SOFTWARE TOOLS FOR NEXT-GEN DESIGN

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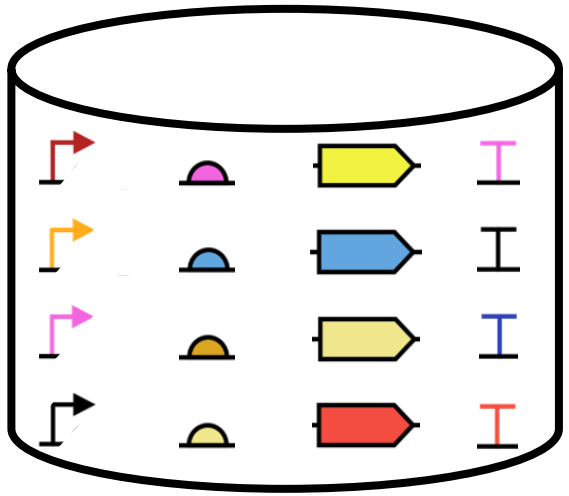
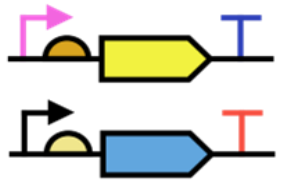
COMBINE 2018

How to Encode Many Possible Designs for a 4-Gene Cluster?

