

[0004] One reason for this is that existing electronic systems for managing, storing, and viewing experimental data do not specify the experimental protocols used in a machine-readable form amenable to computerized analysis and reasoning. Thus, even when a computer has access to raw experimental data, it lacks a rich understanding of the experimentation that generated the raw data. For example in the Indigo Electronic Lab Notebook (“ELN”), the experimental protocol is just free text. *See, e.g.,* EPAM Life Sciences, *Indigo ELN User Guide Version 1.2*, Figure 18, bottom right panel. Thus, information regarding the experimental setup in the Indigo ELN is not machine parsable and one cannot programmatically validate or relate the experimental protocol information embodied by the free text to other information stored in the system. One consequence of this, as is observed in many fields, is that it is not possible to verify the completeness of the experimental protocol information contained in the free text. Another consequence of this is the inability to link experimental protocol information and resulting experimental data together, making it impossible to implement an efficient, reliable, and scalable general framework for linking experiments together.

SUMMARY

[0005] The disclosure provides, in some embodiments, systems and methods for data analysis of experimental data. The analysis can include reference data that are not directly generated from the present experiment, which reference data may be values of the experimental parameters that were either provided by a user, computed by the system with input from a user, or computed by the system without using any input from a user. Another example of such reference data may be information about the instrument, such as the calibration method of the instrument.

[0006] In one embodiment, a system is provided for analyzing data obtained from a laboratory experiment, comprising a processor, memory, and program code that comprises an experiment module configured to store values for experimental parameters for executing an experiment; and generate instructions for carrying out an experiment technique with the values for the experimental parameters, wherein the generating of the instructions for carrying out the experiment technique comprises generating a protocol object representing the experiment, wherein the protocol object directs and coordinates production of a new physical sample; placing, into a queue, the protocol object; and generating an experiment protocol when the protocol object is removed from the queue, wherein the experiment

protocol is programmatically linked to a laboratory sample, the experimental parameters, sensors, or tracking devices, and the experiment protocol is dynamically altered in response to received laboratory information, wherein the received laboratory information comprises information from one or more laboratory instruments, or information from the laboratory sample; an orchestration module configured to process the experiment protocol to coordinate execution of the experiment; a data module configured to store results from the experiment; an instrument module configured to display a listing of control experiments run on the instrument and a maintenance record for the instrument relevant to the experiment; an environment module configured to store environmental conditions under which the experiment was run; and a data visualization module configured to display a visual representation of the results stored in the data module, wherein the visual representation further comprises representation of one or more reference data point selected from the group

consisting of the values for the experimental parameters, the information about the instrument and the environmental conditions, wherein the system enables a user to explore information pertaining to the experiment while the user is presented with an experiment panel displayed by the experiment module, by: (1) allowing the user to click on the identification of the environmental record and thereby invoking the environment module to display environmental conditions under which experiment was conducted and (2) allowing the user to click on the identification of the instrument and thereby invoking the instrument module to display the listing of control experiments run on the instrument and the maintenance record for the instrument relevant to the experiment.

[0007] Another embodiment provides a system for analyzing data obtained from a laboratory experiment, comprising a processor, memory, and program code comprising an experiment module configured to display identification of a laboratory sample used in an experiment, identification of an instrument for carrying out the experiment, identification of a data set generated from the experiment, and identification of an environmental record that comprises measurement of environmental conditions when and where the experiment was conducted; and generate instructions for carrying out an experiment technique with the values for the experimental parameters, wherein the generating of the instructions for carrying out the experiment technique comprises generating a protocol object representing the experiment, wherein the protocol object directs and coordinates production of a new physical sample; placing, into a queue, the protocol object; and generating an experiment protocol when the protocol object is removed from the queue, wherein the experiment protocol is programmatically linked to the laboratory sample, sensors, or tracking devices, and the experiment protocol is dynamically altered in response to received laboratory information, wherein the received laboratory information comprises information from the instrument, or information from the laboratory sample; an orchestration module configured to process the experiment protocol to coordinate execution of the experiment; a data module configured to display data extract or visualization to represent a data set, identification of an experiment that generated the data set, and identification of an analysis performed on the data set; an instrument module configured to display a listing of experiments carried out on an instrument, a listing of control experiments run on the instrument, and a maintenance record for the instrument; an analysis module configured to display identification of a data set for which an analysis was made, and an analysis summary or figure that represents a result of the analysis; and an environment module configured to display environmental conditions when

and where an experiment was conducted, wherein the system enables a user to explore information pertaining to an experiment while the user is presented with an experiment panel displayed by the experiment module, by: (1) allowing the user to click on the identification of a data set generated from the experiment on the experiment panel, and thereby invoking the data module to display identification of an analysis performed on the data set on a data panel, which allows the user to click on the identification of analysis performed on the data set to invoke the analysis module to display an analysis summary or figure that represents a result of the analysis on an analysis panel; (2) allowing the user to click on the identification of an environmental record and thereby invoking the environment module to display environmental conditions when and where the experiment was conducted; and (3) allowing the user to click on the identification of an instrument for carrying out the experiment and thereby invoking the instrument module to display, on an instrument panel, a listing of control experiments run on the instrument, and a maintenance record for the instrument relevant to the experiment.

