Synthetic Biology

Intent Parser: A Tool for Codification and Sharing of Experimental Design

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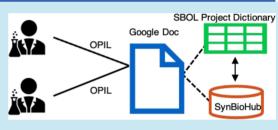
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ABSTRACT: Communicating information about experimental design among a team of collaborators is challenging because different people tend to describe experiments in different ways and with different levels of detail. Sometimes, humans can interpret missing information by making assumptions and drawing inferences from information already provided. Doing so, however, is error-prone and typically requires a high level of interpersonal communication. In this paper, we present a tool that addresses this challenge by providing a simple interface for incremental formal



codification of experiment designs. Users interact with a Google Docs word-processing interface with structured tables, backed by assisted linking to machine-readable definitions in a data repository (SynBioHub) and specification of available protocols and requests for execution in the Open Protocol Interface Language (OPIL). The result is an easy-to-use tool for generating machine-readable descriptions of experiment designs with which users in the DARPA SD2 program have collected data from 80 208 samples using a variety of protocols and instruments over the course of 181 experiment runs.

KEYWORDS: experiment design, design automation, OPIL, SynBioHub, data standards

INTRODUCTION

Many biological experiments are described in text documents, such as laboratory notebooks, which capture information such as the purpose, execution, and results of an experiment. In such descriptions, however, authors typically present information in a highly personal and idiosyncratic manner at varying levels of detail, often omitting critical information. Consequently, this lack of consistency often leads to a variety of issues related to reproducibility, including attempts to compare experimental reports created by different authors or to build upon those results in new work. Humans can sometimes infer sufficient information to interpret such informal documentation of experiment designs, but this is typically an *ad hoc*, challenging, and error-prone process that is not particularly susceptible to automation.

Ambiguity can be greatly reduced if experiment designs are represented in a more structured form. To this end, a number of communities have adopted "minimum information" standards, such as MIAME¹ for microarray experiments, MIFlowCyt² for flow cytometry experiments, or MIBBI³ for general biomedical experiments. A similar approach has recently been proposed with the intent of increasing the reproducibility of bacterial growth and productivity experiments.⁴ These minimum information standards provide rubrics for ensuring that information is reported about certain aspects of a class of experiment, but much of the information about experiment design is often still in the form of opaque blocks of natural language text. More precise specifications can be formulated using machine-readable representations such as Synthetic Biology Open Language⁵ (SBOL), defining the terms used in a description with publicly available resources such as the biomedical ontologies in OBO Foundry⁶ and repositories of reagents (*e.g.*, PubChem⁷), genetic designs (*e.g.*, SynBioHub⁸), proteins (*e.g.*, UniProt⁹), etc. Making use of these tools, however, is difficult for many investigators, as they typically require a high degree of fluency in knowledge representation and software engineering.

However, a "middle ground" approach combining both accessibility and representational precision has been known at least as far back as Winograd's SHRDLU system,¹⁰ using machine feedback and prompting to shape human input into a semistructured form that can be readily interpreted and checked by machines. Several prior tools have attempted to bridge this gap with respect to experiment metadata by offering more user-friendly approaches to annotation with semantic information (*e.g.*, RightField,¹¹ Excemplify,¹² and the CEDAR workbench¹³). All of these tools, however, are focused on the definition of terms rather than representing the larger-scale design of an experiment. They are also primarily focused on annotation of data after the fact rather than proactively as part of

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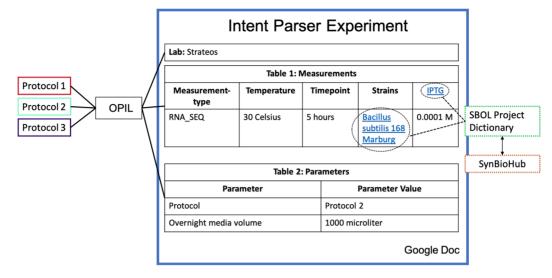


Figure 1. Data sources for Intent Parser. Google Docs provides the core document editing interface and hosts the Intent Parser add-on. Laboratories offer protocols to execute using the Open Protocol Interface Language (OPIL), which are used to generate table templates for describing experiment requests. OPIL is also used to check requests for errors and submit requests to laboratories. Terms are grounded *via* links to the SynBioHub repository through the SBOL Project Dictionary interface.

