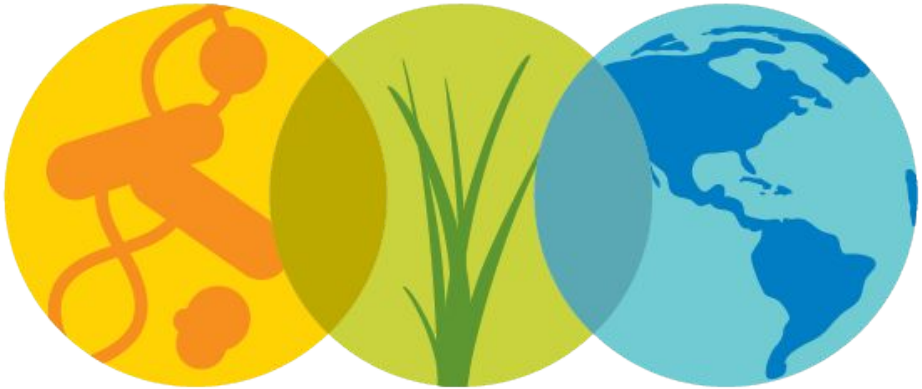
KBase Automation

Group 26 - Senior Design

Client/Advisor: Dr. Myra Cohen

Jake Veatch, Daulton Leach, Daniel Way, Sergey Gernega, Hunter Hall, Caleb Meyer



KBase

PREDICTIVE BIOLOGY

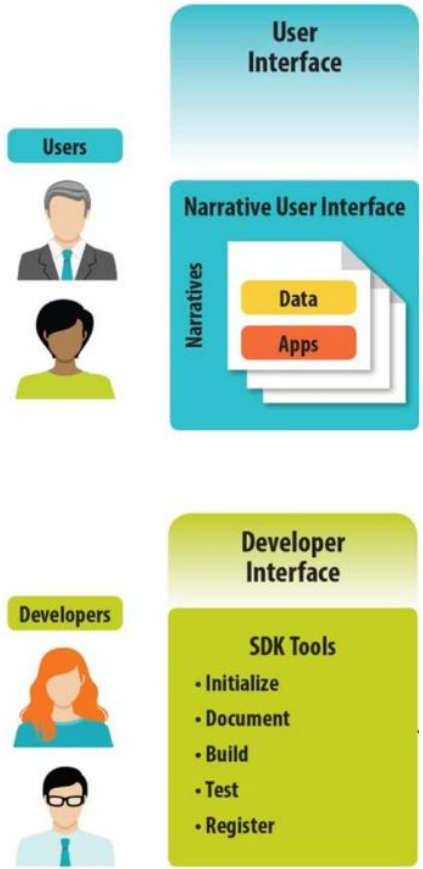
DOE Systems Biology Knowledgebase

https://www.kbase.us/acknowledgements/

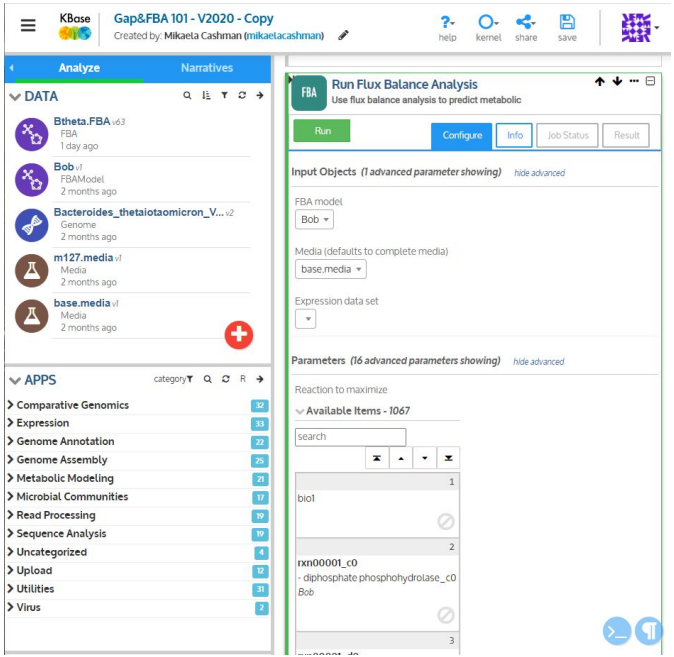
KBase Ecosystem

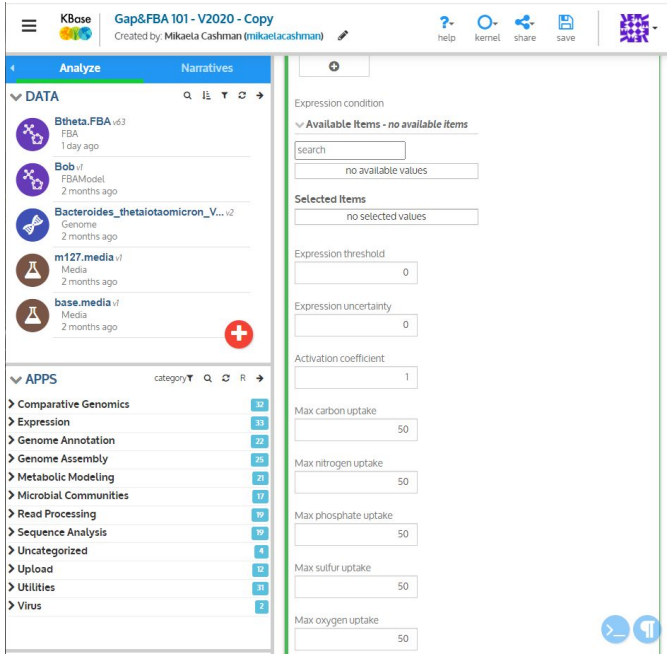
- **Web Application**
  - Non-technical (BIOLOGISTS)

- Software Development Kit (SDK)
  - Technical
  - Not the focus



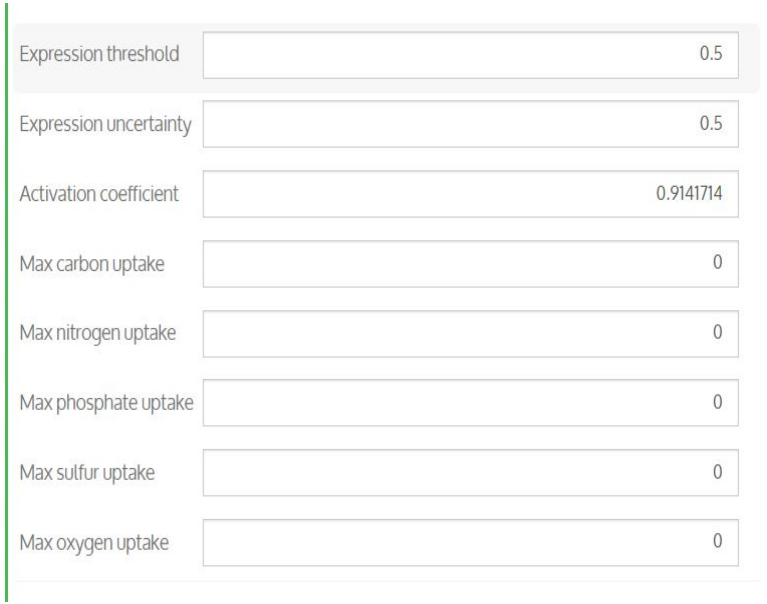
The Flux Balance Analysis (FBA)





Problem

- Manual configuration
  - Which of these 100 solutions does organism X grow best?
- Take minutes to run
- Can’t run tests sequentially (Web App)
- Exponential combination of inputs to test
  - 10 booleans = 2^10 = 1,024 combinations
  - 8 floats with a range of 0-100 is infinite
- Why not use the SDK?
  - We are trying to mimic the user when testing
  - We want to keep it simple for the non-technical users



Project Motivation

1. Primary
    a. Automate programming experiments
    b. Run experiments sequentially
    c. Result - increase efficiency of biologists

2. Side Effect (Secondary)
    a. Tool can be used to test KBase as system
    b. Certain experiment configurations affect / break Kbase?

