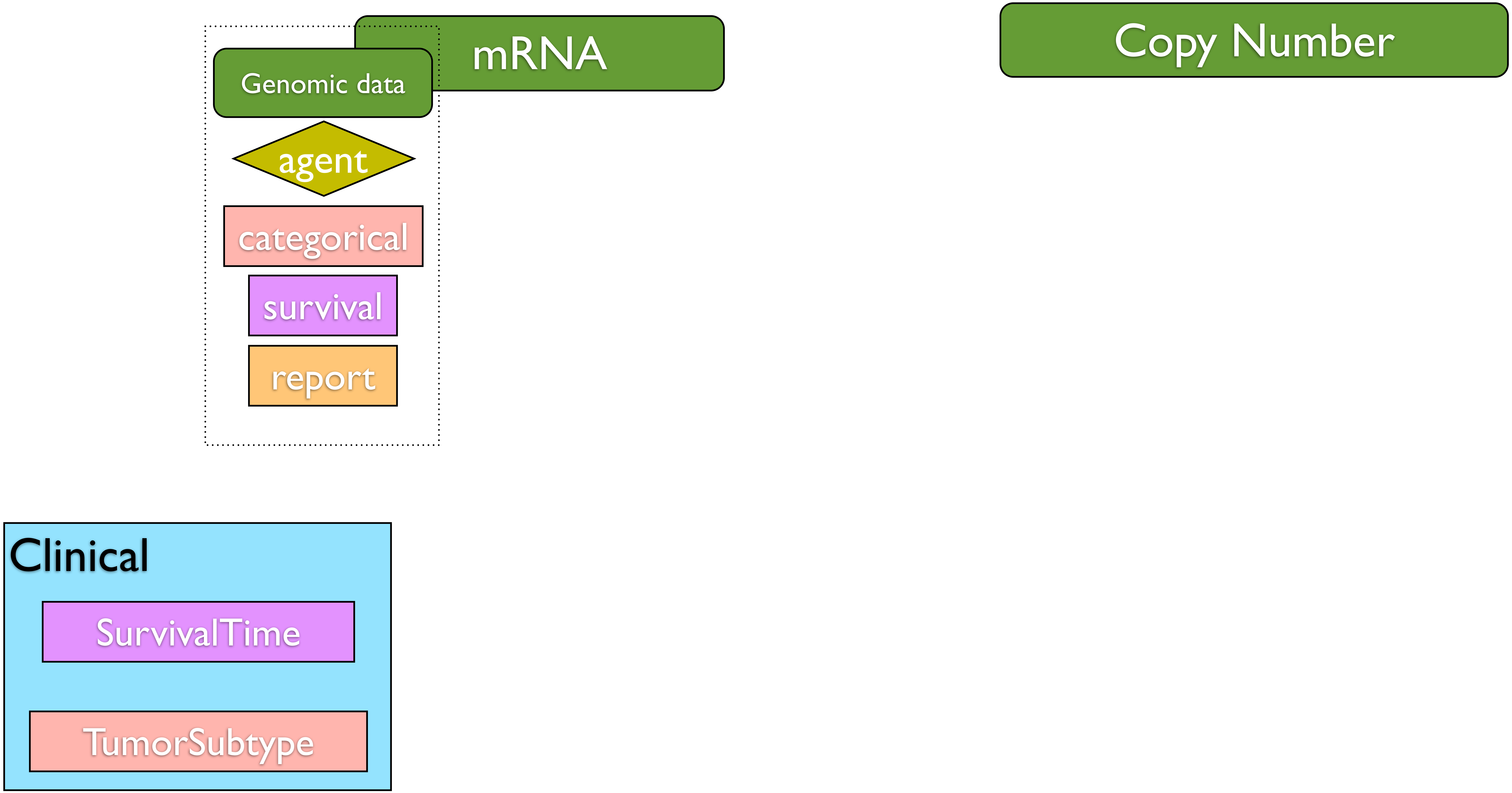
Paradigm on pathway 2

Paradigm on pathway n

Merge all output, create summary plots

FOXM1 transcription factor network -- 247 samples
Inferred Activity
Cellular Entities
Mean activity in patient samples
4
3
2
1
0
-1
-2
-3
-4

- Each E-step takes 1-200 hours (depending on pathway DB, number of samples)
- Don’t know number of EM steps ahead of time, dynamically add jobs until convergence
- Simple Python wrapper around obtuse C++ program



