Roboliq
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## **Preface**

This manual will show you how to write high-level protocols that can be executed on multiple robotic platforms. We introduce *Roboliq*, a software system for automating lab protocols using liquid handling robots. Roboliq support high-level commands that make it much easier to write automation protocols, especially complex ones. It then generates the low-level commands that for your robot system (currently only Tecan Evoware).

### Structure of the manual

- Chapter 1 "Introduction" gives a quick overview of how to use Roboliq.
- Chatper 2 "Quick start" is a practical walk-through for writing Roboliq protocols and compiling them.
- Chapter 3 "Input formats" describes several formats that Roboliq accepts for writing protocols.
- Chapter 4 "Robot configuration" describes how to write robot configurations that Roboliq uses to turn high-level commands into low-level instructions.
- Chapter 5 "Simple Protocols" describes the contents of simple Roboliq protocols.
- Chapter 6 "Advanced Protocols" describes the features available for more sophisticated protocols.
- Chapter 7 "Design tables" describes a how to represent experimental designs in a tree or table format, and how these can be used to concisely define complex experiments.

### Additional documentation

Roboliq has several other documentation sources that might be of interest to you:

- Protocol reference documentation for the commands and type available in Roboliq protocols
- Processor API programmer documentation for Roboliq's protocol processor
- Evoware API programmer documentation for Roboliq's Evoware backend

### Software information and conventions

Roboliq accepts several input formats, but in this manual we will use YAML. YAML is a very popular format for writing software configuration files. If you are not familiar with it yet, please checkout this page on Wikipedia.

Some of the advanced programmable features of Roboliq are demonstrated with JavaScript. Most users won't require knowledge of JavaScript, but if you do need it, there are many good tutorials online.

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Many many many thanks to Prof. Joerg Stelling for his guidance during my PhD research developing Roboliq. Fabian Rudolf was instrumental in determining which features are most relevant for biologists. Michael Kaltenbach provided sage statistical advice while developing the most sophisticated protocols we tested. Daniel Meyer and Urs Senn provided critical technical support in the lab. Oskari Vinko, Charlotte Ramon and Elena Karamaioti were wonderfully helpful guinnea pigs when testing Roboliq's usability.

## Chapter 1

## Introduction

### 1.1 Motivation

Roboliq aims to make it easier to use liquid handling robots for automation in biological laboratories.

It lets you write protocols that are portable between labs, and it compiles the protocols for execution by liquid handling robots.

The only supported backend is for Tecan Evoware robots, but other backends can also be added.

### 1.2 Get started

This guide presumes some familiarity with the command line terminal. You can install Roboliq by following these steps:

- 1. Install nodejs, which lets you execute Javascript programs.
- 2. If you're using Microsoft Windows, install the cygwin terminal, which will be used for typing in commands.
- 3. Copy the Roboliq repository to your computer.
- 4. Open the terminal, navigate to the directory where you copied the Roboliq repository, and run npm install to download Roboliq's software requirements.

Furthermore, the unit tests can be run by running by running npm test, and the documentation can be generated by running npm run docs.

## 1.3 Usage

The typical steps in running a Roboliq protocol on a Tecan Evoware robot are:

- 1. Write a configuration for your lab or use one which has been written by someone else.
- 2. Write a script for your protocol using the Roboliq syntax and commands.
- 3. Compile your script and configuration to create a program (.ESC) to be executed by your robot.
- 4. Open the Tecan Evoware script (.ESC) in Evoware, and run it.
- 5. Load Roboliq's measurement data into R or another statics program to analyze the data.

## Chapter 2

# **Quick Start**

Let's get started with a hands-on walk through. We'll begin with a very basic protocol and build up from there as follows:

- 1. a protocol that doesn't require any configuration or backend
- 2. a protocol with a minimal configuration
- 3. a protocol with a backend
- 4. a protocol compiled for Evoware
- 5. running the server and getting the data during execution of an Evoware script

### 2.1 The simplest protocol

We'll test a simple protocol to show you how to run the software.

1. Navigate to the protocols subdirectory and type this code into a file named walkthrough1.yaml (or copy the file walkthrough1-sample.yaml):

```
roboliq: v1
description: test that doesn't require configuration
steps:
   command: system.echo
   text: Hello, World!
```

2. Open the terminal, and navigate to the directory where you copied the Roboliq repository.

```
cd ~/Desktop/Ellis/roboliq/
```

3. Run Roboliq from the terminal, passing walkthrough1.yaml as input:

```
npm run processor -- protocols/walkthrough1.yaml
```

If there were no errors, you can now find a file named protocols/walkthrough1.out.json. The output file contains a lot of information: in addition to your script, it also contains the core configuration data that comes with Roboliq by default. If you open the file, you can find a steps property which looks like this:

```
"steps": {
   "1": {
      "command": "system._echo",
      "value": "Hello, World!"
   },
```

```
"command": "system.echo",
"value": "Hello, World!"
}
```

You can see a substep with the command system.\_echo. Commands that begin with an underscore are "final" instructions that will be passed the backend without further processing. It may be confusing that the original command (system.echo) and its properties appear after the subcommand, but this is just an artifact of how JavaScript always prints numeric properties first in JSON data.

An important difference between system.echo and system.echo is that system.echo is a higher level command that can handles variables, whereas system.echo just takes the value verbatim.

4. Run the command above again, but this time add the -P compiled argument to put the output in a separate compiled folder.

```
npm run processor -- protocols/walkthrough1.yaml -P compiled/
```

This will automatically create a subfolder named compiled/walkthrough1 and it will save the file compiled/walkthrough1/walkthrough1.out.json. It's important to have a separate folder for every experiment in order to properly organize measured data for each experimental run.

Now you know how to run the software and write a basic protocol. Let's continue to the next step, where we'll see how to create a basic robot configuration file.

### 2.2 A protocol with a minimal configuration

The robot configuration file lets you specify the capabilities of a robot. Let's start building such a configuration – this task can be quite technical and complicated, so we'll keep it basic here.

