

# Getting started with the E. Coli Whole Cell Model on Sherlock: A Brief Tutorial

March 31, 2016

## 1 Basics

This document is an introduction to running the whole-cell E.coli model on the Sherlock computing cluster. In addition to setup and a tutorial on modifying the model, it will include a brief primer on some of model knowledge base fitting in later sections.

First a basic note on file locations. The knowledge base and the code that fits the knowledge base is located in the `wcEcoli/reconstruction/ecoli/` directory. The input information files are in `wcEcoli/reconstruction/ecoli/flat`, and the code that loads it into an object is in `knowledge_base_raw.py`.

Processes are located in `wcEcoli/models/ecoli/processes/`. Each process represents one part of the cell's function, and they are modeled separately in short time steps and then the results of each time step are integrated between modules before initiating the next time step. RNA polymerase elongation is the process used below as an example. Other processes include translation elongation, transcription initiation, and metabolism.

Each process has three components: `initialize` (called only once at the beginning of a simulation), `calculateRequest` (called at the beginning of each timestep), and `evolveState` (called after resources are allocated at each timestep).

*In initialize:* get needed parameters from the knowledge base, get views of bulk and unique molecules (bulk molecules are indistinguishable from each

other, e.g. inactive RNAP molecules, unique molecules can be distinguished from each other, e.g. active RNAP molecules are each assigned to a location on the genome), create a view so that you can get counts, change counts, and change properties.

*In calculateRequest:* request the resources that you want for that timestep (don't request all unless you are certain that another process doesn't need this resource as well, don't forget about metabolism).

*In evolveState:* perform the process, update counts, and update masses (mass must be conserved between steps).

If you want to save new values to be analyzed at the end of the simulation, you must write this information out as a listener. Listeners are programs which record information during the simulation. To add a listener, add the file to `wcEcoli/models/ecoli/listeners/`, and both add an import statement and add the listener to `_listenerClasses` in `wcEcoli/models/ecoli/sim/simulation.py`.

To change the cells initial conditions, change `wcEcoli/models/ecoli/sim/initial_conditions.py`

## 2 Setup

This tutorial assumes you have setup access to the Sherlock cluster. If necessary before following the proceeding steps, do the following setup:

1. Email the research computing staff at `research-computing-support@stanford.edu`, and cc Professor Covert. Request access to the Sherlock cluster, and ask Professor Covert to confirm your request in the email.
2. Follow the setup instructions for logging in to Sherlock on `http://covert.stanford.edu/computational\_resources/sherlock/home/`.
3. Follow all setup instructions in the `wcEcoli/README.md` file (also on the web at `https://github.com/CovertLab/wcEcoli/blob/master/README.md`). In particular, make sure you run

---

```
cd $HOME/wcEcoli
module load wcEcoli
```

```
make compile
```

---

Once done with setup and these basic tutorials on Sherlock and the cluster, return to here to complete the example.

## 3 Example: varying trascription rate

### 3.1 Background

Genes encoding for stable RNA are transcribed at a faster rate in E. Coli. In the model (prior to this tutorial), all genes were transcribed at the same rate of 42nt/s. In this tutorial, we will change the model so that genes for rRNA and tRNA are transcribed at 80nt/s while everything else is still transcribed at 42nt/s.

The code has inevitably evolved since I wrote this tutorial, so lets get on the same page by going back to an older version of the code. Lets do this tutorial on a new branch. cd into your wcEcoli directory and type:

---

```
git checkout wholecell-tutorial
git checkout -b tutorial wholecell-tutorial
```

---

(This gives you your own copy of the `wholecell-tutorial` branch named `tutorial` which you can commit to.)

We need to make sure the output from the model goes to the SCRATCH filesystem (which is larger) rather than SHERLOCK.HOME. We'll need to make a symbolic link between the output directory of your wcEcoli directory and a directory in SCRATCH. Within your wcEcoli diretory, there should be a folder named out/. The model puts its outputput in this folder, so we can basically tell the computer to send anything placed in this folder to SCRATCH instead.