Genomic data

agent

categorical

survival

report

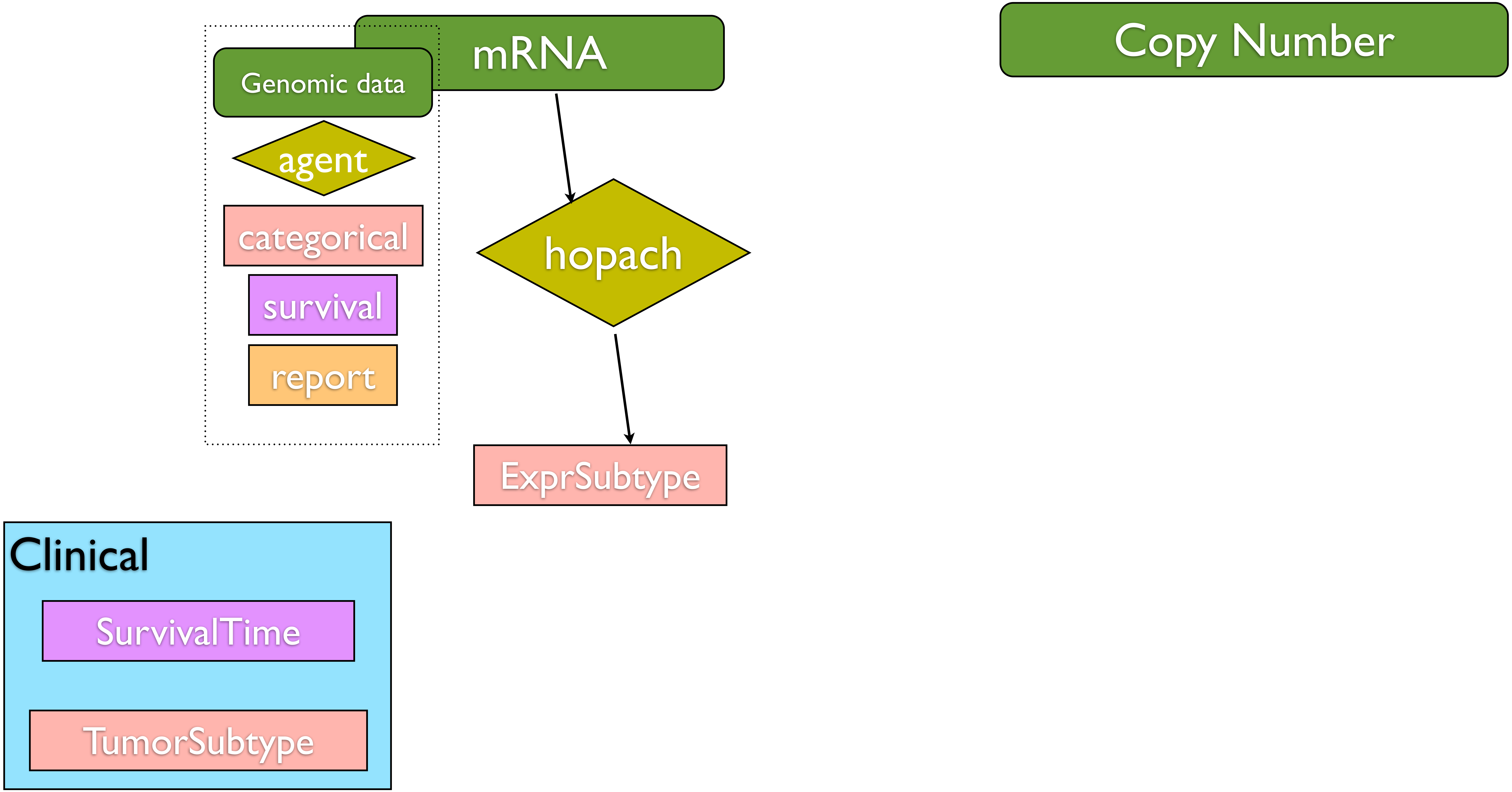
mRNA

Copy Number

Clinical

SurvivalTime

TumorSubtype



Copy Number

Genomic data

mRNA

agent