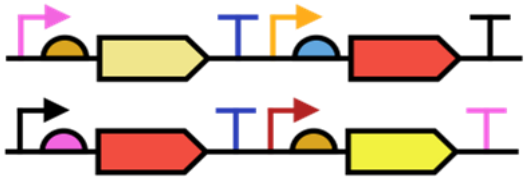


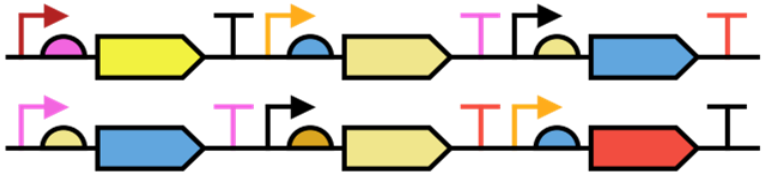
16 Parts

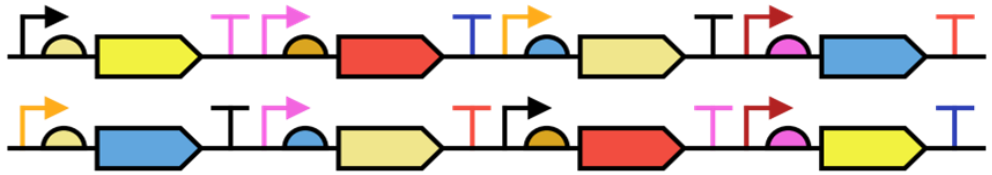


684,544