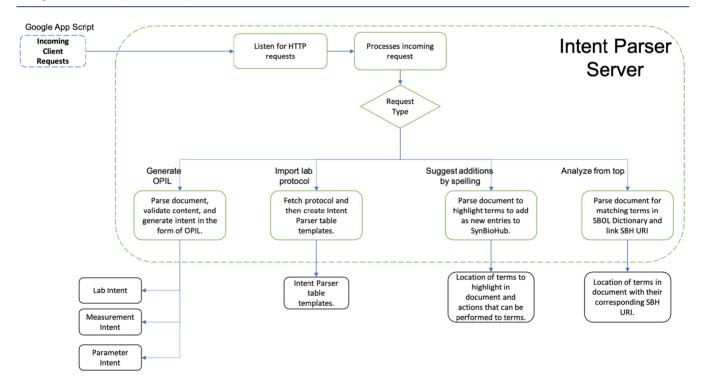


Figure 2. High-level behavior diagram for Intent Parser: software clients (including the Google Docs plugin) send four classes of RESTful requests for processing by the back-end server.

the actual experiment execution process, which means that there is no good way to check the correctness of the annotations.

We have begun to address this challenge with the development of Intent Parser, a tool for collaborative generation of automation-friendly experiment designs that is ready for execution in the laboratory. Intent Parser combines a wordprocessing interface with structured tables and assisted linking to definitions to provide a simple interface for incremental formal codification of experiment designs. This tool can help synthetic biology collaborations by reducing the time and skills required to produce precise experiment designs, enabling automatic checking for errors and ambiguities, supporting automated execution of experiments, and simplifying the interpretation of experimental data, all of which will increase the overall reproducibility and ability to transfer experimental results.

INTENT PARSER

Before Intent Parser's architecture is described, it is important to understand the data used by Intent Parser. There are three data sources, as shown in Figure 1. Google Docs provides the basic word-processing user interface for describing experiments along with an add-on architecture that Intent Parser uses to add pubs.acs.org/synthbio

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0.100, 0.183, 0.265, 0.348, 0.430, 0.513, 0.596, 0.678, 0.761, 0.843, 0.926, 1.009, 1.091, 1.174, 1.257, 1.339, 1.422, 1.504, 1.587, 1.670, 1.752, 1.835, 1.917, 2.000 %	PLATE_READ ER	PLAIN, CSV	3	Bacillus subtilis 168 Marburg	6, 7, 8 hours	30 celsius	216			M9 Glucose CAA (a.k.a. M9 Glucose Stock)

Figure 3. Screenshot of Intent Parser in action on a document from the DARPA SD2 program, showing a measurement table with reagents linked to definitions in SynBioHub. The navigation panel on the right suggests links to add, in this case a link for the term "Glucose" (document location not shown), providing both a best guess and potential alternatives.

functionality to the document. The Intent Parser add-on for Google Docs extends this interface to add functionality for generating structured descriptions of experiment designs, linking experiment designs to specifications of their components, checking for errors, and submitting experiments to be executed. Communication with laboratories is implemented *via* Open Protocol Interface Language (OPIL), a data model for communicating lab capabilities and experiment requests. Finally, semantic grounding (*i.e.*, machine-readable definitions) for design components is implemented using the SynBioHub⁸ data repository and its SBOL Project Dictionary interface.¹⁴ All of these components are publicly available on GitHub under free and open source licenses.¹

Figure 2 shows the high-level behavior model for the Intent Parser back-end server that implements these relationships. Software clients (including the Google Docs plugin) send requests by means of RESTful calls to Intent Parser to the backend server. Requests fall into four classes: generate OPIL, import lab protocol, suggest additions by spelling, and analyze from top. "Generate OPIL" requests are used to process the contents of an experimental design as described in a Google Doc. The processed content is validated, and the corresponding intent is generated. Valid generated intent can then be used to request an experiment execution. "Import lab protocol" requests are used to fetch lab protocols for an experiment and to generate template tables for users to describe their own experiment. "Suggest additions by spelling" requests are used to discover new terms by scanning the Google Doc for unrecognized words and then prompting a user to see whether they should be linked and inserted into SynBioHub so others can refer to the same terms. Finally, "analyze from top" requests process documents to identify and link terms that match entries found in SynBioHub or the SBOL Project Dictionary.