categorical

survival

report

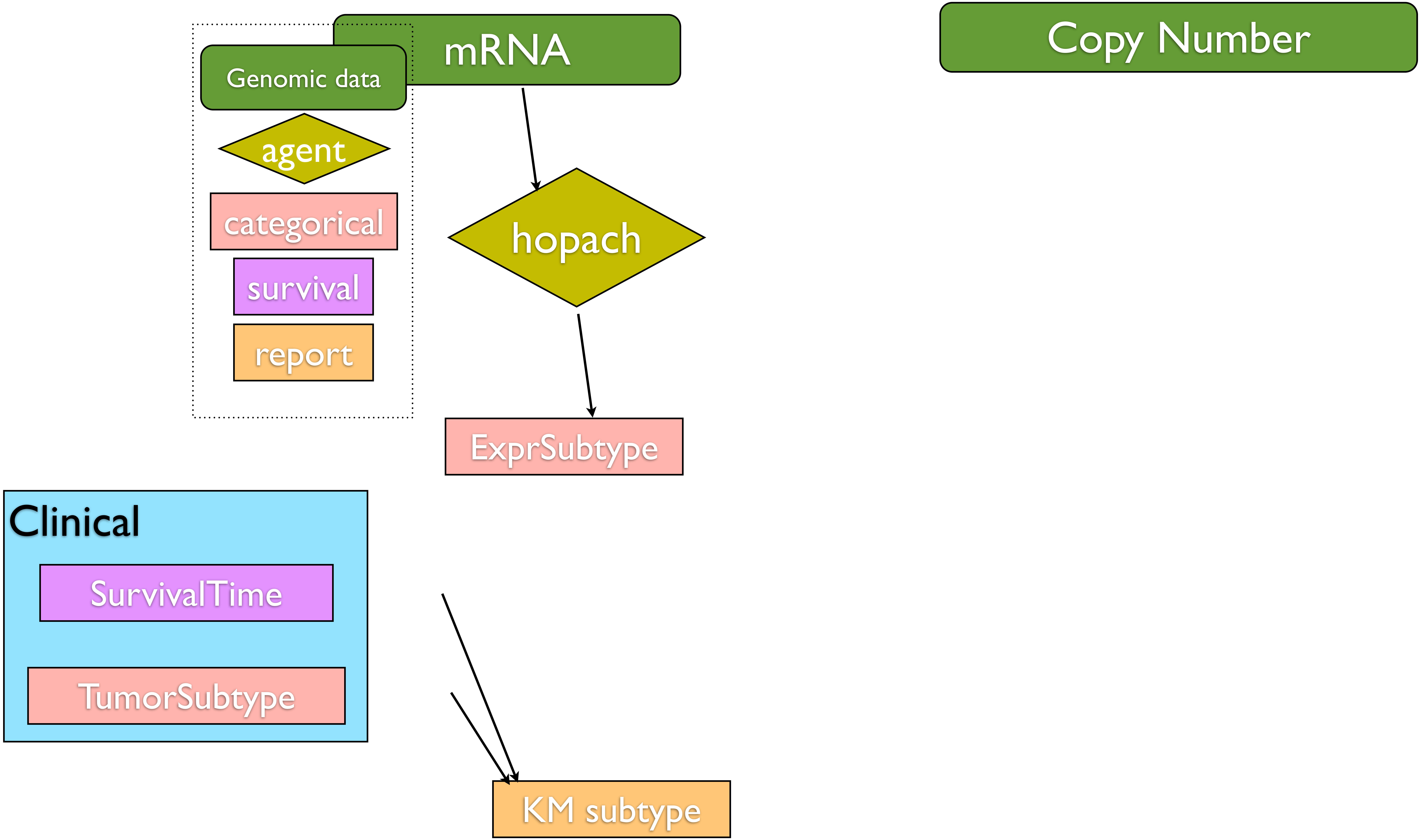
hopach

ExprSubtype

Clinical

SurvivalTime

TumorSubtype



mRNA

Copy Number

Genomic data

agent

categorical

survival