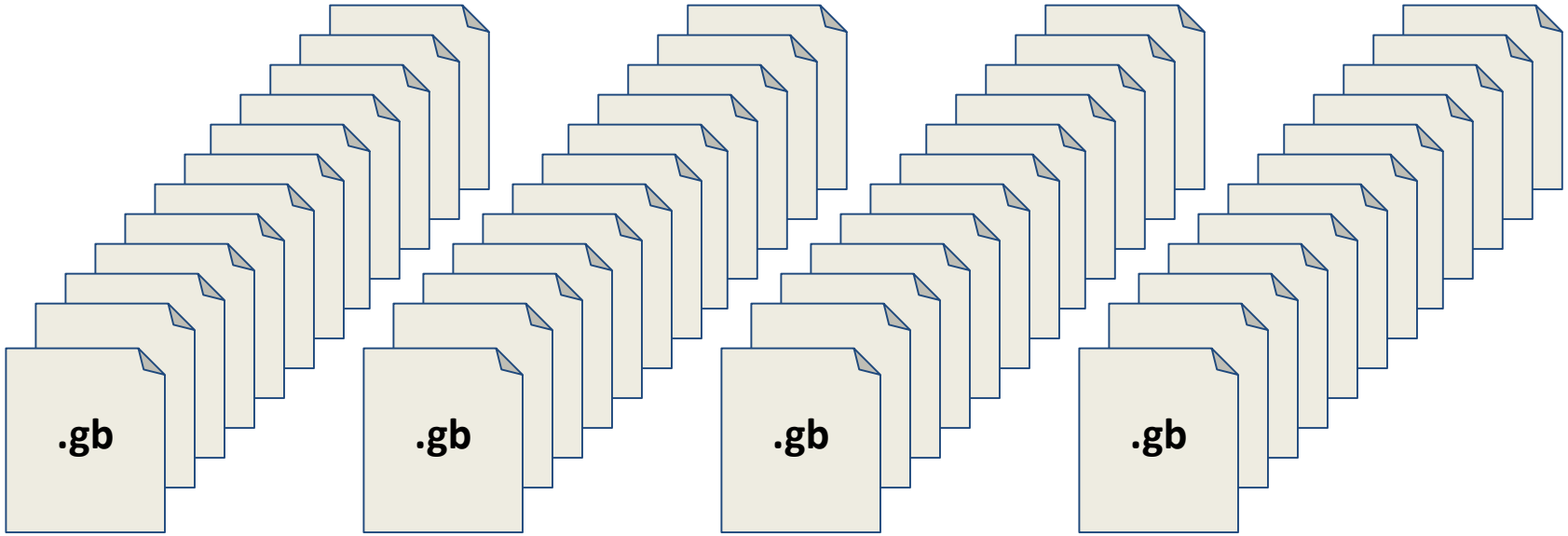
Design Variants







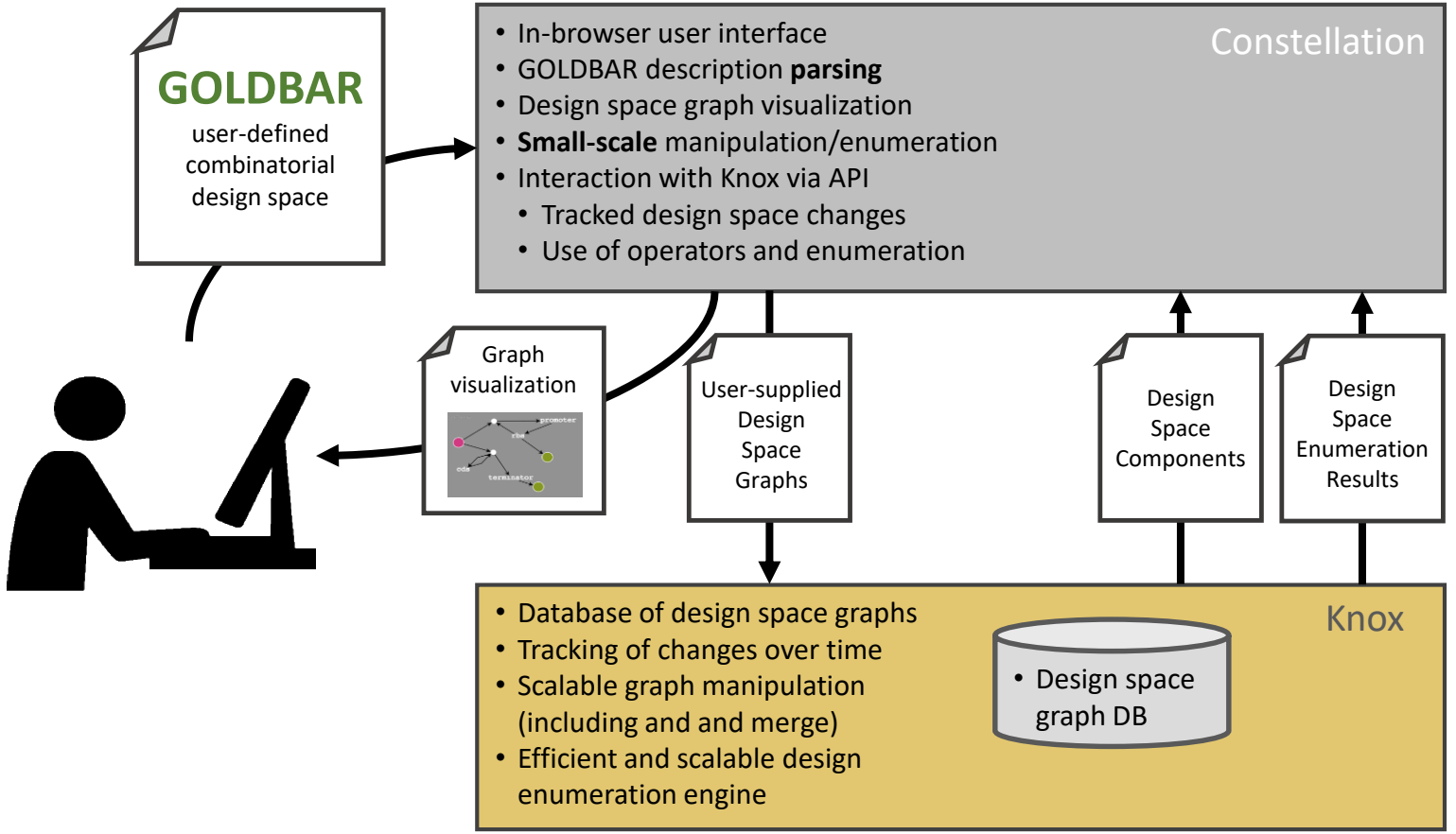
Space-Efficient Design, Storage, and Visualization Solution is Necessary