User-Friendly Editing in Google Docs. A key goal of Intent Parser is to ensure that the tool is user-friendly, building on features with which experimentalists are familiar and expanding the functionality of the tool to fit their needs. To achieve this goal, we talked with a number of experimentalist stakeholders (primarily potential users in the DARPA SD2 program) about their current practices and found that many expressed experiment designs using physical notebooks, word-processing documents (*e.g.*, Microsoft Word, Google Docs, electronic notebooks), or spreadsheets (*e.g.*, Microsoft Excel). These experiment designs would typically include tables to define the combinations of conditions to be tested, the measurements to be taken, and key parameters for protocols,

such as incubation time or temperature. We thus selected Google Docs as a front-end user interface for Intent Parser because it provides a simple and familiar environment for collaborative document creation and editing, including insertion of tables to describe samples, measurements, and protocols.

Google Docs also provides an application programming interface (API) and the ability for users to install Google add-ons for third-party applications to process, edit, and run on contents described in a document. This allowed us to extend the functionality of Google Docs with a menu for Intent Parser operations, providing users with the ability to insert template tables for protocol description, link terms, and perform validation and execution of their designed experiments. Once installed, this add-on provides a menu of operations that can be performed on any Google Doc, with each menu item invoking a corresponding request to the Intent Parser back-end server. Users conceiving of an experiment write up an experiment description in a Google Doc and invoke requests around two workflows: (1) grounding document text with links to definitions in SynBioHub and (2) defining, validating, and exporting experiment requests that make use of those definitions. These requests can be made at any time, supporting an incremental and collaborative approach to experiment design. Examples of these workflows are provided in detail in the Supporting Information.

Grounding Terminology with SynBioHub. Intent Parser connects intuitive human descriptions of experiment design elements to precise machine-readable specifications by means of a set of user interface options for grounding terminology (i.e., providing a shared reference definition) with SynBioHub.⁸ SynBioHub is a synthetic biology knowledge store built around SBOL,¹⁵ an open-data standard used for representing *in silico* biological designs. SBOL can represent not only genetic designs but also reagents, strains, and the design of experimental samples, grounding all terms with URIs that refer either to SBOL data structures or ontologies and semantic data stores such as ChEBI, UniProt, and PubChem, allowing consistent data exchange without loss of information and supporting reproducibility. Figure 3 shows an example of linking information found on SynBioHub to names and terminologies on a Google Doc. The linking interface makes use of SynBioHub's search capability to make suggestions of potential alternatives based on fuzzy matching to the text that is being linked.

Linking terms in the description of an experiment to SBOL stored in an instance of SynBioHub also helps to overcome challenges related to naming. There are often many ways to refer to a particular resource, and which one is used often varies among laboratories or even within a lab. For example, experiment descriptions may refer to L-arabinose in shorthand such as "arabinose", "arab", "ara", or "A+". Likewise, one lab may refer to strains "X" and "Y" while another refers to the same strains as "strain1" and "strain2". Linking to SynBioHub provides a common reference point for looking up information about a term's usage within experiments as well as links to public ontology definitions (*e.g.*, in UniProt or PubChem) and also a place to record name alternatives used by humans and/or laboratory information management systems (LIMS). Intent Parser also makes use of the SBOL Project Dictionary interface,¹⁴ a tool based on Google Sheets that assists teams in collecting and categorizing such aliases in SynBioHub.

Finally, linking with SynBioHub also allows users to know what resources are available to reference within their experiment design. Linking terms to entities in SynBioHub enables a form of validation that can check whether a user's experiment design is ready to be requested for execution. For example, if a user wants to run experiments for strains X and Y in media A, B, and C with 0, 0.1, 0.2, 0.5, and 1.0 μ M Ara but the strains specified in the experiment are not linked to an existing entity within SynBioHub, then the requesting experiment fails validation. In this case, the user is prompted to link ambiguous information to SynBioHub, which may also require adding the appropriate entries there in the first place (e.g., if they are missing a labspecific alias). This ensures not only that the specifications for experiments are well-defined but also that information about the experiment is curated ahead of time, allowing metadata to be prepositioned in support of later analysis of experimental results. Furthermore, the system of lab-specific aliases also prompts user actions to ensure that the appropriate strains and reagents are acquired so that the experiment can actually be carried out.