First go to SCRATCH and create a folder in which to place the output. Run the following command:

---

```
cd $SCRATCH
```

---

Now make a directory to hold the output. You can call it whatever you want, here is one option:

---

```
mkdir wcEcoli_out
```

---

Return to wcEcoli home with

---

```
cd $HOME/wcEcoli
```

---

To create the symbolic link, we first need to delete the existing out/ directory if it is present. Do this with:

---

```
rmdir out/
```

---

If there is no out/ directory, then running the rmdir command won't hurt but isn't necessary. Now run this command to make the symbolic link. Change the name of the directory to the one you made on SCRATCH if it's different.

---

```
ln -s $SCRATCH/wcEcoli_out out
```

---

Now let's try running the unmodified model to make sure it works. First, make sure you are on a compute node on Sherlock. If you are, you will see the computer number next to your shell cursor, something like this:

---

```
sunetid@sh-8-30:~/wcEcoli/$
```

---

If you are on a login node, you will see

---

```
sunetid@sherlock-ln03:~/wcEcoli/$
```

---

If so, return to the sherlock tutorial to see how to use srun to log in to a compute node. It will be something like this:

---

```
srun -p mcovert --ntasks-per-node=1 --pty bash -l
```

---

Once you are in a compute node, ensure you are in your wcEcoli directory.

---

```
cd $HOME/wcEcoli
```

---

Now queue up a simple run of the model.

---

```
DESC="Tutorial run, starting code with unmodified parameters."  
python runscripts/fw_queue.py
```

---

Run the tasks in the queue until finished:

---

```
rlaunch rapidfire
```

---

## 3.2 Add a new parameter to the model

First, lets add a new elongation rate to the knowledge base. In reconstruction/ecoli/flat is a tsv called `growthRateDependentParameters.tsv`. Add a new column for the fast rna polymerase rate (estimate that it is double the normal rate). The normal rate at each growth rate is stored in the column `'rnaPolymeraseElongationRate'`. This command will generate the file with the new column appended, or edit the file in a different way if desired.

---

```
awk '{if(NR==1){print $0 "\t" "rnaPolymeraseElongationRateFast
(units.nt/units.min)}else{print $0 "\t" ($9*2)}}'
growthRateDependentParameters.tsv > temp && mv temp
growthRateDependentParameters.tsv
```

---

Alternatively, you could open the .tsv file in a spreadsheet editor and add the new column by hand.

To check that the parameter was added, examine the knowledge base object in ipython.

---

```
ipython
import reconstruction.ecoli.knowledge_base_raw as kbr
kb=kbr.KnowledgeBaseEcoli()
kb.growthRateDependentParameters[0]
```

---

You should see the 'rnaPolymeraseElongationRateFast': 78 [nucleotide/min]' entry in the resulting dictionary.

### 3.3 Create a new process

Lets split the transcript elongation process into a slow process and a fast process. Go to models/ecoli/processes/ :

---

```
cd models/ecoli/processes/

cp transcript_elongation.py transcript_elongation_fast.py

mv transcript_elongation.py transcript_elongation_slow.py
```

---

Now we need to add these processes to the simulation, so that they actually get called. Lets go back to the wcEcoli directory. Open models/ecoli/sim/simulation.py and change line 19 to read:

---

```
from models.ecoli.processes.transcript_elongation_slow import
    TranscriptElongationSlow
```

---

Then add a line just under this:

---

```
from models.ecoli.processes.transcript_elongation_fast import  
    TranscriptElongationFast
```

---

Under process classes, add TranscriptElongationFast and change TranscriptElongation to TranscriptElongationSlow. `_processClasses` should now look like this:

---

```
    _processClasses = (  
        Metabolism,  
        RnaDegradation,  
        TranscriptInitiation,  
        TranscriptElongationSlow,  
        TranscriptElongationFast,  
        PolypeptideInitiation,  
        PolypeptideElongation,  
        Replication,  
        ProteinDegradation,  
        Complexation,  
        AtpUsage  
    )
```

---

### 3.4 Change the model output

Now lets change the listeners to record output from these new processes. We write data to listeners, and the listener is responsible for recording the data to the file, as well as transforming it as necessary (calculating averages, for example). The transcription submodels write to three listeners: GrowthLimits, RnapData, and TranscriptElongationListener. We need to make several changes in order to correctly log transcription data. The fast and slow transcription submodels need to both write to the same listener attributes, so we need to set them up to add data together, rather than overwriting one another's output.

