EE/CprE/SE 491 WEEKLY REPORT 5

3/15/2021 - 3/29/2021

Group number: 26

Project title: Automated Configuration Testing Framework for KBase

Client &/Advisor: Myra Cohen

*Team Members/Role:* 

Daulton Leach: Scrum master / Developer

Hunter Hall: Development

Sergey Gernega: Development

Caleb Meyer: Development

Jake Veatch: Development

**Daniel Way: Development** 

#### • Weekly Summary

The team got the project updated with KBase's FBA version 2. Our project is built on top of the KBase platform and we interact specifically with the FBA. This means any changes to the FBA GUI would have a significant impact on our project. While it doesn't change often, a big change occurred this sprint causing us to rework some things and modularize them for the future. We restructured and abstracted the input types to allow us to update the application in the future much easier. We finished implementing complex variables and have begun testing them. We began implementing a headless mode for the application to hide the background workings of the KBase platform. We added garbage collection so that after each FBA run, we collect and clear out output to not overwhelm Kbases servers. We also added the ability to read multiple jobs from a single input file as the first steps towards allowing multiple jobs to run at once.

## o Past week accomplishments

 $\cdot$  Daniel Way: Continued analysis and development of concurrent card processing. Specifically, investigating how to prevent jobs' sequences from interfering with one-another.

· Jake Veatch: Implemented functionality to allow running multiple jobs from a single configuration file. Can spin up a list of jobs from a single file, adding each to the queue to be run by the job manager.

 $\cdot$  Caleb Meyer: Implemented functionality to delete the leftover narrative cards that are generated every time the FBA is run. This keeps the interface clean and prevents the extra cards from bogging down the speed of the system.

Ilux Variability Analysis	Minimize Flux	All Single Kos	
Activation Coefficient [0,1]	*Carbon Uptake [0,100]	*Nitrogen Uptake [0,100]	
*Phosphate Uptake [0,100]	*Sulfur Uptake [0,100]	*Oxygen Uptake [0,100]	
Reaction to Maximize	Expression Threshold [0,1]	Expression Uncertainty [0,?]	
Gene Knockouts	Media Supplement	Custom Flux Bounds	
ReactionKnockouts	Expression Condition		
	Read from file	Delete Results Card	
All Random Values	Number of Jobs	Controlled Random	
* Signals a required field. No	default value		

 $\cdot$  Hunter Hall: Found a bug in the GUI form during the selecting of the text fields and areas. Began implementation for the bug fix.

• Sergey Gernega: Helped refactor GUI from JTextFields to JTextAreas for variables affected by version 2.0 FBA upgrade. Changed singleton variables to linked lists and vise versa for affected variables from version 2.0 FBA upgrade. Helped debug known issues with clearing out previous param entries in KBase.

Run		
Flux Variability Analysis	Minimize Flux	All Single Kos
Activation Coefficient [0, 1]	*Carbon Uptake [0,100]	*Nitrogen Uptake [0,100]
*Phosphate Uptake [0,100]	*Sulfur Uptake [0, 100]	*Oxygen Uptake [0,100]
Reaction to Maximize	Expression Threshold [0, 1]	Expression Uncertainty [0,?]
Gene Knockouts	Media Supplement	Custom Flux Bounds
ReactionKnockouts		
	Expression Condition	]

 $\cdot$  Daulton Leach: Refactored file inputting and main GUI classes. Investigated minor errors within the GUI/GUI Interactions. Found the source of the randomization bug (planning to fix this week). Finished implementing file reading from the GUI's perspective.

{ "jobs": [	Minimum FBA Narrative - Created March 14, 2021 ?- O E- Created by: Senior Design - ISU, Team 26 (isu_seniordesign_sdmay2126)		
1	Narratives	Selected Items	
"fluxVariabilityAnalysis": true,	Nanatives	no selected values	
"minimizeFlux": true,	Q LE ▼ 2 →	no selected values	
"simulateAllSingleKos": true,			
"activationCoefficient": 0.5,	↓v41	Expression threshold	
"maxCarbonUptake": 1.0.		1.0	
"maxNitrogenUptake": 1.0,	- the table to produce a Marco		
"maxPhosphateUptake": 1.0,	s_thetaiotaomicron_Vv2	Expression uncertainty	
"maxSulfurUptake": 1.0,		1.0	
"maxOxygenUptake": 1.0,	avi		
"reactionToMaximize": "validReaction",	u vi	Activation coefficient	
"expressionThreshold": 1.0,		0.5	
<pre>"expressionUncertainty": 1.0,</pre>	t v7	0.5	
"geneKnockouts": [		Max carbon uptake	
"geneKnockout"			
],	del vi	1.0	
"mediaSupplements": [	$\bullet$		
"mediaSupplement"	filledt	Max nitrogen uptake	
], "customFluxBounds": [		1.0	
"customFluxBounds"	category▼ Q 😂 R 🗲		
],	mics 32	Max phosphate uptake	
"reactionKnockouts": [		1.0	
"reactionKnockout"	33		
],	n [22]	Max sulfur uptake	
"deleteCard": true,	25	1.0	
"expressionCondition": "expCondition"	g 25		
}	ities 19	Max oxygen uptake	
1	19	1.0	
}	20		