Our Solution

- Take inputs from user either through a GUI or a file
- Automate browser functionality.
- Use a Job/Runner style to allow jobs to run sequentially
- Collect output from job(s) and return the output to the user in a file
- Output is viewable to catch errors and view configuration results

Selenium

- Browser automation software
- Primary use is automation of web applications, but can be extended to any task that needs to be repeated numerous times automatically.

Perfect fit for running multiple Flux Based Analysis experiments (FBAs)

Intended Users

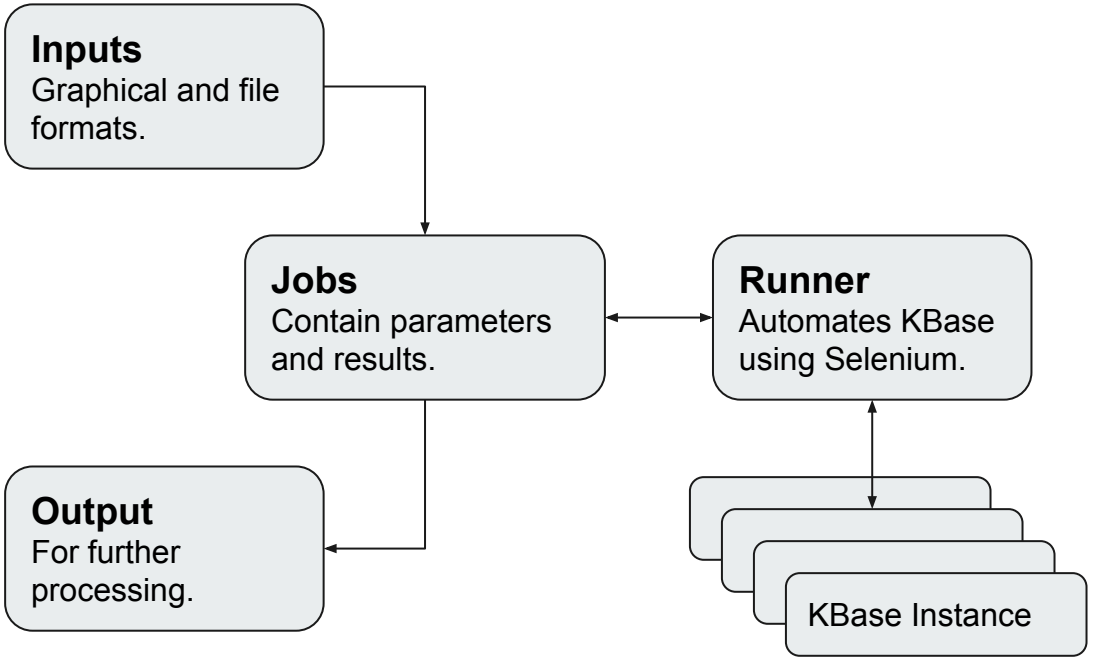
1. Biologists
    a. Allows biologists to view results from running many simulations to determine the desired outcome. Allows the Biologist to play with and configure the parameters to their likings. Can run X simulations at a time and try to find the preferred results.
2. KBase Developers
    a. Projects output collection will flag errors and allow the developers to easily find and replicate bugs to allow for simpler debugging

Realistically: Anyone with proper KBase credentials.

Architecture

Core objectives:

- Inputs, outputs, jobs, and runners should be modular
- System should be extensible for future formats and KBase application types



Requirements

Functional:

- Configure Selenium to interface with KBase apps
- User sets parameters to automate using Selenium
- App will sample the configuration space from set parameters
- Automate the testing of sample configurations
- Collect output data from KBase
- Users will be able to randomize inputs
- All inputs from the KBase GUI will be available

Non-Functional:

- Will not noticeably disrupt KBase traffic flow
- App GUI will have similar layout as KBase GUI

Environmental:

- Will require a valid and active KBase account
- Standalone application that can be executed from the users desktop
- Must be run on device which supports Selenium

Standards Followed

IEEE 12207-2017 - ISO/IEC International Standard - Information Technology - Software Life Cycle Processes

This standard holds the purpose of defining a lifecycle standard for software projects from design, development, deployment, testing, and acquisition standpoints.