First, we need to update the listeners to zero out the relevant attributes each time step, so that we can add to them from each model. Open `models/ecoli/listeners/growth_limits.py` and add the following lines to the end of

tableAppend(...), at line 100:

---

```
self.ntpRequestSize = np.zeros(len(self.ntpIds), np.float64)
self.ntpAllocated = np.zeros(len(self.ntpIds), np.float64)
self.ntpUsed = np.zeros(len(self.ntpIds), np.float64)
```

---

We need to make two changes to models/ecoli/listeners/rnap\_data.py. At line 73, update the lines that read:

---

```
self.rnapStalls = np.zeros(0, np.int64)
self.ntpCountInSequence = np.zeros(21, np.int64)
self.ntpCounts = np.zeros(21, np.int64)
```

---

To read:

---

```
self.rnapStalls = np.empty(0, np.int64)
self.ntpCountInSequence = np.empty(0, np.int64)
self.ntpCounts = np.empty(0, np.int64)
```

---

This initialises some arrays we'll be writing to to be completely empty, which allows us to append to them without having a bunch of leading data we don't want. Next, we reset the relevant attributes as in GrowthLimits. Add the following to the bottom of tableAppend(...), at line 119:

---

```
self.rnapStalls = np.empty(0, np.int64)
self.ntpCountInSequence = np.empty(0, np.int64)
self.ntpCounts = np.empty(0, np.int64)
self.expectedElongations = 0
self.actualElongations = 0
self.didTerminate = 0
self.terminationLoss = 0
```

---

Finally, we need to update models/ecoli/listeners/transcript\_elongation\_listener.py. Add to the bottom of tableAppend(...) at line 47:

---

```
self.countRnaSynthesized =
    np.zeros(self.countRnaSynthesized.shape,
              self.countRnaSynthesized.dtype)
```

---



### 3.5 Modify a process

Now let's modify the new processes. Open `models/ecoli/processes/transcript_elongation_slow.py` and change all references of `TranscriptElongation` to `TranscriptElongationSlow`.

Next create a Boolean vector that is `True` at the indices of transcripts that should be elongated at the slow rate and `False` at the indices of transcripts that should be elongated at the fast rate. In the `initialize` function add the following line (after line 70):

---

```
self.slowRnaBool =  
    ~(sim_data.process.transcription.rnaData["isRRna5S"] |  
      sim_data.process.transcription.rnaData["isRRna16S"] |  
      sim_data.process.transcription.rnaData["isRRna23S"] |  
      sim_data.process.transcription.rnaData["isTRna"])
```

---

`isRRna5S`, `isRRna16S`, `isRRna23S`, and `isTRna` are properties of `rnaData`, which is found in the simulation data set (`sim_data`). These are vectors of Boolean values. The tilde inverts the boolean value, so this creates a vector that is `False` for all 5S rRNA, 16S rRNA, 23S rRNA, and tRNA, and `True` for everything else. Now let's change the view onto the active rna polymerases to a view onto only the active rna polymerases that are on transcripts that should be elongated at the slow rate. Change the definition of `self.activeRnaPolys` (line 75) to read:

---

```
self.activeRnaPolys = self.uniqueMoleculesView(  
    'activeRnaPoly',  
    rnaIndex = ("in", np.where(self.slowRnaBool)[0]))
```

---

Next, we need to update our writes to the listeners to increment or append, rather than overwrite, the attributes that are updated. First, add a new import at the top of the file (around line 25):

---

```
from wholecell.listeners.listener import WriteMethod
```

---

Second, we need to change our calls to `writeToListener(...)` to either increment (in the case of numeric attributes), or append (in the case of arrays), rather than overwriting. Modify all of the `writeToListener(...)` calls to have

a new parameter at the end: `WriteMethod.increment`, except for the writes to `rnapStalls`, `ntpCountInSequence`, and `ntpCounts`, which instead should have `WriteMethod.append`. Overall, the lines should look like the following (although in the file they are scattered around a bit):