report

hopach

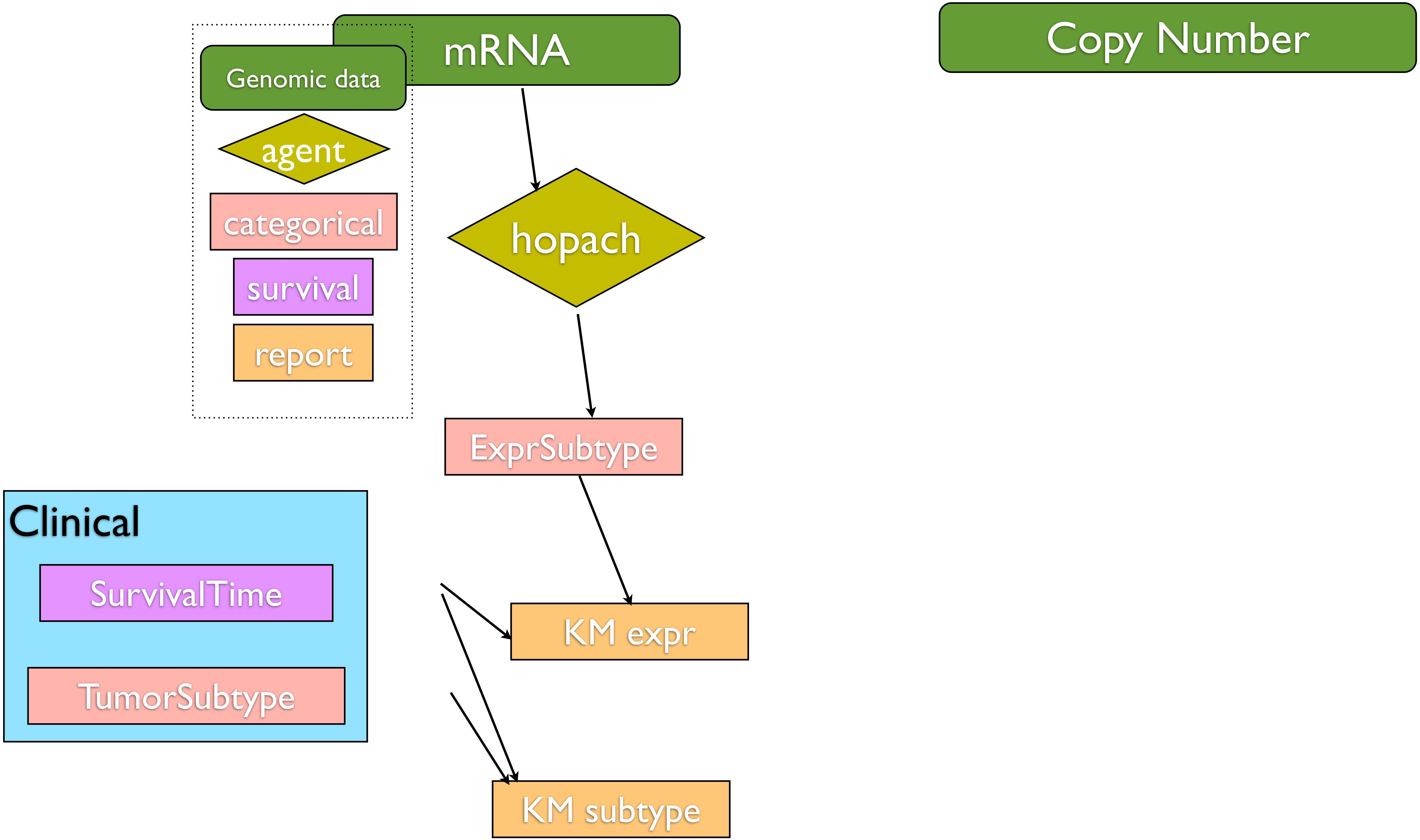
ExprSubtype

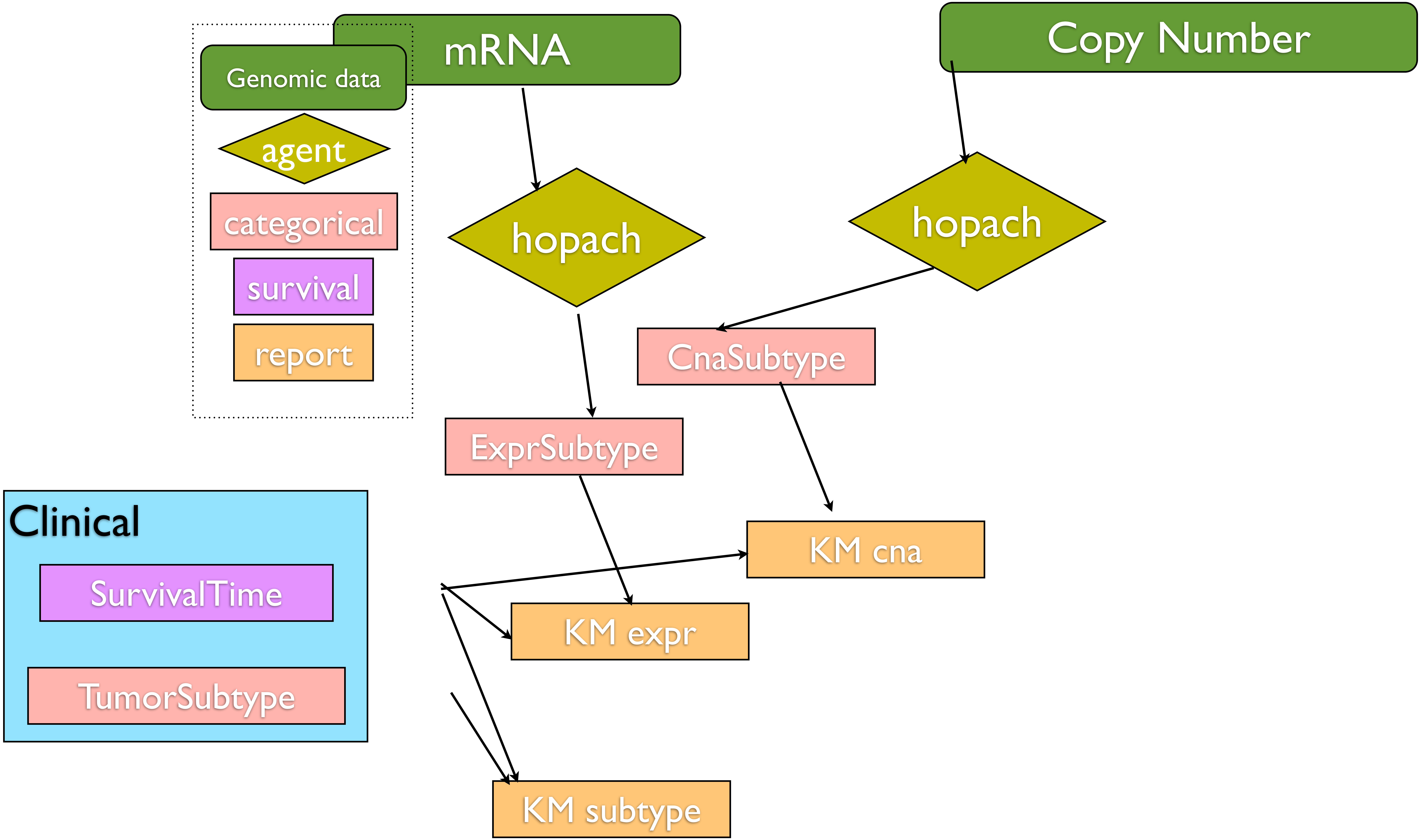
Clinical

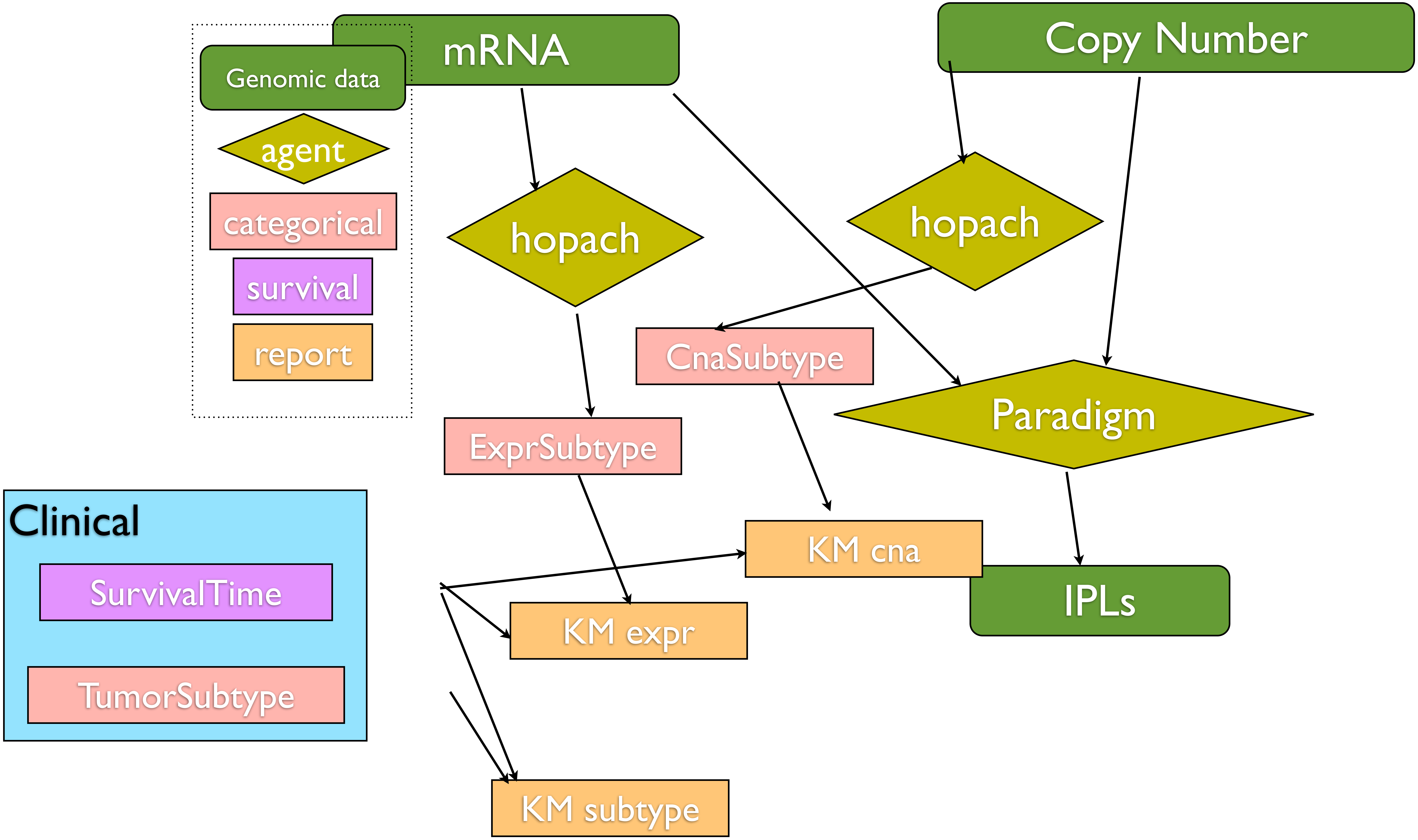
SurvivalTime