684,544 Files

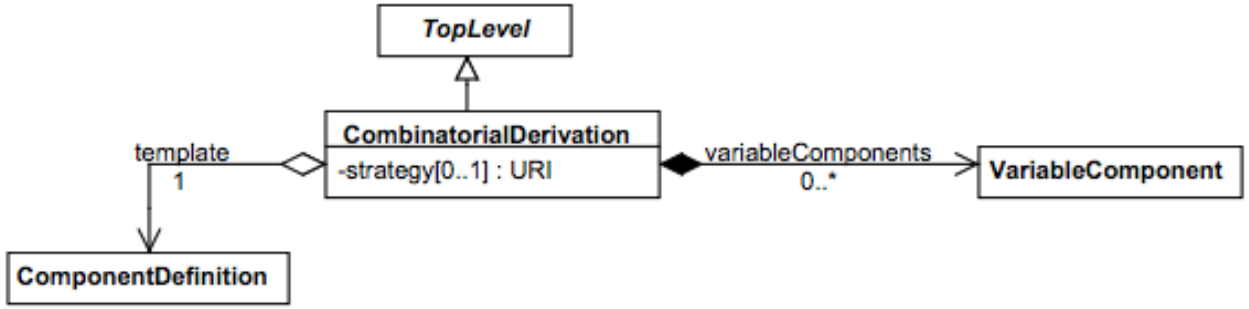
Memory >6 GB

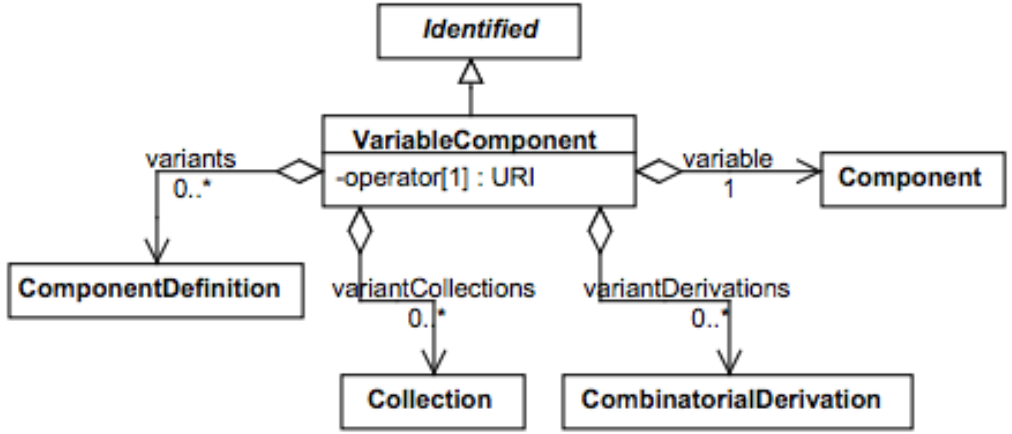
Tools Ecosystem

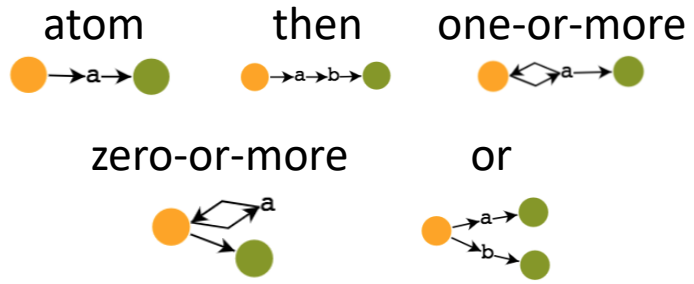


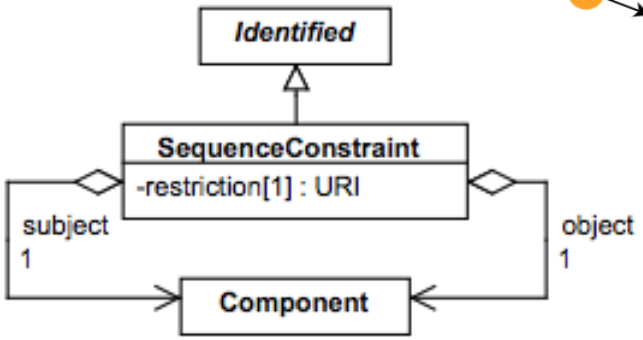
Architecture and interactions between GOLDBAR, Constellation, and Knox components. The individual implemented components will comprise an infrastructure that supports an interactive, responsive experience for users, whether they are doing rapid prototyping or engaging in large-scale design space exploration.

SBOL 2.2 Combinatorial Data Model









Operator URI	Description
http://sbols.org/v2#zeroOrOne	No more than one Component in the derived ComponentDefinition SHOULD have a wasDerivedFroms property that refers to the template Component.
http://sbols.org/v2#one	Exactly one Component in the derived ComponentDefinition SHOULD have a wasDerivedFroms property that refers to the template Component.
http://sbols.org/v2#zeroOrMore	Any number of Component objects in the derived ComponentDefinition MAY have wasDerivedFroms properties that refer to the template Component.
http://sbols.org/v2#oneOrMore	At least one Component in the derived ComponentDefinition SHOULD have a wasDerivedFroms property that refers to the template Component.