---

```

self.writeToListener("GrowthLimits", "ntpRequestSize",
    maxFractionalReactionLimit * sequenceComposition,
    WriteMethod.increment)

self.writeToListener("GrowthLimits", "ntpAllocated",
    self.ntps.counts(), WriteMethod.increment)

self.writeToListener("TranscriptElongationListener",
    "countRnaSynthesized", terminatedRnas, WriteMethod.increment)

self.writeToListener("GrowthLimits", "ntpUsed", ntpsUsed,
    WriteMethod.increment)
self.writeToListener("RnapData", "rnapStalls", rnapStalls,
    WriteMethod.append)
self.writeToListener("RnapData", "ntpCountInSequence",
    ntpCountInSequence, WriteMethod.append)
self.writeToListener("RnapData", "ntpCounts", ntpCounts,
    WriteMethod.append)
self.writeToListener("RnapData", "expectedElongations",
    expectedElongations.sum(), WriteMethod.increment)
self.writeToListener("RnapData", "actualElongations",
    sequenceElongations.sum(), WriteMethod.increment)
self.writeToListener("RnapData", "didTerminate",
    didTerminate.sum(), WriteMethod.increment)
self.writeToListener("RnapData", "terminationLoss",
    (terminalLengths - transcriptLengths)[didTerminate].sum(),
    WriteMethod.increment)

```

---

This is all we need to change in this file. Now lets open the fast transcript elongation file `models/ecoli/processes/transcript_elongation_fast.py`. Similarly to what we did in the slow elongation file, lets change all references of `TranscriptElongation` to `TranscriptElongationFast`.

Now, lets create the opposite of the Boolean vector that we created in the `transcript_elongation_slow`. In the `initialize` function add the following line

(after line 70):

---

```
self.fastRnaBool =
    sim_data.process.transcription.rnaData["isRRna5S"] |
    sim_data.process.transcription.rnaData["isRRna16S"] |
    sim_data.process.transcription.rnaData["isRRna23S"] |
    sim_data.process.transcription.rnaData["isTRna"]
```

---

Now lets change the view onto the active rna polymerases to a view onto only the active rna polymerases that are on transcripts that should be elongated at the fast rate (line 75):

---

```
self.activeRnaPolys = self.uniqueMoleculesView(
    'activeRnaPoly',
    rnaIndex = ("in",
        np.where(self.fastRnaBool)[0])
)
```

---

Finally, lets change the elongation rate. Change line 59 to read:

---

```
self.elngRate =
    kb.rnaPolymeraseElongationRateFast.asNumber(units.nt / units.s)
    * self.timeStepSec
```

---

Update the writeToListener(...) lines to match the changes you made in TranscriptElongationSlow, above. Now data from both submodels will be recorded in the whole cell output.

Now we can run a simulation and rRNA and tRNA would be transcribed at the new fast rate, while everything else was transcribed at the same slow rate before. Follow these steps to run the new simulation code:

Queue up the tasks in fireworks:

---

```
DESC="Tutorial run, adding different RNA polymerization rate for
r- and t- RNAs." python runscripts/fw_queue.py
```

---

Run the tasks in the queue until finished:

---

```
rlaunch rapidfire
```

---

To check for the success of your simulation, open the /out/ folder, and the folder timestamped to the simulation just run, then click through to the output plots. Specifically look at the rnapActiveFraction plot. This should be around 20%. Is it? Also look at the massFractionSummary plot. Does everything roughly double in one cell cycle? If not, why might that be?

### 3.6 Changing the fitting

Even though we've changed the model, the simulation will be initialized the same way as before. This is a problem because before running a simulation, we need to fit several initial parameters including the initial counts of RNA polymerases and the activation rate of the RNA polymerases. Because some things are now being transcribed at a faster rate, we should need fewer RNA polymerases to make the same number of transcripts. Additionally, if some things are being transcribed more quickly, then RNA polymerases will be inactivating more quickly. In order to maintain a constant ratio of active to inactive RNA polymerases (experimentally shown to be around 20%), the activation rate must also increase now.