Specifying Experiment Requests with OPIL. In addition to grounding individual terms, Intent Parser needs to be able to convey how these terms are organized into a complete experiment design and needs to know what sorts of experiment designs a laboratory is expected to be able to execute. For this purpose, it uses the Open Protocol Interface Language (OPIL),² a representation of protocol requests in terms of sample designs (in SBOL), measurements, and parameters. This data model provides a standard interface for any laboratory that wishes to interact with Intent Parser, making it simple to add new laboratories and new protocols.

Intent Parser extracts experiment designs from the Google Doc by looking for tables following a specific format, for which templates can be generated from an add-on menu item. The Intent Parser server collects information about the protocols available to run at each laboratory in OPIL format, which is then used to generate table templates for the user to specify experiments. Validation and export requests are sent to the Intent Parser server to validate the contents of Intent Parser tables parsed from the Google Doc. Validation follows the rules generated from OPIL specifications to check for required information and uses SynBioHub and the SBOL Project Dictionary to validate that all of the terms extracted from the table are properly grounded. From these, the server generates both a report on validity and an OPIL representation of the experiment design, which can then be sent to a laboratory to request execution. Examples are provided in the Supporting Information to illustrate the difference between a structured document with tables generated, linked, and validated using Intent Parser and an semistructured document from before the introduction of Intent Parser.

The use of OPIL allows Intent Parser to present a consistent interface for use of the protocols from multiple different laboratories as long as their interfaces can be translated into OPIL. As with SBOL, OPIL also makes the nature of a request precise, drawing on external ontology terms and forcing potentially open descriptions to be mapped onto a constraining rubric that makes them readily described and inspected in tabular form.

CASE STUDY: DARPA SD2 PROGRAM

The DARPA Synergistic Discovery and Design (SD2) program aimed to accelerate scientific discovery by machine-assisted integration of the experimental design—build—test—learn loop and tested these aims *via* a collaboration of over 100 researchers across more that 20 different organizations. In SD2, Intent Parser was used by both data scientists and "bench" synthetic biology practitioners to define and request experiments *via* Google Docs.

Stakeholders, including data scientists, subject matter experts, and experimental laboratories, were consulted to help determine a format for experiment requests that was sufficiently general to specify experiment designs spanning multiple challenge problems, protocols, laboratories, and experiment designs as well as to support specific constraints from the SD2 program organization and organizational infrastructure. In the final format used by Intent Parser for SD2, the information recorded in these experiment requests includes the name of the lab to execute the experiment; which measurements are to be taken and at what time points; amounts of reagents, strains, and media to be used in each sample; and experimental conditions and parameters such as culturing temperature. As users described the experiment, they also checked its validity and required number of samples with the validation feature in Intent Parser. Finally, when the experiment design was validated and all of the collaborating parties were satisfied with the design, the users requested execution through Intent Parser. Because these experiments were generated systematically with grounded definitions, metadata assignment and analysis were greatly simplified and accelerated, enabling faster analysis and more effective sharing of data and analyses across the SD2 program.

Initially, making new protocols available for execution required significant development. Three protocols were onboarded during this phase, taking an average of just over 2 weeks per protocol. Table 1 shows the development time for

 Table 1. For Pre-OPIL Protocols, Time from Initiation of an

 Experiment Request for a New Protocol to the Beginning of

 Intent Parser-Aided Execution

protocol name	experiment request start	protocol executed
Growth Curves	10/28/2019	11/11/2019
Time Series	10/30/2019	11/26/2019
Obstacle Course	01/03/2020	01/14/2020

each of these three protocols, as measured from the time when the first experiment request for the protocol began to be authored to the time when the first experiment was executed in a laboratory. Once the initial protocol development was completed, subsequent executions required no changes and were able to proceed immediately through the Intent Parser for lab execution. After the introduction of OPIL, protocol pubs.acs.org/synthbio

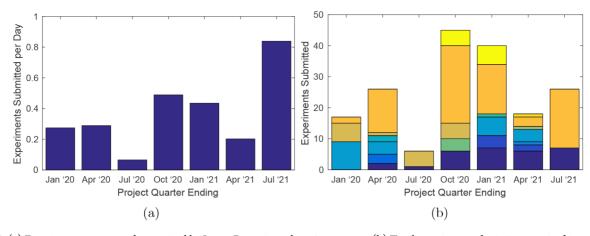


Figure 4. (a) Experiment counts per day received by Intent Parser in each project quarter. (b) Total experiment submissions received in each project quarter by Intent Parser, broken out by color to indicate authorship.

onboarding into Intent Parser was automated, and for the remaining 18 protocols there was no significant lag between the time when a protocol became available in a lab API and the time the protocol was available through Intent Parser.