We will write the robot configuration in JavaScript; this way, we can later use helper function that will simplify configuring some of the equipment. Please copy the code below to a file named config/walkthrough2a-config.js

```
// This variable lets us export our configuration to Roboliq
module.exports = {
  // The targetted version of Roboliq
  "roboliq": "v1",
  // The configuration objects
  "objects": {
    // The top namespace for things in "our lab"
    "ourlab": {
      "type": "Namespace",
      // The namespace for things on our robot "mario"
      "mario": {
        "type": "Namespace",
        // An object to represent Mario's controller software
        // An `Agent` object executes instructions, such as operating equipment.
        "controller": {
          "type": "Agent"
        // The robot's "arm", used for moving labware
        "transporter1": {
          "type": "Transporter",
        // The namespace for mario's "sites" -- i.e., where it can place the
```

```
// labware. In this case, we have just two sites, named P1 and P2.
        "site": {
          "type": "Namespace",
          "P1": { "type": "Site" },
          "P2": { "type": "Site" }
     },
      // Namespace for labware models in our lab
      "model": {
        "type": "Namespace",
        // A 96-well plate model with 8 rows and 12 columns
        "plateModel_96well": {
          "type": "PlateModel",
          "label": "96 well plate",
          "rows": 8,
          "columns": 12
     }
   }
  },
  // The logical predicates for our configuration (see explanation in text below)
  "predicates": [
   // -----
   // Transporter logic
   // -----
   // Declare a site model siteModel 1
   {"isSiteModel": {"model": "ourlab.mario.siteModel 1"}},
    // Our 96-well plate can be placed on top of siteModel_1
   {"stackable": {"below": "ourlab.mario.siteModel_1", "above": "ourlab.model.plateModel_96well"}},
   // Both sites, P1 and P2, are assigned to siteModel_1
   {"siteModel": {"site": "ourlab.mario.site.P1", "siteModel": "ourlab.mario.siteModel_1"}},
   {"siteModel": {"site": "ourlab.mario.site.P2", "siteModel": "ourlab.mario.siteModel_1"}},
    // The list of sites that we can move labware between directly (i.e. without needing to go through
   {"siteCliqueSite": {"siteClique": "ourlab.mario.siteClique1", "site": "ourlab.mario.site.P1"}},
   {"siteCliqueSite": {"siteClique": "ourlab.mario.siteClique1", "site": "ourlab.mario.site.P2"}},
    // Let Roboliq know that mario's controller can use transporter1 to move
   // labware around on siteClique1.
   // The `program` property provides an additional specification for how the
    // transporter should move or grip the labware (not always necessary)
    {"transporter.canAgentEquipmentProgramSites": {
        "agent": "ourlab.mario.controller",
        "equipment": "ourlab.mario.transporter1",
        "program": "Narrow",
        "siteClique": "ourlab.mario.siteClique1"
   }}
  ٦
};
```

The logic for labware transportation is somewhat complex – to understand it, you'll need to know the following concepts:

- site: a location where the transporter can place labware
- site model: basically a list of labware that a site can accept; since some sites will accept the same set of labware, they can share the same "site model".

- stackable: this mean that one thing can be placed on top of another thing. In particular, it specified which labware models can go on top of which site models.
- site clique: a set of sites that that permit direct movement of labware among all members of the clique. This concept is a bit tricky. A simple robot configuration might just have a single clique that includes all of its sites. But more complex configuration may need to prohibit some movements. For example, we might have sites on the left of the bench and sites on the right, which are partially blocked by equipment in the middle. If each side of the bench has its own transporter arm and there is a single site in the middle that both arms can reach, then we could define two clicks: the left clique would contain all sites on the left plus the middle site, and the right clique would contain all sites on the right plus the middle site. This would ensure that Roboliq never generates instructions to directly move a plate from the left side to the right side, but rather first navigates through the middle site.

Now write a script to verify that we can move a plate between the two bench sites. Save this file as protocols/walkthrough2a.yaml or use the file protocols/walkthrough2a-sample.yaml.

```
roboliq: v1
description: Move plate from site P1 to P2
objects:
   plate1:
     type: Plate
     model: ourlab.model.plateModel_96well
     location: ourlab.mario.site.P1
steps:
   command: transporter.movePlate
   object: plate1
   destination: ourlab.mario.site.P2
```

Process the script by running this command from the terminal:

```
npm run processor -- config/walkthrough2a.js protocols/walkthrough2a.yaml -P compiled/
```

Or if you just want to run the sample files which are already present:

```
npm run processor -- config/walkthrough2a-sample.js protocols/walkthrough2a-sample.yaml -P compiled/
```

## 2.3 A BSSE protocol for mario

Now we'll run a protocol on the real robot (named mario). In our lab, mario has already been configured.

For this example, we'll simply dispense water into each well of a 96-well plate, seal it, and shake it. Create a new file ~/Desktop/Ellis/roboliq/charlotte01.yaml and write a script like this:

```
# version of Roboliq being used
roboliq: v1
# description of this protocol; the pipe symbol "/"" allows for multi-line text
description:
  Dispense a liquid into each well of a
  96-well plate, seal it, and shake it.
objects:
                                           # the set of materials used in this protocol
  plate1:
                                           # an object named "plate1"
                                           # which is a type of plate
   type: Plate
   model: ourlab.model.plateModel_96_round_transparent_nunc # whose model is defined in the configura
   location: ourlab.mario.site.P3
                                           # which the user should place at the location "P1"
  waterLabware:
   type: Plate
   model: ourlab.model.troughModel 100ml
   location: ourlab.mario.site.R6
```

```
contents: [Infinity 1, water]
    type: Liquid
    wells: waterLabware(A01 down D01)
steps:
  1:
    command: pipetter.pipette
    sources: water
    destinations: plate1(all)
    volumes: 40 ul
    cleanBetween: none
    command: sealer.sealPlate
    object: plate1
    command: shaker.shakePlate
    object: plate1
    program:
      duration: 10 seconds
```

Make sure your in the directory ~/Desktop/Ellis/roboliq/roboliq-processor, and run the command: npm start -- ../protocols/charlotte01.yaml

## Chapter 3

# Input formats

Roboliq accepts four input formats:

- JSON
- YAML
- JavaScript Node.js module that outputs an object
- JavaScript Node.js module that outputs a function

JSON stands for JavaScript Object Notation. It is a simple format for encoding software data, and it has gradually become the defacto format of choice for transfering data on the web.

YAML is a JSON-like format that is more legible. Due to its superior legibility, this manual usually displays protocols in YAML.