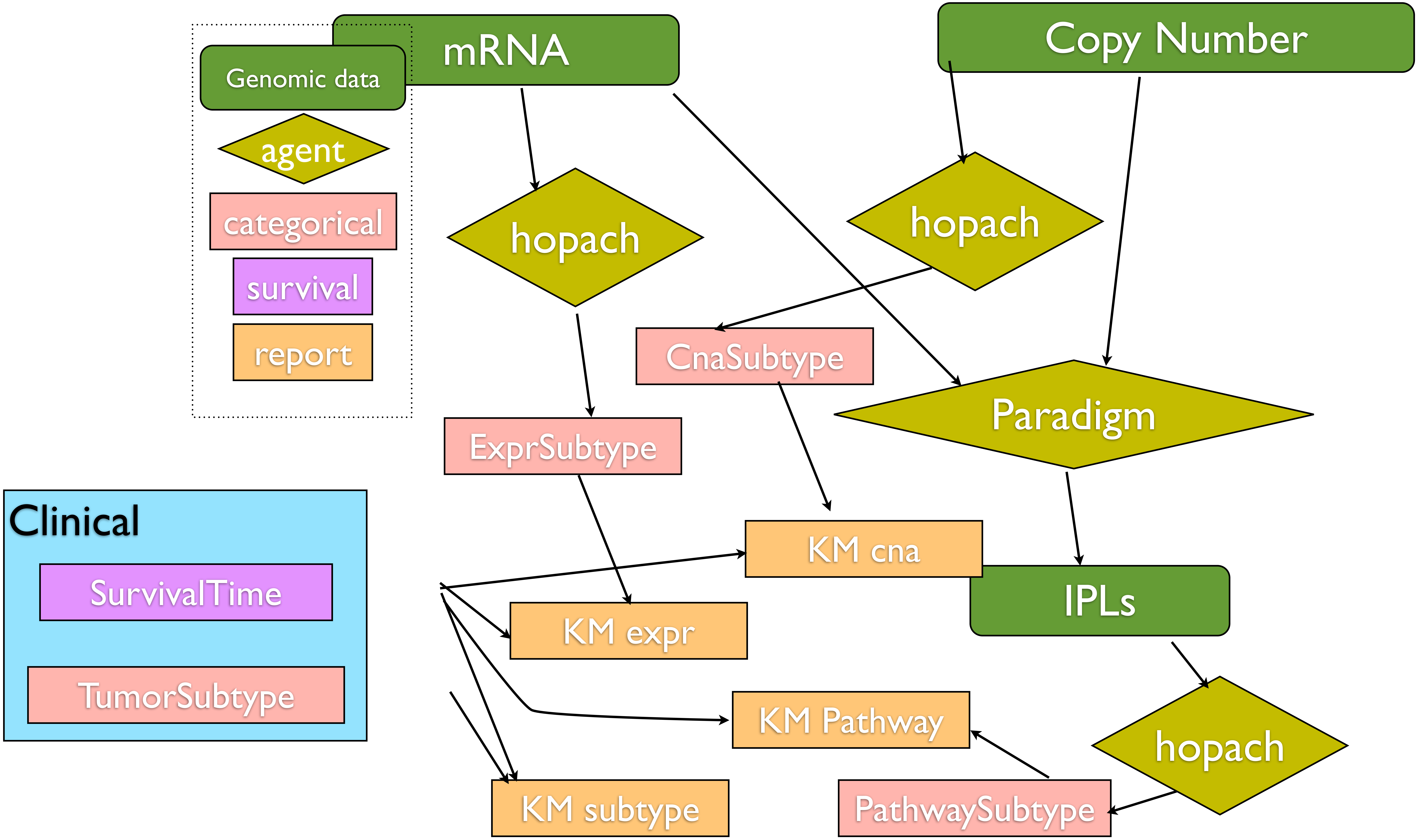
TumorSubtype

KM subtype


mRNA
Copy Number
Genomic data
agent
categorical
survival
report
hopach
ExprSubtype
Clinical
SurvivalTime
TumorSubtype
KM expr
KM subtype