We calculate the number of RNA polymerases that we need initially by writing an equation for the rate of change of some RNA  $R_i$  (rate of synthesis rate of degradation = rate of dilution due to growth):

$$\frac{dR_i}{dt} = \frac{k_{elong}}{L_i} P_i(t) - \frac{\ln(2)}{h_i} R_i(t) = \frac{\ln(2)}{\tau_d} R_i(t)$$

$L_i$  is the length of transcript  $i$ ;  $P_i$  is the number of RNA polymerases actively transcribing  $R_i$  at time  $t$ ;  $h_i$  is the half life of  $R_i$ ;  $\tau_d$  is the length of the cell cycle;  $k_{elong}$  is the transcript elongation rate. Right now this is a constant value for all transcripts. We want to change this to be different for rRNA and tRNA. Lets change this in the code. Open the file reconstruction/ecoli/fit\_sim\_data\_1.py and go to the setRNAPCountsConstrainedByPhysiology function. This is what we need to change. Lets add the Boolean vectors for fast and slow transcripts. Right at the beginning of this function definition (after the docstring), add these two lines:

---

```
fastRnaBool = kb.process.transcription.rnaData["isRRna5S"] |
               kb.process.transcription.rnaData["isRRna16S"] |
```

```
kb.process.transcription.rnaData["isRRna23S"] |  
kb.process.transcription.rnaData["isTRna"]  
slowRnaBool = ~fastRnaBool
```

---

Lets break up the calculation of nActiveRnapNeeded into nActiveRnapNeededforFast and nActiveRnapNeededforSlow. Change the nActiveRnapNeeded calculation to read:

```
nActiveRnapNeededforSlow =  
  calculateMinPolymerizingEnzymeByProductDistributionRNA(  
    rnaLengths[slowRnaBool],  
    sim_data.growthRateParameters.rnaPolymeraseElongationRate,  
    rnaLossRate[slowRnaBool])
```

---

Add a line under this for the calculation for the fast transcripts:

```
nActiveRnapNeededFast =  
  calculateMinPolymerizingEnzymeByProductDistributionRNA(  
    rnaLengths[fastRnaBool],  
    sim_data.growthRateParameters.rnaPolymeraseElongationRateFast,  
    rnaLossRate[fastRnaBool])
```

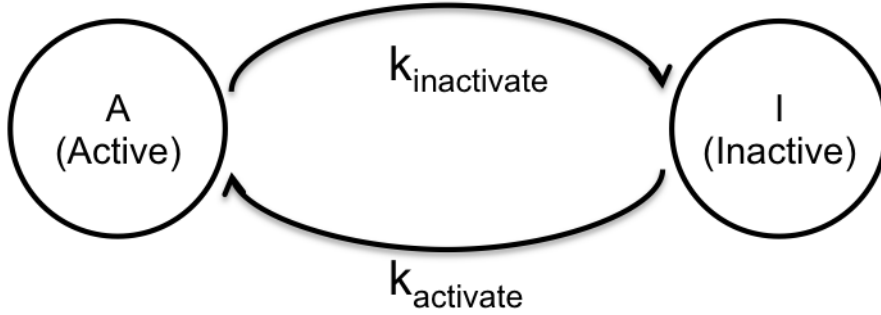
---

Below this, add a line to calculate the total number of RNA polymerases needed:

```
nActiveRnapNeeded = nActiveRnapNeededforFast +  
  nActiveRnapNeededforSlow
```

---

Now lets change the calculation of the RNA polymerase activation rate. In the model, an RNA polymerase can either be active or inactive:



To calculate the rate of activation,  $k_{activate}$ , we write an equation for the rate of change of the number of RNAP active at steady state:

$$\frac{dA}{dt} = k_{activate}I - k_{inactivate}A = 0$$

This gives us that

$$k_{activate} = k_{inactivate} \frac{A}{I}$$

We know from experiments the fraction of RNA polymerases that are active,  $f_{active}$ :

$$f_{active} = \frac{A}{A + I}$$

Using that

$$f_{active} = 1 - f_{inactive}$$

We can rearrange and solve for the rate of activation:

$$k_{activate} = k_{inactivate} \left( \frac{f_{active}}{1 - f_{active}} \right)$$

We can calculate the rate of inactivation from the elongation rate, the transcript lengths, and the synthesis probabilities:

$$k_{inactivate} = \frac{k_{elong}}{L_i} \cdot \frac{1}{p_{synth}}$$

We want to change the elongation rate to be a vector, rather than a constant:

$$k_{inactivate} = \frac{k_{elong,i}}{L_i} \cdot \frac{1}{p_{synth}}$$

Now lets do this in the code. In reconstruction/ecoli/fitkb1.py, in the fitRNAPolyTransitionRates function (on line 483), at the top add the following lines. The tilde operator inverts the booleans.