JavaScript is the lingua-franca of the web, and Node.js is the most popular platform for running JavaScript applications outside of browsers. You probably won't need JavaScript for Roboliq, unless you get into more advanced applications. If you do use JavaScript, your module may either 1) output a JavaScript object (i.e. module.exports = myOjbect;) or 2) a function that accepts configuration parameters and returns an object (i.e. module.exports = function(options) { ... return myOjbect; };).

There are many good online tutorials for the above formats, so please search for one if you encounter confusion.

## Chapter 4

# Robot configuration

In order for Roboliq to compile your protocol for your robot setup, it needs to know how the robot is configured. This is the most complicated part of Roboliq – it requires advanced technical knowledge or your robot and some programming skill. Once the configuration has been specified, future users don't need to be concerned with it.

So if someone else has configured Roboliq for your robot already, then you should probably just proceed to the next chapter. However, if you need to write the configuration, this chapter is for you.

### 4.1 Evoware configuration

(If you are not using an Evoware robot, you can skip this section.)

Roboliq supplies a simplified method for configuring Evoware robots. You will need to create a JavaScript file in which you define an EvowareConfigSpec object, and then have it converted to the Roboliq protocol format. Your config file will have the following structure:

```
const evowareConfigSpec = {
  // Lab name and robot name
  namespace: "YOUR LAB ID",
  name: "YOUR ROBOT ID",
  // Compiler settings
  config: {
   TEMPDIR: "TEMPORARY DIRECTORY FOR MEASUREMENT FILES",
   ROBOLIQ: "COMMAND TO CALL ROBOLIQ'S RUNTIME",
   BROWSER: "PATH TO WEB BROWSER"
  },
  // Bench sites on the robot
   MYSITE1: {evowareCarrier: "CARRIER ID", evowareGrid: MYGRID, evowareSite: MYSITE},
  },
  // Labware models
  models: {
   MYPLATEMODEL1: {type: "PlateModel", rows: 8, columns: 12, evowareName: "EVOWARE LABWARE NAME"},
 },
  // List of which sites and labware models can be used together
 siteModelCompatibilities: [
```

```
sites: ["MYSITE1", ...],
   models: ["MYPLATEMODEL1", ...]
 . . .
],
// List of the robot's equipment
equipment: {
 MYEQUIPMENT1: {
   module: "EQUIPMENT1.js",
   params: {
   }
  }
},
// List of which lid types can be stacked on which labware models
lidStacking: [
 {
   lids: ["lidModel_standard"],
   models: ["MYPLATEMODEL1"]
],
// List of the robot's robotic arms
romas: [
   description: "roma1",
   // List of sites this ROMA can safely access with which vectors
    safeVectorCliques: [
              { vector: "Narrow", clique: ["MYSITE1", ...] },
          ]
 },
  . . .
],
// Liquid handing arm
liha: {
 // Available tip models
 tipModels: {
   MYTIPMODEL1000: {programCode: "1000", min: "3ul", max: "950ul", canHandleSeal: false, canHandleCe
  },
  // List of LIHA syringes (e.g. 8 entries if it has 8 syringes)
  syringes: [
   { tipModelPermanent: "MYTIPMODEL1000" },
  ],
  /\!/ Sites that the LIHA can access
  sites: ["MYSITE1", ...],
  // Specifications for how to wash the tips
  washPrograms: {
    // For Example: Specification for flushing the tips with `programCode == 1000`
   flush_1000: { ... },
```

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```
},
  // Additional user-defined command handlers
  commandHandlers: {
    "MYCOMMAND1": function(params, parsed, data) { ... },
  },
  // Optional functions to choose among planning alternatives
  planAlternativeChoosers: {
    // For Example: when the `shaker.shakePlate` command has
    // multiple shakers available, you might want to use
    // the one name `MYEQUIPMENT1`
    "shaker.canAgentEquipmentSite": (alternatives) => {
            const l = alternatives.filter(x => x.equipment.endsWith("MYEQUIPMENT1"));
            if (1.length > 0)
                return 1[0];
        }
  }
};
const EvowareConfigSpec = require('roboliq-evoware/dist/EvowareConfigSpec.js');
module.exports = EvowareConfigSpec.makeProtocol(evowareConfigSpec);
```

The details about evowareConfigSpec are in the Evoware API documenation, and an extensive example can be found in roboliq-processor/tests/ourlab.js. This information is probably enough to configure your Evoware robot, and you can skip the rest of this chapter unless you need to setup a different kind of robot.

### 4.2 Components

A configuration is a JavaScript object with the following properties:

- roboliq: specifies the version of Roboliq.
- schemas: JSON Schema definitions for all object and commands.
- objects: specifies the objects provided by the robot.
- commandHandlers: specifies the functions that handle protocol commands, for example by generating low-level commands from high-level commands.
- predicates: specifies the *logical predicates* used by Roboliq's A.I. to figure out how to compile some high-level commands to low-level commands for this configuration.
- objectToPredicateConverters: specifies functions that generate logical predicates based from objects.
- planAlternativeChoosers: specifies functions that can choose a specific plan among various alternative plans
- planHandlers: specifies the functions that transform logical tasks into commands.

The first four properties are easy for the average JavaScript programmer to understand: they are straight-forward JSON values or JavaScript functions. In contrast, the last four properties (predicates, objectToPredicateConverters, planAlternativeChoosers, and planHandlers) rely on concepts from Artificial Intelligence, which will require more effort to grasp.

### 4.2.1 roboliq

As with protocols, the first property of a configuration should be roboliq: v1.

#### 4.2.2 schemas

For every command and object type, Roboliq requires a schema that defines its properties. By convention, object types begin with an upper-case letter, and commands begin with a lower-case letter. The schemas are written in a standardized format, which you can learn more about at JSON Schema.

Normally, the schemas required for your robot should be automatically provided by your chosen backend and the equipment you select. The schemas property is a hash map: its keys are the command names and object type names; its values are the respective JSON schemas. You will not need to write schemas unless you are creating new commands or objects types for Roboliq. An example schema is provided below in the commandHandlers section.

### 4.2.3 objects

The objects property of a configuration is the same as describe for protocols in the Quick Start chapter. However, robot configurations usually contain complex objects, such as measurement devices, whereas protocols usually only define fairly simple labware. Furthermore, the configuration may contain information that's required for the backend compiler. The object schemas are described in the documentation for standard Roboliq objects and for Evoware objects.

*Namespaces*. Because a robot "contains" its devices, sites, and permanent labware, we use Namespace types to build nested objects. For example, if our lab is named "bsse", we have a robot named "bert", and it has a site named "P1", this could be encoded as follows:

```
objects:
  bsse:
  type: Namespace
  bert:
   type: Namespace
  site:
    type: Namespace
  P1:
    type: Site
   ...
```

We can then reference the site in the protocol as bsse.bert.site.P1.

#### 4.2.4 commandHandlers

A command handler is a JavaScript function that processes command parameters and returns information to Roboliq about the command's effects, sub-commands, and user messages.

Command handlers are supplied by various modules. Roboliq's command modules are in the subdirectory roboliq-processor/src/commands, and Evoware's command modules are in the subdirectory roboliq-evoware/src/commands. The API documentation contains information about the available commands.

If you want to write your own command handler, you can add it to commandHandlers as a property. The property name should be the name of the command, and the value should be the command handler function. For example, let's make a simplistic function called my.hello that tells an Evoware robot to say "Hello, YOURNAME!". First we'll defined the schema for the new command:

```
schemas: {
   "my.hello": {
    description: "Say hello to someone",
    properties: {
```

```
name: {
    description: "Name to say hello to",
    type: "string"
    }
},
    required: ["name"]
}
```

This schema lets Roboliq know that there's a command named my.hello.

### 4.3 Logic components

Roboliq uses an Articifial Intelligence method called Hierarchical Task Network (HTN) Planning. In particular, it uses a SHOP2 implementation written by Warren Sack in JavaScript.

### 4.3.1 predicates

A predicate defines a "true statement". For example, the following predicate is named sealer.canAgentEquipmentProgramMode and it lets Roboliq know that the robot agent ourlab.mario.evoware can use the sealer ourlab.mario.sealer with the labware model ourlab.model.plateModel\_96\_round\_transparent\_nunc at site ourlab.mario.site.ROBOSEAL with the internal program file PerkinElmer\_weiss.bcf.

The general form for predicates is:

```
predicateName:
  object1: value1
  object2: value2
   ...
```

The values are usually object names, and predicates often define true relationships among objects. All of the predicates together form a database of true statements about the "world" in which the protocol will run. They are used by certain command handlers to automatically figure out valid operations without the user needing to specify the low-level details. (Currently, the end-user documentation does not contain details about which predicates are used by which commands, but it can be found in the command handler source code.)

Here is an example excerpt of using the predicate database to find all valid sealers from the sealer.sealPlate command handler:

The function commandHelper.queryLogic() will find all solutions the predicates array, filling in the missing values as necessary. If more than one alternative solution is present, it will choose one of them. The solution can either by chosen by a appropriate function planAlternativeChoosers, or else Roboliq simply picks the first item in the alternatives list.

### 4.3.2 objectToPredicateConverters

Roboliq's AI needs predicates describing the available objects. These are generated dynamically by the functions supplied in <code>objectToPredicateConverters</code>. It is a map from an object type to a function that accepts a named object and returns an array of predicates. For example, here is Roboliq's converter for <code>Plate</code> objects:

This converter creates between 4 and 6 predicates for every plate object: isLabware lets the AI know that the plate is a kind of labware, isPlate says that the plate is a plate, model says which labware model the plate has, and location says where the plate is located. Furthermore, plateIsSealed will be present if-and-only-if the plate is sealed.

You'll only need to create additional object-to-predicate converters if you want to extend Roboliq's object types, or perhaps if you create an advanced command that required additional logic.

### 4.3.3 planHandlers

Plan handlers are functions that convert from a planning action to a Roboliq command (usually a low-level command). It is a map from an action name to a function that accepts that action parameters and returns

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an array of commands. The function also accepts the parameters of the parent command (the one that generated the plan), and the protocol data, in case those are needed to compute the new command.

An example use-case is using the transporter.movePlate command to move a plate into a closed centrifuge: the planning algorithm will include an action to open the centrifuge first, and then the transporter.movePlate command will call the appropriate function in planHandlers to create the required sub-command.

### 4.4 Conclusion

Configuring a robot can be complicated. First of all, it requires a lot of detailed knowledge about your robot. Secondly, it involves a lot of interdependencies. For example, in order to support a new labware model, you'll need to add the model to the models list (easy), but you also need to update the list of site/model compatibilities, the list of safe transport vectors, and perhaps the list of which models accept lids or can be stacked on top of each other.

It's certainly do-able, but you're likely to encounter some frustrations if you need to trouble-shoot why you get compiler errors when trying to use your new model, for example.

## Chapter 5

# Simple Protocols

Roboliq was developed to help automate protocols on liquid handling robots, especially for lab experiments in molecular biology. This chapter will explain the four properties in simple protocols and how to write write them.

First consider this short example – it uses Roboliq version "v1"; it defines a Plate named sourcePlate; and it instructs us to shake the plate:

```
roboliq: v1
description: Shake a plate, just because we can
objects:
    sourcePlate:
        type: Plate
steps:
    1:
        command: shaker.shakePlate
        object: sourcePlate
```

The protocol consists of *properties* and *values*. A *property* is a name followed by a semicolon and then a *value*. In the above example, we see the following properties and values:

- 1) The first property is roboliq, and it has a string value of v1 which indicates we're using Roboliq version 1.
- 2) The second property is description, whose value is also a text string.
- 3) The third property is objects, which defines the materials we'll use in the protocol. In contrast to the previous properties, the *value* starts on the next line and is indented by two spaces. This means that the value of objects is another set of properties: sourcePlate is the name of a material whose type property is set to Plate.
- 4) The forth property is steps, which defines the steps to be performed. Its *value* is usually a numbered set of steps, and each numbered step is assigned properties as well: in this case, step 1 has the properties command: shaker.shakePlate and object: sourcePlate which tell Roboliq to shake the plate named sourcePlate.

Most of your protocols will have those four basic properties, and perhaps additional properties as well.

Next we will describe the objects and steps properties in more detail.

### 5.1 Objects

In order to add more objects, just give them a name and assign them the appropriate properties. Here we extend objects to include another plate for mixing named mixPlate:

```
objects:
    sourcePlate:
    type: Plate
    mixPlate:
    type: Plate
```

Objects are the things that can be used in the protocol's steps, including labware, liquids, and equipment. Each object requires a type property (e.g. Plate in the example above) – the two most common types used in protocols are:

- Plate: for defining labware, including tubes and troughs.
- Liquid: for defining liquids.

A complete list of types can be found in the Commands & Types documentation, but most of them are only used in robot configurations rather than in protocols.

In addition to the type property, object have other properties as well (also available in the type documentation), and all objects have an optional description property that you can use to add your own notes about the object. Here are examples of the two main object types to indicate that a liquid named specialMix is in all wells on plate1:

```
objects:
   plate1:
     type: Plate
     description: Plate to be used for initial mixing
     model: ourlab.roboto.model.96microwell
     location: ourlab.roboto.P1
specialMix:
     type: Liquid
     description: Our special mad-scientist mix
     wells: plate1(all)
```

## 5.2 Steps

A *step* is either a command or a numbered list of sub-steps, and a protocol's **steps** property specifies the steps that should be taken during the protocol. Here is an example with two numbered steps in which a plate is sealed and shaken:

```
steps:
1:
    command: sealer.sealPlate
    object: plate1
2:
    command: shaker.shakePlate
    object: plate1
```

A command is indicated by a command property, such as the commands sealer.sealPlate and shaker.shakePlate above. Besides the command property, you will need to specify additional properties to tell the command exactly what to do. In the above example, the line object: plate1 tells the command to act on plate1.

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Command names have two parts separated by a period. First is the command category, which contains related commands. Second is the actual command name. Roboliq's standard commands are listed in the Command documentation, and Evoware's special commands are listed in the Evoware Command documentation.

Steps can also be given a description property that let's you explanation what's happening for someone else who reads the protocol (or for yourself later after you've forgotten). Step can also be given a comment property, which is intended to be used as programmer comments that aren't of interest to others.

Here is an example that contains nested steps, descriptions and commands - it is the same as the previous example, but applied to two plates:

```
steps:
1:
    description: "Handle plate1"
1:
        command: sealer.sealPlate
        object: plate1
2:
        command: shaker.shakePlate
        object: plate1
2:
        description: "Handle plate2"
1:
        command: sealer.sealPlate
        object: plate2
2:
        command: shaker.shakePlate
        object: plate2
2:
        command: shaker.shakePlate
        object: plate2
```

### 5.3 Conclusion

Simple protocols can be writen using four properties: roboliq, description, objects, and steps. The roboliq property indicates the version of Roboliq, and description lets you document what the protocol does. In objects you specify the labware and liquids used in the protocol. And in steps you create a list of numbered commands; the steps can be nested and documented however you prefer. You can find documentation for the objects and commands in the Commands & Types documentation.

## Chapter 6

# **Advanced Protocols**

Advanced protocols can contain many more elements than the simple protocols described in the previous chapter. In this chapter we'll discuss parameters, objects, data properties, variable scope, substitution, directives, and template functions.

### 6.1 Parameters

Parameters are named values that you define at the beginning of a protocol. You can then use the parameter name instead of the value later in the protocol. In this partial example, a VOLUME parameter is defined which is used in the pipetter.pipette step:

```
parameters:
    VOLUME:
        description: "amount of water to dispense"
        value: 200 ul
...
steps:
    1:
        command: pipetter.pipette
        sources: water
        destinations: plate1(all)
        volumes: $#VOLUME
```

A parameter should be given a description and a value. Notice that \$# prefixes VOLUME in the step; \$# tells Roboliq to substitute in a parameter value. Substitution is discussed in more detail later in this chapter.

## 6.2 Objects

There are several more object types you might want to use in advanced protocols:

Data: for defining a data table. The Data type facilitates complex experimental designs, and you can read more about it in the next section and in the chapter on Design Tables.

Variable: For defining references to other variables. Variables are not particularly useful in Roboliq, but they could potentially be used to easily switch between objects in case you have, for example, two water sources water1 and water2. In that case you could have a water variable whose value to set to the source you want to use:

```
objects:
   water1: ...
   water2: ...
   water:
    description: "water source"
       type: Variable
    value: water1
steps:
   1:
       command: pipetter.pipette
       sources: water
       destinations: plate1(all)
       volumes: 50 ul
```

Template: You can use a template to define re-usable steps. Here is a toy example for a template named dispenseToPlate1 which creates a pipetter.pipette command that transfers a volume of water to all wells on plate1:

```
objects:
  plate1:
    type: Plate
  dispenseToPlate1:
    description: "template to dispense `volume` ul of water to all wells on plate1"
    type: Template
    template:
      command: pipetter.pipette
      sources: water
      destinations: plate1(all)
      volumes: "{{volume}}"
steps:
  1:
    command: system.call
    name: dispenseToPlate1
    params:
      volume: 10 ul
    command: system.call
    name: dispenseToPlate1
    params:
      volume: 50 ul
```

This protocol will first dispense 10ul to all wells, then another 50ul to all wells – not actually a useful protocol, but it illustrates the point. In the system.call command, the name of the template is specified along with the parameters template parameters. Templates are expanded using the Handlebars template engine, which is the reason for the "{{" and "}}" delimiters in the line volumes: "{{volume}}".

### 6.3 Data

Roboliq supports data tables to enable complex experiments. Conceptually, a data table is like a spread sheet of rows and named columns, where each row represents some "thing", a each column represents a property. In Roboliq, a data table is an array of JSON objects: each object is a row, and each property is a column. Normally all the objects will have the same set of properties (but this is not required).

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Data tables are supported by a Data type, a data property, a data() directive, and a set of data.\* commands.

### 6.3.1 Data type

You can define a data table using the Data object type. Here's an example where each row has a well, a liquid source, and a volume:

```
objects:
  data1:
    type: Data
    value:
        - {well: A01, volume: 10 ul, source: liquid1}
        - {well: B01, volume: 10 ul, source: liquid2}
        - {well: A02, volume: 20 ul, source: liquid1}
        - {well: B02, volume: 20 ul, source: liquid2}
```

You can define as many data tables as you want in a protocol.

### 6.3.2 data property

After defining a data table, you need to "activate" it for usage. This is done using the data property, which understands the following parameters:

- source: this is the name of a Data object.
- where: this is an optional boolean mathjs expression that is evaluated for each data row only rows for which the expression evaluates to true are activated.
- orderBy: an optional array of column names for ordering rows. The ordering behavior is the same as the \_.sortBy function in lodash.

Any step can be given a data property to make a table available in that step and its sub-steps. Here's an example application:

```
steps:
1:
    data: {source: data1}
    command: pipetter.pipette
    sources: $$source
    destinationPlate: plate1
    destinations: $$well
    volumes: $$volume
```

The data property activates our data table data. The command pipetter.pipette can now access the data columns by using the \$\$-prefix along with the column name. So the above example is essentially equivalent to this:

```
steps:
1:
    command: pipetter.pipette
    sources: [liquid1, liquid2, liquid1, liquid2]
    destinationPlate: plate1
    destinations: [A01, B01, A02, B02]
    volumes: [10 ul, 10 ul, 20 ul, 20 ul]
```

#### 6.3.3 data.\* commands

Roboliq's data.\* commands provide two commands for more sophisticated handling of data tables: data.forEachRow and data.forEachGroup.

data.forEachRow lets you run a series of steps on each row of the data table. For each row, the command activates a new data table containing only that row, and it runs its sub-steps using that new table. Here's a toy example:

```
steps:
  1:
    data: {source: data1}
    command: data.forEachRow
    steps:
      1:
        command: pipetter.pipette
        sources: $source
        destinationPlate: plate1
        destinations: $well
        volumes: $volume
      2:
        command: fluorescenceReader.measurePlate
        object: plate1
        output:
          joinKey: well
```

In this case, the sub-steps will be repeated 4 times, once for each row. That mean each well will be dispensed into and measured before moving onto the next well. Notice that here only a single \$-prefix was used rather than the double \$\$-prefix for the column variables. When a data table is activated, Roboliq will check if any of the columns have all the same value; if so, that property and value will be automatically added to the current scope (see the next section about Scope). Scope variables are accessible via the \$-prefix. Since the data.forEachRow command activates each row individually, all of its columns will be added to the scope.

data.forEachGroup lets you operate on groups of rows at a time. You provide a groupBy property for it to group by, and then for each group it activates a new data table with those rows and runs its sub-steps using that new table. Here's another toy example:

```
steps:
  1:
    data: {source: data1}
    command: data.forEachGroup
    groupBy: source
    steps:
      1:
        command: pipetter.pipette
        sources: $source
        destinationPlate: plate1
        destinations: $$well
        volumes: $$volume
      2:
        command: fluorescenceReader.measurePlate
        object: plate1
        output:
          joinKey: well
```

Since there are two unique source values in data1, the data.forEachGroup command will create two new data tables for it sub-steps:

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First table:

```
- {well: A01, volume: 10 ul, source: liquid1}
- {well: A02, volume: 20 ul, source: liquid1}
```

Second table:

```
- {well: B01, volume: 10 ul, source: liquid2}
- {well: B02, volume: 20 ul, source: liquid2}
```

So the sub-steps will be repeated twice, once for new data table. Notice that here we used the single \$-prefix for source, but the double \$\$-prefix for well and volume. Because the values of the well and volume columns are not the same in all rows, they are not automatically added to the scape, and we can't use the single \$-prefix.

### 6.3.4 data() directive

The data() directive lets you assign a modified version of your data table to a property value. It will be easier to explain this in the section on Substitution, so we'll postpone the discussion till the end of this chapter.

### 6.4 Scope

Scope is the set of currently active variables in a step. These usually come from one of two sources: 1) the data directive and commands, as discussed above, or 2) a loop command like system.repeat, which lets you add an index variable to the scope of the sub-steps.

The scope is a kind of stacked-tower structure. When a step pushes variables into scope, they are available to that step's command and all substeps; however, they are not available to sibling or parent steps.

### 6.5 Substitution

Substitution lets you work with parameters and data tables by inserting their values into the protocol. Roboliq supports three forms: template substitution, scope substitution, and directive substitution.

### 6.5.1 Scope \$ substitution

In scope substition, an expression starting with \$ is replaced with a value from the scope. There are various forms of replacement, which we'll dive into now.

#### \$#...: pre-scope substitution for parameter values

Parameters are not actually part of the scope, and they are accessible outside of steps as well. This means that they can be used in other parameter values and in object definitions, which is not the case for normal scope variables. You can substitute the value of a parameter named MYPARAM by with \$#MYPARAM.

#### \${...}: javascript expression

Roboliq will substitute in the result of a JavaScript expression. The JavaScript expression has access to:

- The scope variables
- \_: the lodash module and its many functions.
- math: the mathjs module and its many functions.

Note that any value JSON value may be returned, whether it's a string, number, boolean, array, or object.

#### (...): mathis calculation

The mathjs module provides a fairly broad range of math operations and is able to handle of units, such as volume. The mathjs expression has access to the current scope variables.

#### \$...: scope value substitution

Here you just name the scope variable, and Roboliq will substitute in its value.

If you have activated a data table using the data property, then you can use \$colName to get an array of all the values in the column named colName. Furthermore, if any of the data columns are filled with the same value, then that value is added to the scope as \$colName\_ONE, where colName is the actual name of the column. For example, if the active data table has a column named plate whose entries are all plate1, then \$plate1\_ONE = "plate1".

**NOTE**: Scope substitution can only be used as a parameter value, but not as a parameter name or part of a longer string. The following uses are invalid:

- text: "Hello, \$name": Roboliq only supports scope substitution for an entire value, so the name value will not be substituted into this text.
  - You can use template substitution for this purpose instead.
- \$myparam: 4: Roboliq does not support scope substitution for property names. You can use template substitution for this purpose instead.

#### Examples

Let's look at examples of \$-substitutions. Consider this protocol:

```
roboliq: v1
parameters:
  TEXT: { value: "Hello, World" }
objects:
  data1:
    type: Data
    value:
      - {a: 1, b: 1}
      - \{a: 1, b: 2\}
steps:
  1:
    data: data1
    command: system.echo
      javascript: "${`${TEXT} ${a} ${__step.command}`}"
      math: "$(a * 10)"
      scopeParameter: $TEXT
      scopeColumn: $b
      scopeOne: $a_ONE
      scopeData: $__data[0].b
      scopeObjects: $__objects.data1.type
      scopeParameters: $__parameters.TEXT.value
      scopeStep: $__step.command
```

The system.echo command will output the object described in its value parameter. The resulting value is this:

```
javascript: "Hello, World 1 system.echo"
math: 10
scopeParameter: "Hello, World"
```

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```
scopeColumn: [1, 2]
scopeOne: 1
scopeData: 1
scopeObjects: "Data"
scopeParameters: "Hello, World"
scopeStep: "system.echo"
```

### 6.5.2 Template 'substitution

Template substitution uses the Handlebars template engine to manipulate text. Template substitution occurs on strings that start and end with a tick ('). Here's a simple example that produces a new string:

```
text: "`Hello, {{name}}`"
```

If the name in the current scope is "John", then this will set text: "Hello, John".