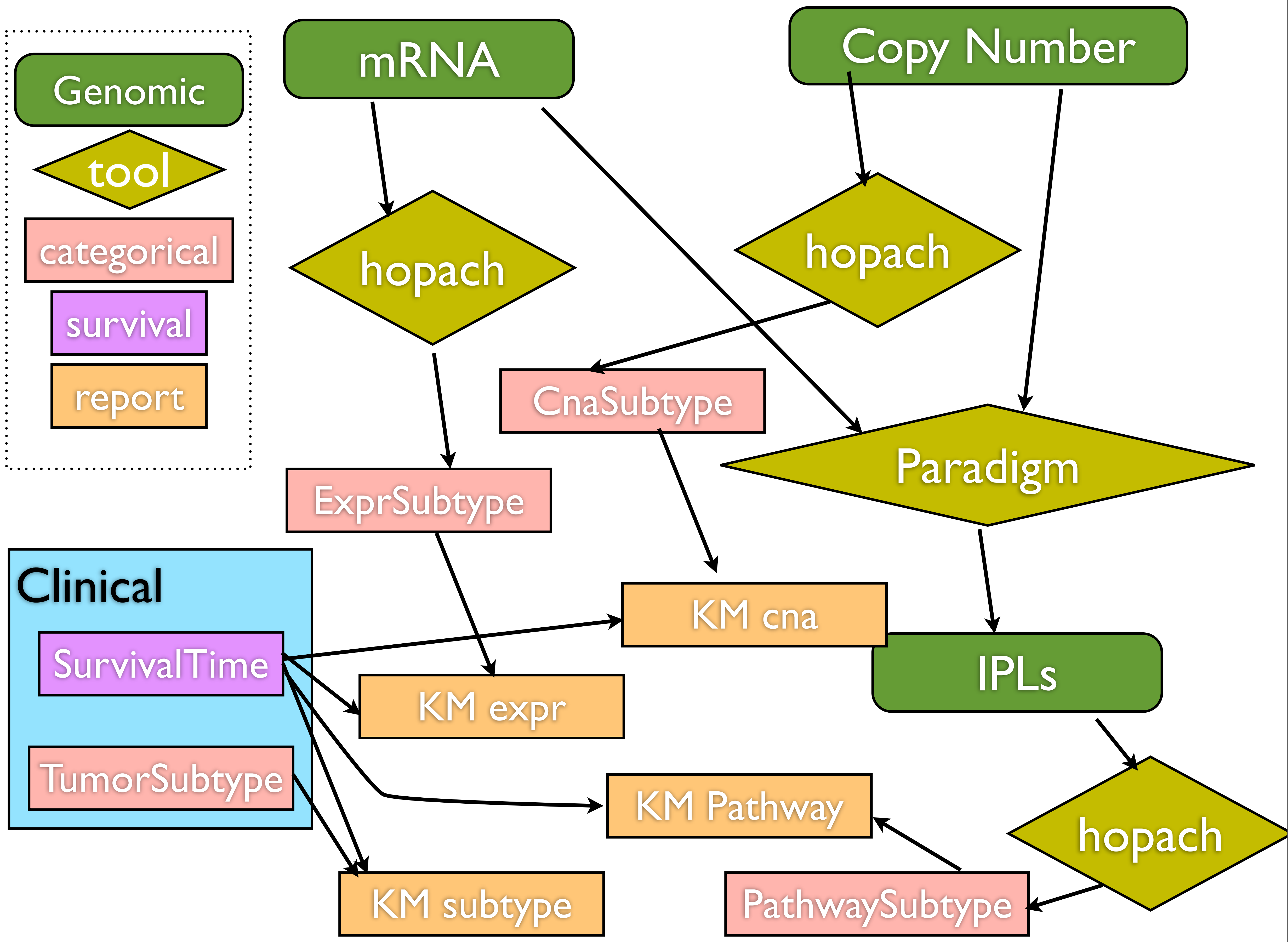

mRNA
Copy Number
Genomic data
agent
categorical
survival
report
hopach
hopach
CnaSubtype
ExprSubtype
Clinical
SurvivalTime
TumorSubtype
KM cna
KM expr
KM subtype


mRNA
Copy Number
Genomic data
agent
categorical
survival
report
hopach
hopach
CnaSubtype
Paradigm
ExprSubtype
Clinical
SurvivalTime
TumorSubtype
KM cna
IPLs
KM expr
KM subtype