---

```
fastRnaBool = (
    sim_data.process.transcription.rnaData["isRRna5S"] |
    sim_data.process.transcription.rnaData["isRRna16S"] |
    sim_data.process.transcription.rnaData["isRRna23S"] |
    sim_data.process.transcription.rnaData["isTRna"])
slowRnaBool = ~fastRnaBool
```

---

Now, delete the elngRate definition (elngRate = kb.rnaPolymeraseElongationRate) and add an elongation rate vector:

---

```
elngRateVector = slowRnaBool *
    sim_data.growthRateParameters.rnaPolymeraseElongationRate +
    fastRnaBool *
    sim_data.growthRateParameters.rnaPolymeraseElongationRateFast
```

---

Delete the calculation of averageTranscriptLength and expectedTerminationRate and add the following three lines:

---

```
expectedTranscriptionTime = rnaLengths/elngRateVector

weightedExpectedTranscriptionTime = units.dot(synthProb,
    expectedTranscriptionTime)

expectedTerminationRate = 1/weightedExpectedTranscriptionTime
```

---

Were done editing this file now. Now the fitting of the initial number of RNA polymerases and the activation rate is fixed.

### 3.7 Running simulations

Now we can run some simulations. Be sure to complete the setup section (2) if you haven't already.

First log in to a sherlock node. Replace 'username' with your username in the command below:

---

```
ssh username@sherlock
```

---

Now log in to a non-login node, so that the simulation can be run in interactive mode (running in interactive mode on a login node can result in getting booted from the cluster). These nodes are covert-lab specific and it's ok to do more serious computation on them.

---

```
srun -p mcovert --ntasks-per-node=1 --time=12:00:00 --pty bash
```

---

Now prepare the fireworks queue with your simulation task.

Once setup is complete, change the DESC description text as desired, and run:

---

```
DESC="Tutorial run, adding different RNA polymerization rate for  
r- and t- RNAs." python runscripts/fw_queue.py
```

---

Now the simulation task is queued up in fireworks and can be launched via:

---

```
rlaunch rapidfire
```

---

After about a minute, this should start producing output looking something like this:

---

```
[mpaull@sh-8-31 ~/wcEcoli]$ rlaunch rapidfire  
2015-06-23 19:09:29,106 INFO Hostname/IP lookup (this will take a  
few seconds)
```

---



```
2015-06-23 19:09:29,814 INFO Created new dir
    /home/mpaull/wcEcoli/launcher_2015-06-24-02-09-29-810292
2015-06-23 19:09:29,817 INFO Launching Rocket
2015-06-23 19:09:32,285 INFO RUNNING fw_id: 12 in directory:
    /home/mpaull/wcEcoli/launcher_2015-06-24-02-09-29-810292
2015-06-23 19:09:32,289 INFO Task started:
    {{wholecell.fireworks.firetasks.initKb.InitKbTask}}.
Tue Jun 23 19:09:32 2015: Instantiating unfit knowledgebase
Tue Jun 23 19:09:32 2015: Saving unfit knowledgebase
2015-06-23 19:09:32,292 INFO Task completed:
    {{wholecell.fireworks.firetasks.initKb.InitKbTask}}
2015-06-23 19:09:34,950 INFO Rocket finished
2015-06-23 19:09:35,328 INFO Created new dir
    /home/mpaull/wcEcoli/launcher_2015-06-24-02-09-35-326470
2015-06-23 19:09:35,330 INFO Launching Rocket
2015-06-23 19:09:37,772 INFO RUNNING fw_id: 10 in directory:
    /home/mpaull/wcEcoli/launcher_2015-06-24-02-09-35-326470
2015-06-23 19:09:37,775 INFO Task started:
    {{wholecell.fireworks.firetasks.symlink.SymlinkTask}}.
Tue Jun 23 19:09:37 2015: Creating symlink
2015-06-23 19:09:37,777 INFO Task completed:
    {{wholecell.fireworks.firetasks.symlink.SymlinkTask}}
2015-06-23 19:09:40,154 INFO Rocket finished
2015-06-23 19:09:40,531 INFO Created new dir
    /home/mpaull/wcEcoli/launcher_2015-06-24-02-09-40-530368
2015-06-23 19:09:40,533 INFO Launching Rocket
2015-06-23 19:09:42,981 INFO RUNNING fw_id: 9 in directory:
    /home/mpaull/wcEcoli/launcher_2015-06-24-02-09-40-530368
2015-06-23 19:09:42,984 INFO Task started:
    {{wholecell.fireworks.firetasks.fitKb.FitKbTask}}.
Tue Jun 23 19:09:42 2015: Fitting knowledgebase (Level 1)
```