If the template substitution result is enclosed by braces or brackets, Roboliq will attempt to parse it as a JSON object. Here's a trivial example that turns a template substitution into a command, assuming that name is currently in scope:

```
1: `{command: "system._echo", text: "Hello, {{name}}"}`
```

### 6.5.3 Directive () substitution

Directives are substitution functions. The main one is the data() directive, which was briefly mentioned above in the Data section. The other directives are also closely related to Data objects, and they are discussed more in the chapter on Design Tables.

The data() directive lets you assign a modified version of your data table to a property value. The directive can take several properties:

- where: same as for the data property, this lets you select a subset of rows in the active data table.
- map: each row in the data table will be mapped to this value. This is how you can transform your rows.
- summarize: like map, but for summarizing all the rows into a single row. Summarize has a particularity: all column names are pushed into the current scope as arrays, and they are not overwritten by a single common value even if the column only contains a single value.
- join: a string separator that will be used to join all elements of the array (see Array#join in some JavaScript documentation).
- head: if set to true,

Let's consider some examples using the data1 table from above. Here is the table:

```
- {well: A01, volume: 10 ul, source: liquid1}
- {well: B01, volume: 10 ul, source: liquid2}
- {well: A02, volume: 20 ul, source: liquid1}
- {well: B02, volume: 20 ul, source: liquid2}
```

and here are the examples:

```
Directive:
```

```
data(): {where: 'source == "liquid1"'}}
Result:
- {well: "A01", volume: "10 ul", source: "liquid1"}
- {well: "A02", volume: "20 ul", source: "liquid1"}
```

```
Directive:
data(): {map: '$volume'}
Result:
["10 ul", "10 ul", "20 ul", "20 ul"]
Directive:
data(): {where: 'source == "liquid1"', map: '$(volume * 2)'}
Result:
["20 ul", "40 ul"]
Directive:
data(): {map: {well: "$well"}}
Result:
- {well: "A01"}
- {well: "B01"}
- {well: "A02"}
- {well: "B02"}
Directive:
data(): {map: "$well", join: ","}
{\bf Result:}
"A01,B01,A02,B02"
Directive:
data(): {summarize: {totalVolume: '$(sum(volume))'}}
Result:
- {totalVolume: "60 ul"}
Directive:
data(): {groupBy: "source", summarize: {source: '${source[0]}', totalVolume: '$(sum(volume))'}}
Result:
- {source: "liquid1", totalVolume: "30 ul"}
- {source: "liquid2", totalVolume: "30 ul"}
```

## Chapter 7

# Design Tables

Here we use the term *Design Table* to refer to a data table that is designed for an experiment. It should contain all relevant factors for later analyzing the experimental results.

Experiments on microwell plates can easily involve hundreds of unique liquid combinations, so specifying them manually can be tedious and error-prone. Here we present a short-hand for creating design tables.

WARNING: This is very abstract. Don't bother with it if you're looking for something easy. That said, it makes complex experiments much, much easier to design, trouble-shoot, and analyze.

NOTE: In this chapter, we'll uses the following terms interchangeably: column, factor, variable.

### 7.1 First examples

Let's create a design table with a single row like this:

plate	source	destination	volume
plate1	water	A01	25 ul

This table could be used to specify a single pipetting operation that dispenses 25 ul of water into well A01 of plate1. We will specify this in Roboliq as follows:

```
roboliq: v1
objects:
    data1:
        type: Data
        description: First example
        design:
            plate: plate1
            source: water
            destination: A01
            volume: 25 ul
```

In a Roboliq protocol, designs are placed under the objects property. In this case, its name is data1, its type is Data, and it has a description. The design property is where factors are specified.

Let's expand the design table a bit to dispenses 25 ul of water into several destinations.

plate	source	destination	volume
plate1	water	A01	25 ul
plate1	water	B01	25  ul
plate1	water	C01	25  ul

To specify this in Roboliq, we change the destination property to a branching factor:

```
roboliq: v1
objects:
  data1:
    type: Data
    description: First example
  design:
    plate: plate1
    source: water
    destination*: [A01, B01, C01]
    volume: 25 ul
```

Notice the asterisk in **destination\***. An asterisk at the end of a factor name indicates *branching*. Branching factors require an array of values, and for each value in the array, the existing rows are first replicated and then the value is assigned to the factor in that row.

Now let's assign a different volume to each row:

plate	source	destination	volume
plate1	water	A01	25 ul
plate1	water	B01	50  ul
plate1	water	C01	75  ul

To specify this in Roboliq, we change the volume property to an array:

```
roboliq: v1
objects:
    data1:
        type: Data
        description: First example
        design:
        plate: plate1
        source: water
        destination*: [A01, B01, C01]
        volume: [25 ul, 50 ul, 75 ul]
```

When a factor value is an array, a new column is added with those values.