[0008] The present disclosure, in some embodiments, also provides systems, methods, computer-readable media, modules, and means for implementing an integrated system for laboratory experiment design, adjustment, scheduling, compiling, execution, analysis,

CLAIMS:

1. A system for analyzing data obtained from a laboratory experiment, comprising a processor, memory, and program code that comprises:

an experiment module configured to store values for experimental parameters for executing an experiment; and generate instructions for carrying out an experiment technique with the values for the experimental parameters, wherein the generating of the instructions for carrying out the experiment technique comprises:

generating a protocol object representing the experiment, wherein the protocol object directs and coordinates production of a new physical sample;

placing, into a queue, the protocol object; and

generating an experiment protocol when the protocol object is removed from the queue, wherein the experiment protocol comprises machine executable code and is programmatically linked to a laboratory sample, the experimental parameters, sensors, or tracking devices, and the experiment protocol is dynamically altered in response to received laboratory information, wherein the received laboratory information comprises information from one or more laboratory instruments, or information from the laboratory sample, wherein the experiment module is further configured to display, on an experiment panel, an identification of (i) an instrument for carrying out the experiment and (ii) an environmental record that comprises measurement of environmental conditions when and where the experiment was conducted, and the experiment protocol further comprises a human-readable instruction set comprising a dynamic interactive checklist that enables monitoring and confirmation of the experiment;

an orchestration module configured to:

process the experiment protocol to coordinate execution of the experiment;

a data module configured to store results from the experiment;

an instrument module configured to display a listing of control experiments run on the instrument and a maintenance record for the instrument relevant to the experiment;

an environment module configured to store environmental conditions under which the experiment was run; and

a data visualization module configured to display a visual representation of the results stored in the data module,

wherein the visual representation further comprises representation of one or more reference data point selected from the group consisting of the values for the experimental parameters, the information about the instrument and the environmental conditions, wherein the system enables a user to explore information pertaining to the experiment while the user is presented with an experiment panel displayed by the experiment module, by:

(1) allowing the user to click on the identification of the environmental record and thereby invoking the environment module to display environmental conditions under which experiment was conducted; and

(2) allowing the user to click on the identification of the instrument and thereby invoking the instrument module to display the listing of control experiments run on the instrument and the maintenance record for the instrument relevant to the experiment.

2. The system of claim 1, wherein the reference data point further comprises a result from a second experiment.

3. The system of claim 1, wherein the reference data point imposes a limitation on interpretation of the results.

4. The system of claim 3, wherein the reference data point eliminates a portion of the results as not relevant to analysis of the data.

5. The system of claim 3, wherein the reference data point validates or invalidate the results.

6. The system of claim 3, wherein the reference data point serves as standard or control to the results.

7. A system for analyzing data obtained from a laboratory experiment, comprising a processor, memory, and program code comprising:
an experiment module configured to

display identification of a laboratory sample used in an experiment, identification of an instrument for carrying out the experiment, identification of a data set generated from the experiment, and identification of an environmental record that comprises measurement of environmental conditions when and where the experiment was conducted; and generate instructions for carrying out an experiment technique with the values for the experimental parameters, wherein the generating of the instructions for carrying out the experiment technique comprises:

generating a protocol object representing the experiment, wherein the protocol object directs and coordinates production of a new physical sample;

placing, into a queue, the protocol object; and

generating an experiment protocol when the protocol object is removed from the queue, wherein the experiment protocol is programmatically linked to the laboratory sample, sensors, or tracking devices, and the experiment protocol is dynamically altered in response to received laboratory information, wherein the received laboratory information comprises information from the instrument, or information from the laboratory sample;

an orchestration module configured to:

process the experiment protocol to coordinate execution of the experiment;

a data module configured to display data extract or visualization to represent a data set, identification of an experiment that generated the data set, and identification of an analysis performed on the data set;

an instrument module configured to display a listing of experiments carried out on an instrument, a listing of control experiments run on the instrument, and a maintenance record for the instrument;

an analysis module configured to display identification of a data set for which an analysis was made, and an analysis summary or figure that represents a result of the analysis; and

an environment module configured to display environmental conditions when and where an experiment was conducted,

wherein the system enables a user to explore information pertaining to an experiment while the user is presented with an experiment panel displayed by the experiment module, by:

- (1) allowing the user to click on the identification of a data set generated from the experiment on the experiment panel, and thereby invoking the data module to display identification of an analysis performed on the data set on a data panel, which allows the user to click on the identification of analysis performed on the data set to invoke the analysis module to display an analysis summary or figure that represents a result of the analysis on an analysis panel;
- (2) allowing the user to click on the identification of an environmental record and thereby invoking the environment module to display environmental conditions when and where the experiment was conducted; and
- (3) allowing the user to click on the identification of an instrument for carrying out the experiment and thereby invoking the instrument module to display, on an instrument panel, a listing of control experiments run on the instrument, and a maintenance record for the instrument relevant to the experiment.

8. The system of claim 7, wherein the program code further comprises a sample module configured to display the identifications of a first experiment from which the sample is generated and a second experiment that is performed on the sample.

9. The system of claim 7, wherein the displayed analysis summary or figure on the analysis panel allows the user to make adjustment and access to the data set from which the analysis summary or figure is generated.

10. The system of claim 7, wherein the system allows the user to click on the listing of experiments on the instrument panel to view one or more other experiments conducted on the instrument for comparison.