---

Then once the actual simulation starts, you will see:

---

Tue Jun 23 19:10:13 2015: Running simulation

Time (s)	Dry mass	Dry mass	Protein	RNA	Expected
	(fg)	fold change	fold change	fold change	fold change

=====	=====	=====	=====	=====	=====
-------	-------	-------	-------	-------	-------

0	245.19	1.000	1.000	1.000	1.000
---	--------	-------	-------	-------	-------

Warning - converting 'reactionIDs' attribute from ndarray to list  
for JSON serialization.

1	245.27	1.000	1.000	1.000	1.000
2	245.20	1.000	1.000	1.000	1.000
3	244.50	0.997	1.000	1.000	1.001
4	244.52	0.997	1.000	1.000	1.001
5	244.58	0.998	1.001	1.001	1.001
6	244.63	0.998	1.001	1.002	1.001
7	244.64	0.998	1.001	1.003	1.001
8	244.63	0.998	1.001	1.004	1.002
9	244.73	0.998	1.001	1.005	1.002
10	244.79	0.998	1.002	1.007	1.002
11	244.87	0.999	1.002	1.008	1.002
12	244.96	0.999	1.002	1.010	1.002
13	245.08	1.000	1.002	1.012	1.003
14	245.10	1.000	1.002	1.014	1.003
15	245.21	1.000	1.003	1.016	1.003
16	245.32	1.001	1.003	1.018	1.003
17	245.41	1.001	1.003	1.021	1.003
18	245.49	1.001	1.003	1.023	1.003
19	245.59	1.002	1.003	1.026	1.004
20	245.69	1.002	1.004	1.028	1.004
21	245.79	1.002	1.004	1.031	1.004
22	245.89	1.003	1.004	1.034	1.004
23	245.95	1.003	1.004	1.037	1.004
24	246.04	1.003	1.005	1.040	1.005
25	246.14	1.004	1.005	1.043	1.005
26	246.23	1.004	1.005	1.046	1.005
27	246.33	1.005	1.005	1.049	1.005
28	246.41	1.005	1.005	1.052	1.005
29	246.51	1.005	1.006	1.056	1.006
30	246.60	1.006	1.006	1.059	1.006
31	246.70	1.006	1.006	1.062	1.006

32	246.79	1.007	1.006	1.066	1.006
33	246.88	1.007	1.006	1.069	1.006
34	246.98	1.007	1.007	1.073	1.007
35	247.07	1.008	1.007	1.076	1.007
36	247.16	1.008	1.007	1.079	1.007
37	247.26	1.008	1.007	1.083	1.007
38	247.35	1.009	1.007	1.087	1.007
39	247.43	1.009	1.008	1.090	1.008
40	247.52	1.010	1.008	1.094	1.008
41	247.61	1.010	1.008	1.098	1.008
42	247.70	1.010	1.008	1.101	1.008
43	247.79	1.011	1.008	1.105	1.008
44	247.88	1.011	1.009	1.109	1.009
45	247.97	1.011	1.009	1.113	1.009
46	248.05	1.012	1.009	1.116	1.009
47	248.14	1.012	1.009	1.120	1.009
48	248.23	1.012	1.009	1.124	1.009
49	248.31	1.013	1.010	1.128	1.009

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This will take a few minutes to run. At the end you can find the output in the out/timestamp directory (timestamp obviously replaced with the actual timestamp of when you started the simulation). Look at the plots in the /wcEcoli/out/20150623.190922.827654/wildtype\_000000/000000/generation\_-00 0000/000000/plotOut directory (replacing the timestamp directory with your own timestamped directory name).