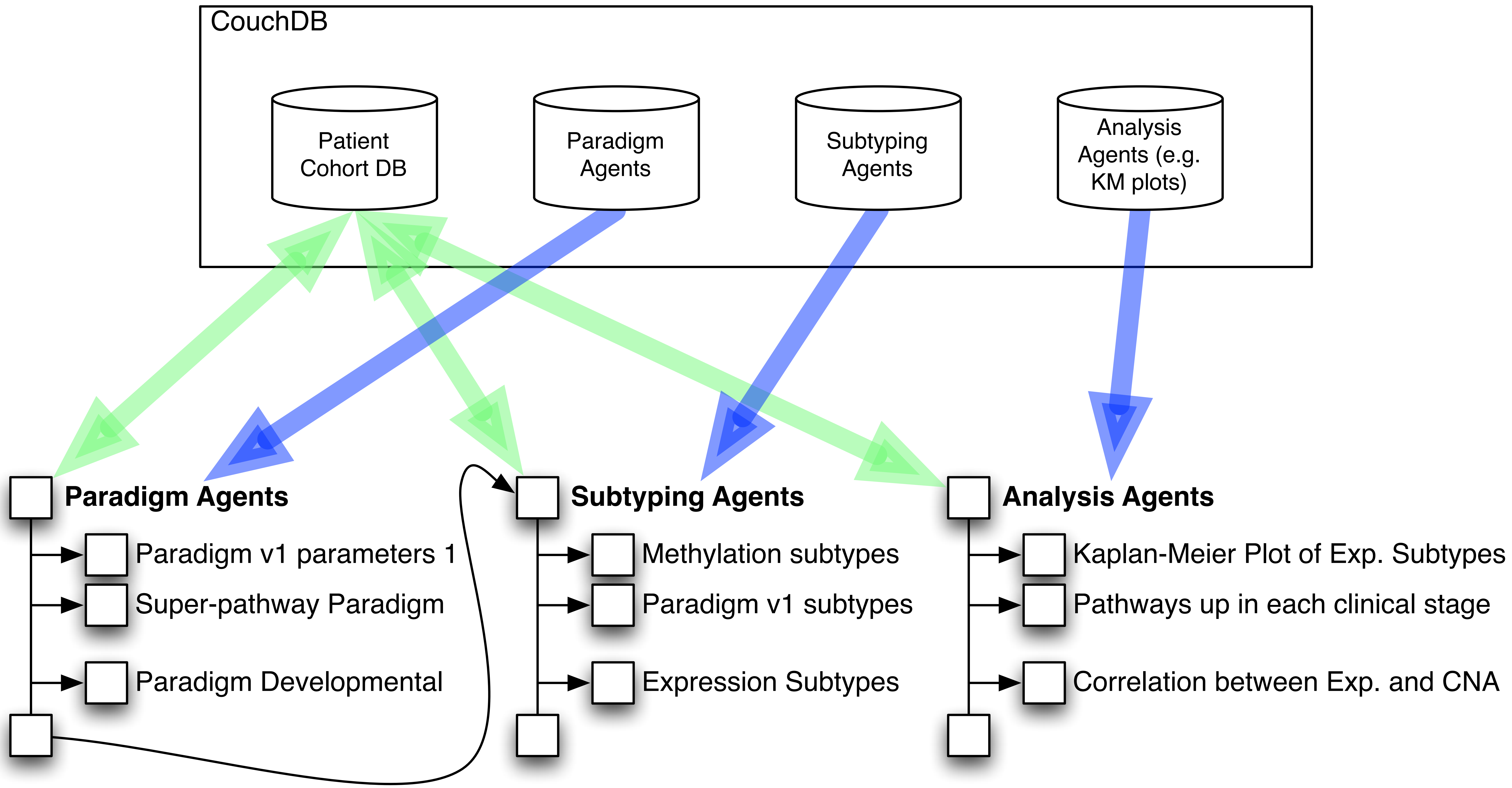

mRNA
Copy Number
Genomic data
agent
categorical
survival
report
hopach
hopach
CnaSubtype
Paradigm
ExprSubtype
Clinical
SurvivalTime
TumorSubtype
KM cna
IPLs
KM expr
KM Pathway
hopach
KM subtype
PathwaySubtype

Longboard

- System for running Paradigm and relevant downstream analyses, built on JobTree
- Unlike other pipeline systems, it's "agent" based– agents run on every input that meets their input filter
- In contrast, other systems require human steering
- Cancer group doesn't have enough people to steer analysis of 20+ cancers in TCGA