Within the SD2 program, Intent Parser was used heavily after its introduction: during an 18 month period, 13 SD2 users from various organizations generated 69 experimental requests in multiple different areas of investigation. Specifically, these users represented three cross-organization working groups, one focused on adaptation of synthetic biology methods to novel chassis organisms, another focused on engineering logic gates in yeast, and the third focused on the development of cell-free riboswitch devices. This collection of experiment requests constituted 61% of all experiments conducted in SD2 after the introduction of Intent Parser (the vast majority of experiments not conducted using Intent Parser were from two other working groups using more specialized workflows where Intent Parser integration was not attempted for nontechnical reasons). Once executed, these requests resulted in a total of 181 individual experiment runs and 80 208 experimental samples executed using four different protocols with data collected using a variety of instruments. Figure 4a shows the rate at which experiment requests were made using Intent Parser over this 18 month period, grouped on the basis of the quarterly project meeting cycle used in SD2. This figure indicates that Intent Parser was actively used since its introduction, with the rate increasing in the latter half of 2020 after the addition of automated execution.

Figure 4b shows the same set of requests in the form of a stacked bar graph of total number of requests colored by author. In addition to the increase in submission rate, we also see an increase in the variety of authors after the addition of automated execution, with six authors submitting experiments before its introduction and 11 authors submitting after its introduction, for a total of 13 authors in the beginning of the period to a total of 11 at the end.

DISCUSSION

Intent Parser provides a user-friendly process for describing experiments, defining the terms used in narrative design descriptions in links to a SynBioHub repository, and generating and validating specifications for wet-lab experiments. Critically, the use of Intent Parser can ensure that information about experiment designs is collected incrementally and proactively as experiments are being designed and executed, such that the cost of formalizing description is low and problems can be detected early.

The positive experiences of users in the SD2 program and the high volume of experiments that they executed with the help of Intent Parser suggest that this approach has value and should continue to be elaborated. Our use of broadly applicable standards means that Intent Parser should also be readily applicable to other related domains without the need for any significant changes. Future directions include improving integration and the user interface, generalizing to other editing interfaces and data stores, increasing the scope of descriptions, and using natural language processing to extract additional semantic content from prose. Finally, at present Intent Parser is configured for private deployments via installation of a script in each document, configured to an organization's SynBioHub instance and SBOL Project Dictionary instance; in the future it could potentially also be made more easily available via publication through the Google Workspace Marketplace.

ASSOCIATED CONTENT

Supporting Information

The Supporting Information is available free of charge at https://pubs.acs.org/doi/10.1021/acssynbio.1c00285.

Tutorial for Intent Parser to show how to use the tool and examples of experimental designs produced by Intent Parser (PDF)

Special Issue Paper

Invited contribution from the 12th International Workshop on Bio-Design Automation.

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Author Contributions

T.N., N.W., D.S., M.W., and J.B. developed the methodology. T.N., N.W., D.S., and M.W. wrote the software. J.B. conceptualized, supervised, and administered the project. T.N. and J.B. wrote the manuscript. T.N., N.W., M.W., and J.B. edited the manuscript.

Notes

The authors declare no competing financial interest.

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ADDITIONAL NOTES

¹Intent Parser: https://github.com/SD2E/experimentalintent-parser. OPIL: https://github.com/SD2E/opil; https:// github.com/SD2E/OPIL-specification/. SynBioHub: https:// github.com/SynBioHub/synbiohub. SBOL Project Dictionary: https://github.com/SD2E/sbol-dictionary-maintainer; https://github.com/SD2E/sbol-dictionary-writer.

²https://github.com/SD2E/opil, https://github.com/SD2E/ OPIL-specification/.

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