### o Pending issues

 $\cdot$  Daniel Way: Understanding the critical zones in our programming, execution, and collection sequences. This is important for concurrency.

· Jake Veatch: NA

· Caleb Meyer: NA

 $\cdot$  Hunter Hall: Working on a way to make the GUI form more responsive to user interaction.

· Sergey Gernega: Try to replicate KBases filtering options for Gene Knockouts bug to

help developers. In this case, KBase should do an exact match, but it only correctly filters half the time.

	kb g.436.pbs.10 filter applied	<b>x • y</b>
	1 kblg.436.att.0 Bacteroides_thetalotaomicron_VPI-5482	0
	2 kb/g.436.att.1 Bacteroides_thetalotaomicron_VPI-5482	0
	3 kblg.436.pbs.0 Bacteroides_thetalotaomicron_VPI-5482	0
	4 kblg.436.pbs.1 Bacteroides_thetalotaomicron_VPI-5482	0
	5 kblg.436.pbs.10 Bacteroides thetalotaomicron VPI-5482	0

 $\cdot$  Daulton Leach: No major issues. Currently working on tracking down a few bugs in some of the features. Most notably, the randomization of variables option has an issue where some of the variables don't default and are passed to the runner in a state that results in program failure. This and a few other small bugs are my main issues as of now.



#### o Individual contributions

NAME	Individual Contributions	<u>Hours this</u> <u>week</u>	<u>HOURS</u> <u>cumulative</u>
Daniel Way	Continued analysis and development of concurrent card processing. Specifically, investigating how to prevent jobs' sequences from interfering with one-another.	14	57
Jake Veatch	Implemented multiple jobs from a single configuration file.	14	53
Caleb Meyer	Implemented deletion of left over narrative cards after each run.	13	54
Hunter Hall	Found a bug in the GUI form during the selecting of the text fields and areas. Began	14	55

	implementation for the bug fix.		
Sergey Gernega	Updated singleton variables to linked lists and vise versa for KBase's FBA version 2.0 upgrade	14	57
Daulton Leach	Helped Daniel and Sergey as needed to get the program updated to FBA2.0. Finished implementing/testing file reading from the GUI. Worked on fixing some edge case bugs/errors within some features.	14	58

# Plans for the upcoming week

 $\cdot$  Daniel Way: Determine critical zones of concurrency, implement basic job distribution within a runner's domain. Add additional thread for cards.

 $\cdot$  Jake Veatch: Updating and preparing documentation for running and configuring project files. Creating means for allowing the users to easily run the application seamlessly.

 $\cdot$  Caleb Meyer: Improve the functionality of resetting the FBA card. Help with bug fixes.

 $\cdot$  Hunter Hall: Implement a bug fix to make the GUI more responsive to user interaction and add functionality to clear out labels when the tab key is pressed in the GUI form to go to the next text field or area.

 $\cdot$  Sergey Gernega: Try to figure out KBases filtering for exact matches by replicating the issue and possibly relaying it to the KBase developers. Work on refactoring and make code more generic so if changes do occur down the line, they would only need to be rewritten in one location.

• Daulton Leach: Working on fixing various bugs within the features of our project. Working on hiding the KBase UI/going into a headless mode once the user has input a job. Updating the GUI/file reader interaction to make it nice for the user. Fix the bug in the randomization feature that causes the program to be in an error state.

## o Summary of weekly advisor meeting

This week we had our biweekly sprint meeting. We demonstrated the new features and got feedback from our advisor on those features. With the end of the semester coming up we talked about each member's plans for the remainder of the semester. We discussed what features we plan to add before then. We also discussed how we are going to leave the project off for next year's senior design team or potentially KBase's development team.