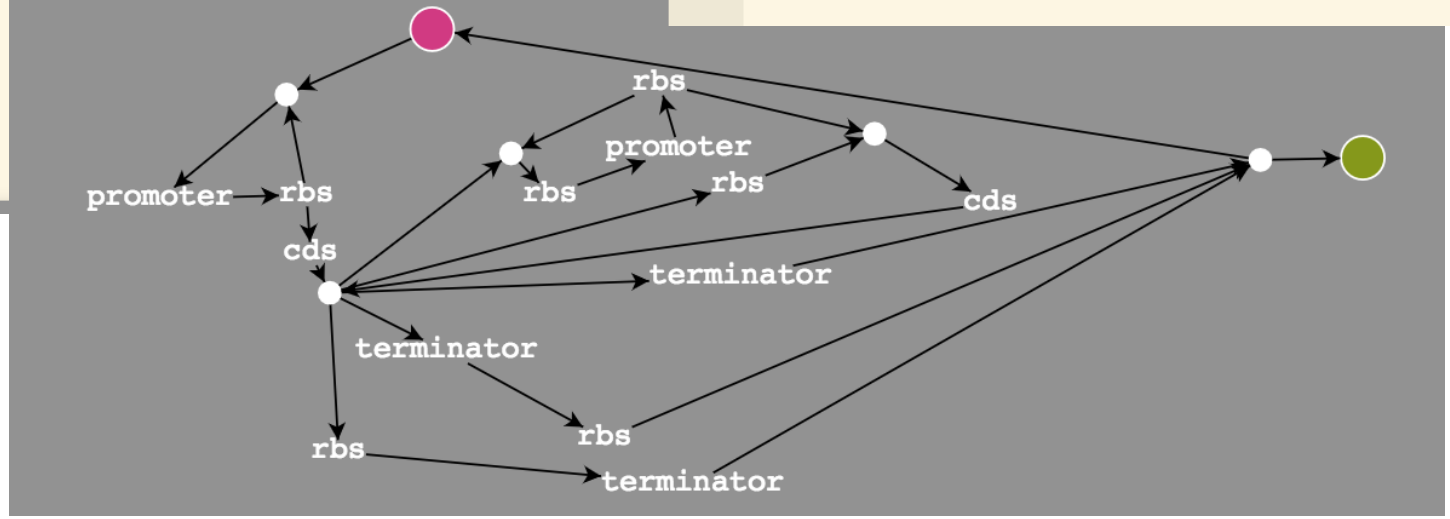
Constellation Demo

Specification

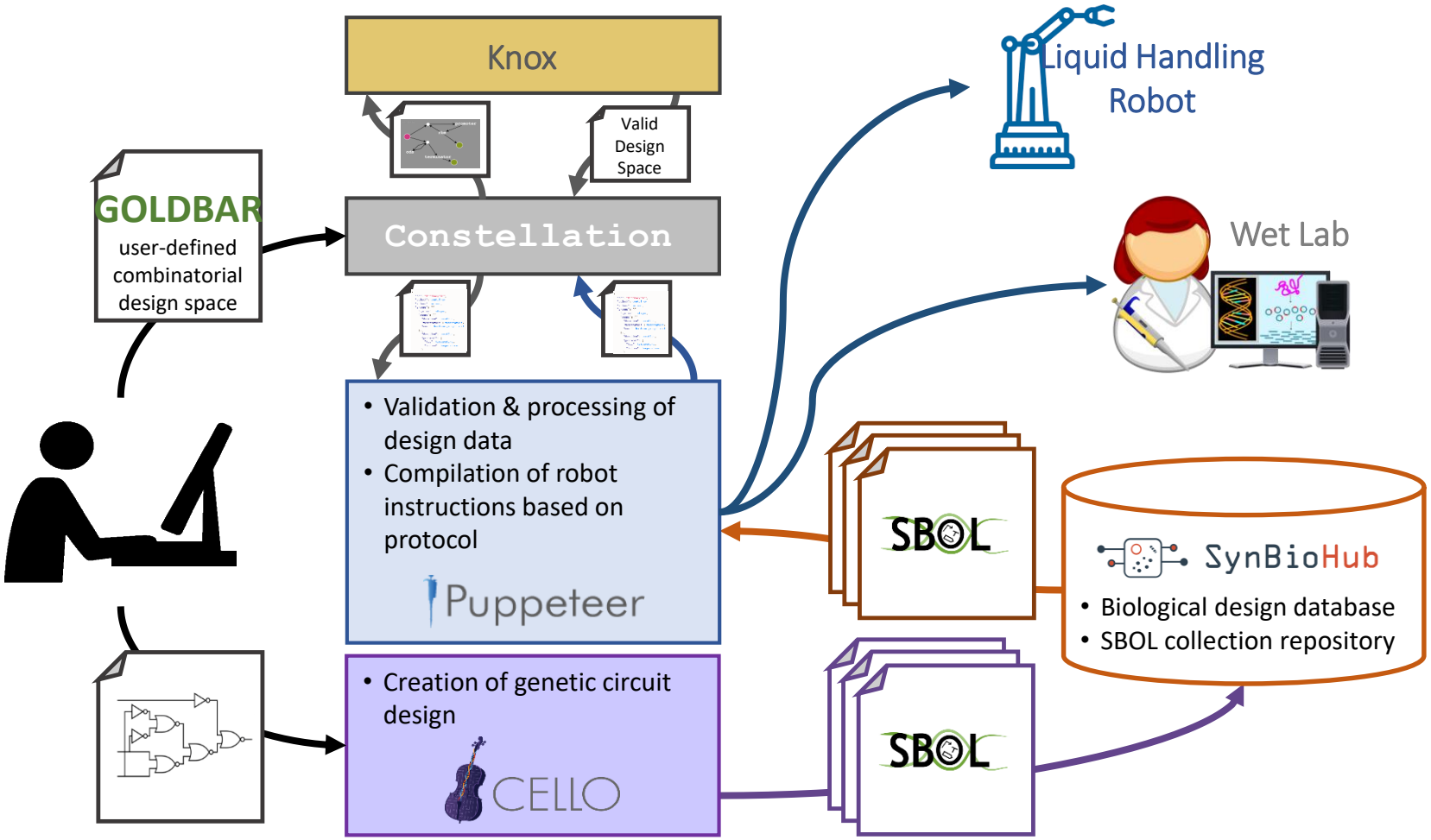
```
one-or-more(
  one-or-more(promoter then rbs) then cds then
    zero-or-more(
      rbs or one-or-more(
        rbs then promoter then rbs
        ) then cds
    ) then
  terminator or (terminator then rbs) or (rbs then terminator)
)
```

Categories

```
{"promoter": ["BBa_R0040", "BBa_J23100"],
 "rbs": ["BBa_B0032", "BBa_B0034"],
"cds": ["BBa_E0040", "BBa_E1010"],
"terminator": ["BBa_B0010"]}
```