IEEE 1028-2008 - IEEE Standard for Software Reviews and Audits

This standard defines five different types of software reviews and audits that can be used in combination to increase the quality of software projects at various stages of their lifecycle.

IEEE 2430-2019 - IEEE Trial-Use Standard for Software Non-Functional Sizing Measurements

This standard defines how to size nonfunctional requirements in software.

Engineering Constraints

- Have to use selenium to manipulate GUI, cannot use SDK.
- Unable to modify KBase in any way
- Future development teams must be able to modify project.

Operational Environment

- Will require a valid and active KBase account
- Must be run on device which supports Selenium
- Standalone application that can be executed from the users desktop

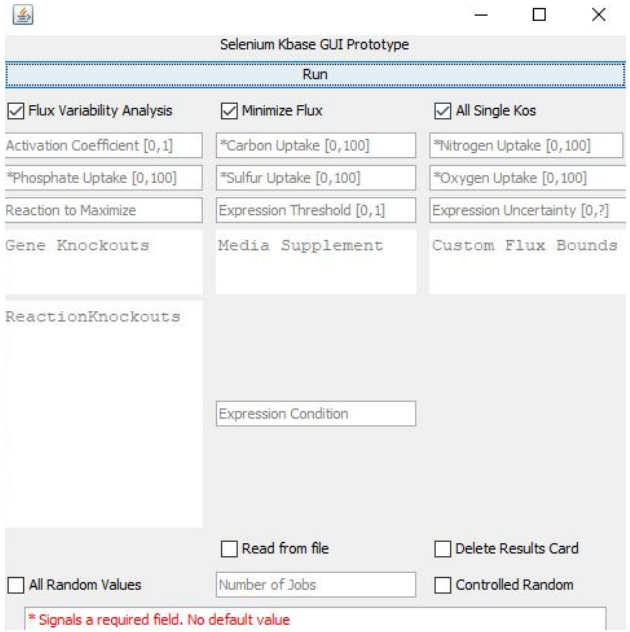
Security Concerns

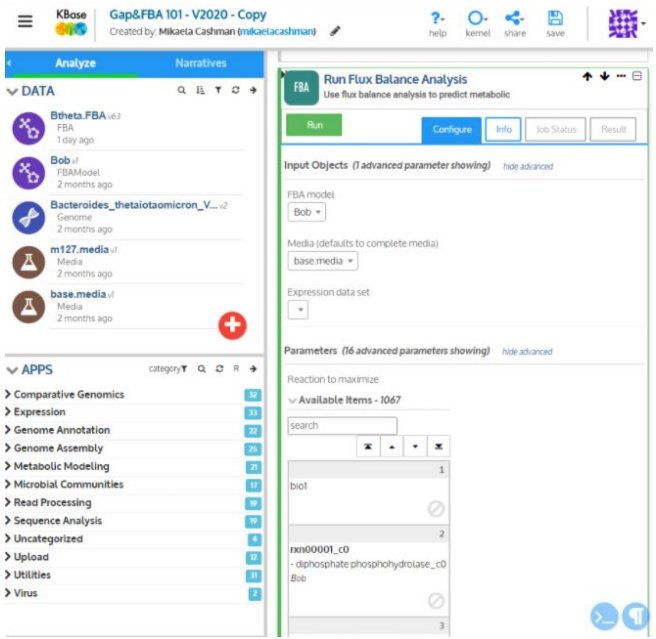
- Less risk - the project is augmented current user capabilities
- User must provide authentication credentials

Testing Plan

- Unit testing
- Continuous integration testing
- Acceptance testing
- Results

Screenshots





DEMO

References

- *IEEE SA - The IEEE Standards Association - Home*, IEEE Standards Association, standards.ieee.org/.
- Arkin AP, Cottingham RW, Henry CS, Harris NL, Stevens RL, Maslov S, et al. KBase: The United States Department of Energy Systems Biology Knowledgebase. Nature Biotechnology. 2018;36: 566. doi: 10.1038/nbt.4163

Questions?

Thank you for your time.