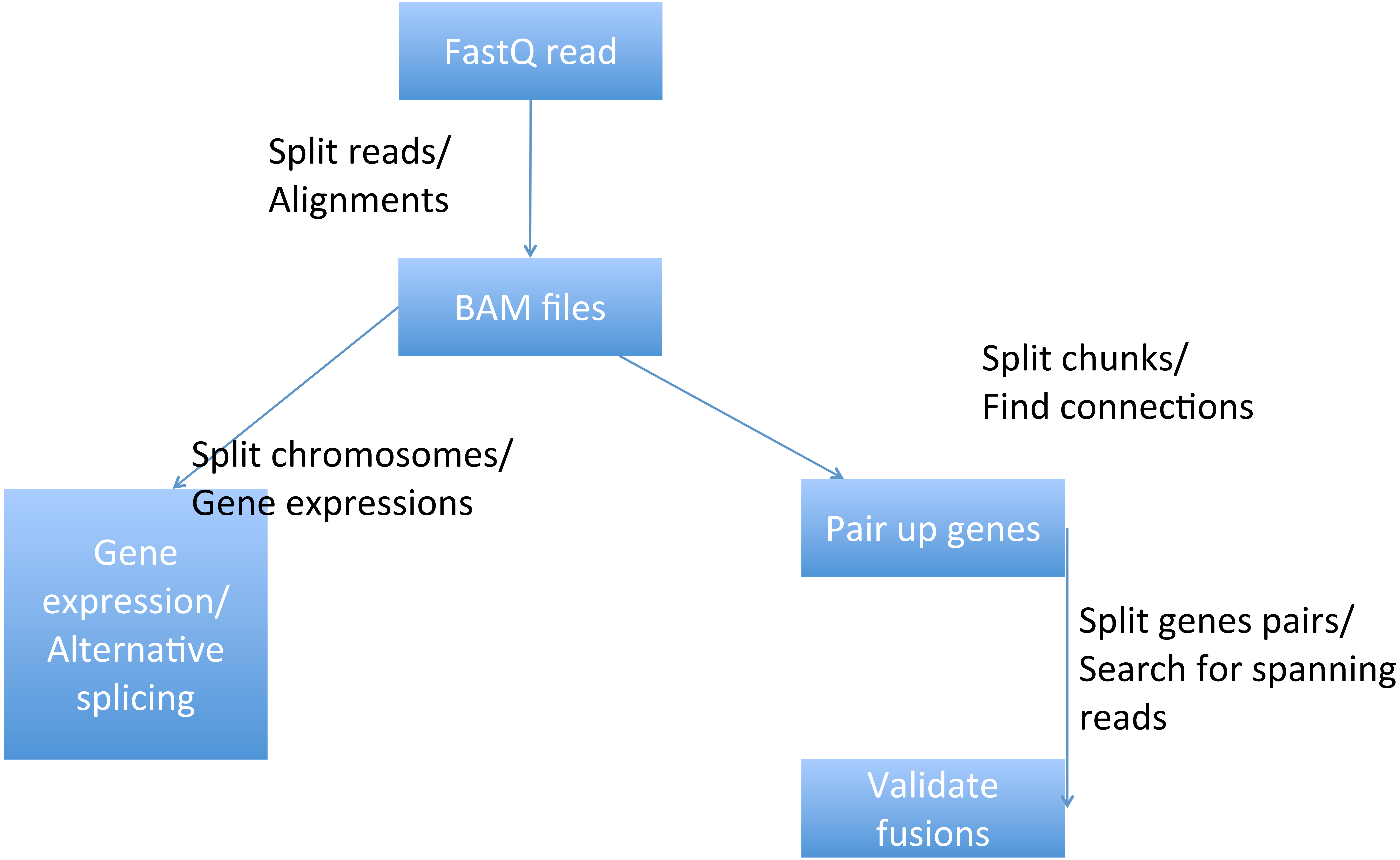


longboardRun.py



Daniel

RNAseq pipeline



FastQ read

Split reads/
Alignments

BAM files

Split chromosomes/
Gene expressions

Gene expression/
Alternative splicing

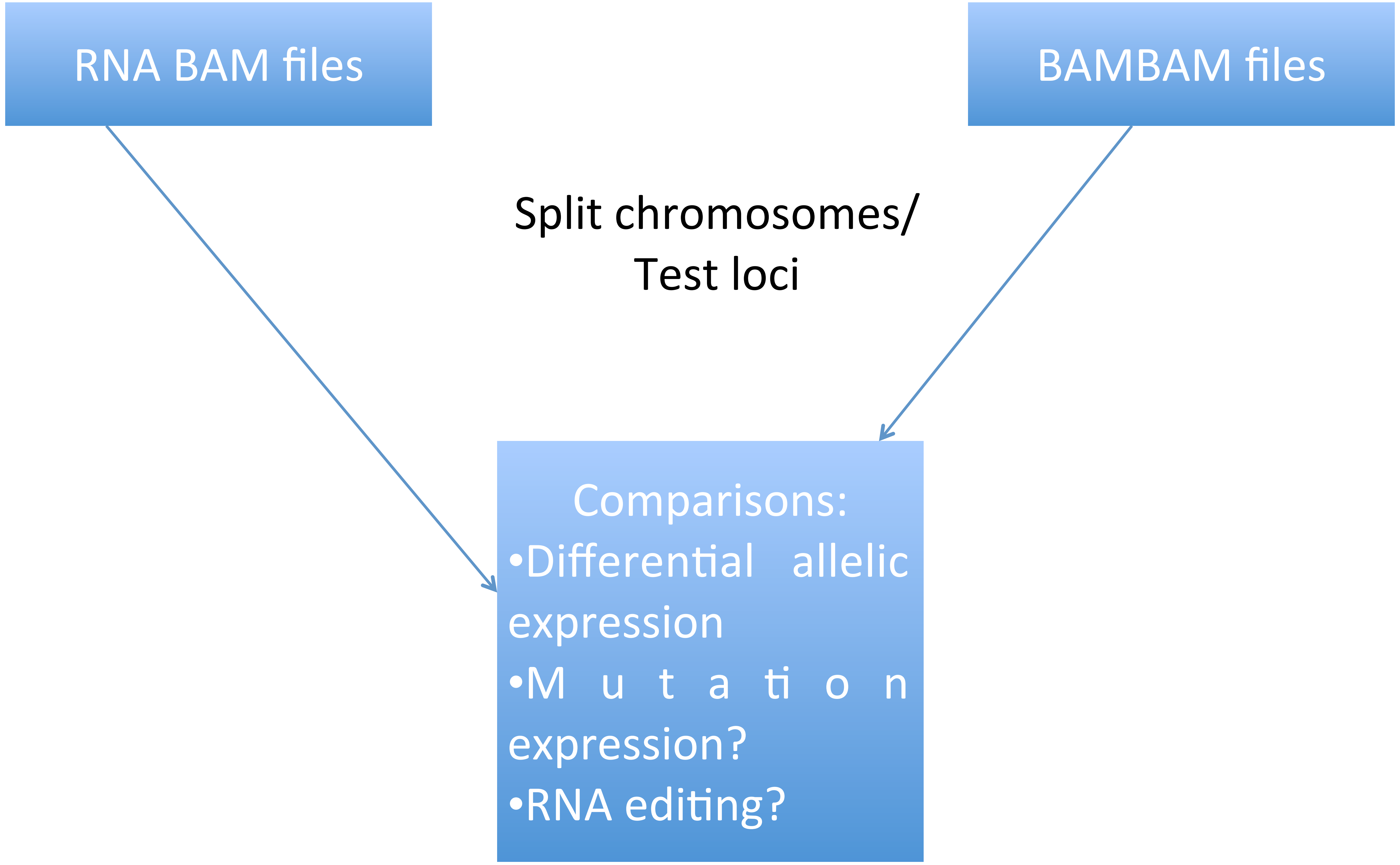
Split chunks/
Find connections

Pair up genes

Split genes pairs/
Search for spanning reads

Validate fusions

RNAseq pipeline 2



RNA BAM files

BAMBAM files

Split chromosomes/
Test loci

Comparisons:

- Differential allelic expression
- Mutation expression?
- RNA editing?