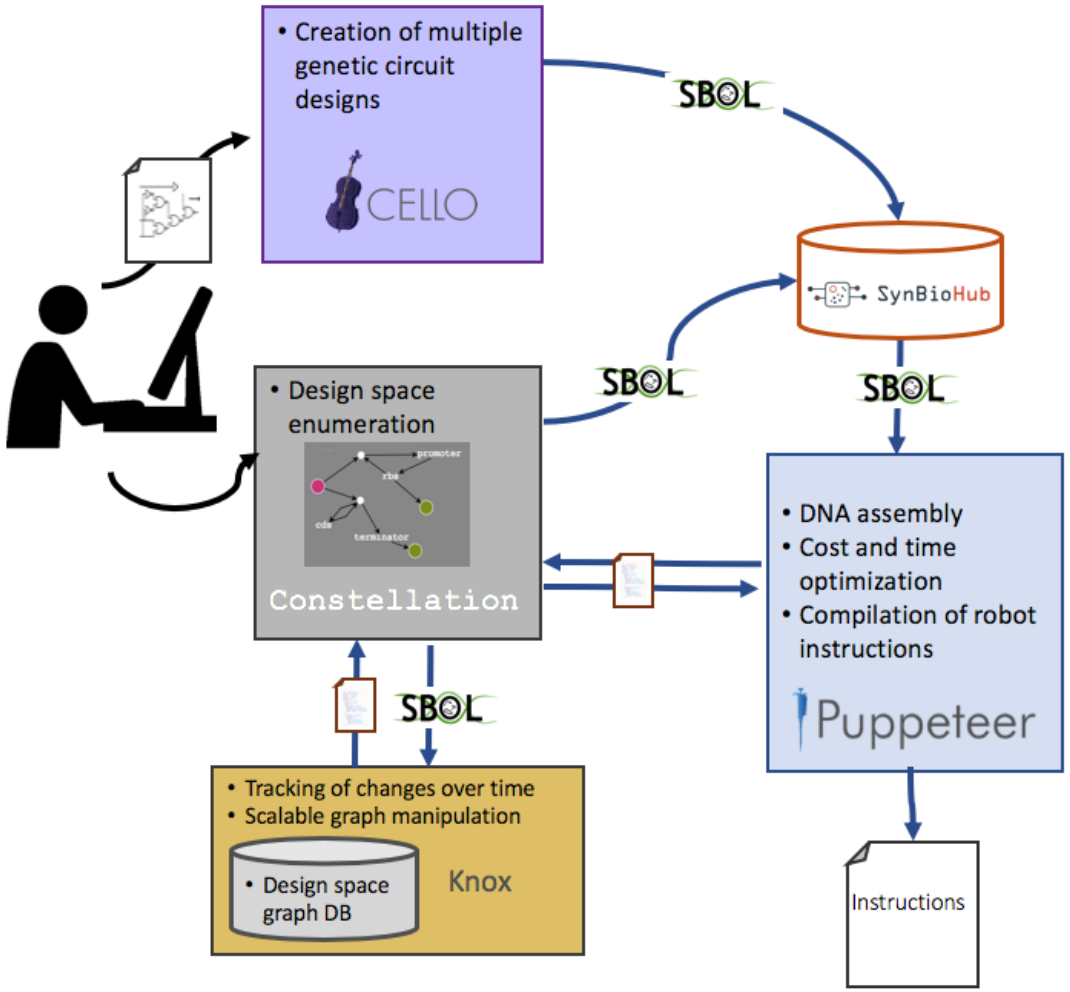
System Architecture in Context



GOLDBAR, Constellation, and Knox within Tool Ecosystem. The implemented tools can already be situated within more complex integrated workflows that begin at the human-directed design phase, populate shared community repositories of designs such as SynBioHub, and generated experimental protocol specifications.

Future Work

- Complete integration via APIs between Constellation and Knox
- End-to-end integrated workflow with Cello, SynBioHub, & Puppeteer
- Case studies for publication



Conclusion

- The formally defined **GOLDBAR** language has been developed to validate design spaces for assembly by merging and intersecting graphs for available parts and intended designs.
- The design space repository system **Knox** has been publicly released and supplemented with the in-browser **Constellation** application for combinatorial design specification and enumeration.
- Using these pieces, we plan to develop a software pipeline that takes as input the designs produced by Cello and biosynthetic gene cluster tools.
- Pipeline will allow users to generate space of designs (**Constellation**), store and validate the design space for assembly (**Knox**), enumerate valid designs (**Knox**/**Constellation**), and yield instructions for assembly by liquid handling robots (**Puppeteer**).

Acknowledgements

/CIDARLAB/knox
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/hicsail/puppeteer

www.constellationcad.org

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