Try it. Copy the above code to a new file in Roboliq's root directory named data1Test.yaml. Open a terminal and change directory to the Roboliq root, and run the following command:

```
npm run design -- --path objects.data1 data1Test.yaml
```

It should produce this output:

```
plate1 water CO1 75 ul
```

Branches can also be specified as integers. If you specify an integer, it creates that many branches which are each given an integer index, as follows:

```
roboliq: v1
objects:
    designInteger:
    type: Data
    design:
        a*: 3
        b*: 3
```

Which creates the following table:

a	b
1	1
1	2
1	3
2	1
2	2
2	3
3	1
3	2
3	3
_	

## 7.2 Nested branching

Nested branching provides a lot of power to the design specification, but it is also where the complexity starts. Consider this table where two sources are nested in each destination, and each source has its own volume:

plate	destination	source	volume	liquidClass
plate1	A01	water	50 ul	Roboliq_Water_Air_1000
plate1	A01	dye	25  ul	Roboliq_Water_Air_1000
plate1	B01	water	50  ul	Roboliq_Water_Air_1000
plate1	B01	$_{ m dye}$	25  ul	Roboliq_Water_Air_1000
plate1	C01	water	50  ul	Roboliq_Water_Air_1000
plate1	C01	dye	25 ul	Roboliq_Water_Air_1000

This can be described in Roboliq as follows:

```
roboliq: v1
objects:
    data2:
    type: Data
    description: Nested example
    design:
        plate: plate1
        destination*: [A01, B01, C01]
        source*:
        water:
```

volume: 50 ul
dye:

volume: 25 ul

liquidClass: Roboliq\_Water\_Air\_1000

Create a file named data2Test.yaml with those contents and run:

```
npm run design -- --path objects.data2 data2Test.yaml
```

Let's walk through this example step-by-step to see how the desired table is achieved.

Step 0: A design starts as a single empty row.

Step 1: plate: plate1

This assigns the value plate1 to the property plate in the first row:

plate plate1

Step 2: destination\*: [A01, B01, C01]

Three copies of the previous row are created, and a column for destination is added to each row, each with its own value:

plate	destination
plate1	A01
plate1	B01
plate1	C01

#### Step 3: source\*

This branch has two keys: water and dye. So to start with, two copies are made of each of the previous three rows. The first copy is updated according to the first key, giving us:

plate	destination	source
plate1	A01	water
plate1	B01	water
plate1	C01	water

Then the conditions embedded under water: are applied to those rows - in this case, volume = 50 ul:

plate	destination	source	volume
plate1	A01	water	50 ul
plate1	B01	water	50  ul
plate1	C01	water	50  ul

For the second table copy, an analogous process sets source = dye and volume = 25 ul:

plate	destination	source	volume
plate1	A01	dye	25 ul

plate	destination	source	volume
plate1	B01	dye	25 ul
plate1	C01	dye	25  ul

Next those two tables are concatenated, giving us:

plate	destination	source	volume
plate1	A01	water	50 ul
plate1	A01	dye	25  ul
plate1	B01	water	50  ul
plate1	B01	dye	25  ul
plate1	C01	water	50  ul
plate1	C01	dye	25  ul

Step 4: liquidClass: Roboliq\_Water\_Air\_1000

Finally, liquidClass = Roboliq\_Water\_Air\_1000 is assigned to all rows:

plate	destination	source	volume	liquidClass
plate1	A01	water	50 ul	Roboliq_Water_Air_1000
plate1	A01	dye	25  ul	Roboliq_Water_Air_1000
plate1	B01	water	50  ul	Roboliq_Water_Air_1000
plate1	B01	dye	25  ul	Roboliq_Water_Air_1000
plate1	C01	water	50  ul	Roboliq_Water_Air_1000
plate1	C01	dye	25  ul	$Roboliq\_Water\_Air\_1000$

### 7.3 Hidden factors

There are generally many ways to achieve the same results. As an example, an alternative way of achieving the same result as above is:

```
roboliq: v1
objects:
  data2:
    type: Data
    description: Nested example
  design:
    plate: plate1
    destination*: [A01, B01, C01]
        .sourceId*:
    - source: water
        volume: 50 ul
        - source: dye
        volume: 25 ul
        liquidClass: Roboliq_Water_Air_1000
```

In this case, the branching factor is <code>.sourceId\*</code> and it's an array. The period prefix hides that column, and the final results are the same as above.

### 7.4 Actions

Roboliq provides various designs "actions" that can be used for more sophisticated values. The most important ones are:

- allocateWells
- range
- calculate
- case

### 7.4.1 allocateWells

Let's take a look at an example:

```
replicate*: 2
well=allocateWells:
  rows: 8
  columns: 12
```

An action is indicated with the "="-infix. So in the case of well=allocateWells, the factor name is well, the action is allocateWells, and the properties are the arguments to the action. In this case, rows and columns tells the plate dimension we want to get wells for, and 2 wells will be allocated since the table has two rows:

```
{replicate: 1, well: A01}
{replicate: 2, well: B01}
```

### 7.4.2 range

The range action gives you an integer sequence. It accepts these arguments:

- $\bullet\,$  from: the integer to start at (optional)
- till: the integer to end at (optional)
- step: the distance between generated integers (default = 1)

Here's an example:

```
a*: 2
b*: 2
c=range: {}
d=range: {from: 10, step: 10}
```

Which produces this result:

a	b	$\mathbf{c}$	d
1	1	1	10
1	2	2	20
2	1	3	30
2	2	4	40

The first range, c, just numbers all the rows starting with 1. The second range, d, starts numbering at 10 and procedes in steps of 10.

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### 7.4.3 calculate

The calculate action takes a string to be parsed by mathjs. The calculation will be made for each row individually. Here's an example:

```
a*: 3
volume=calculate: '(a * 10) ul'
more=calculate: '(50 ul) - volume'
```

And here is the result:

a	volume	more
1	10 ul	40 ul
2	20 ul	30 ul
3	30  ul	20 ul

Alternatively, the calculate action can accept parameters:

• value: the string to parse

• units: the units of the final output

```
a*: 3
volume=calculate:
  value: '(a * 10)'
  units: ul
```

With this output:

a	volume
1	10 ul
2	20 ul
3	30  ul

### 7.4.4 case

A case action takes an array of cases and tests them against each row of the table. The first case whose where statement is missing or evaluates to true will be applied. The individual case items take these arguments:

- $\bullet\,$  where an optional math js statement that will be evaluated on each row
- design a design specification that will be applied to the matching rows

Here's an example:

```
a*: 3
volumeCase=case:
    where: a < 2
    design:
     volume: 10 ul
    design:
     volume: 12354 ul</pre>
```

a	${\bf volume Case}$	volume
1	1	10 ul
2	2	12345  ul

a	volumeCase	volume
3	2	12345 ul

### 7.5 Step and data nesting

You can only load one design per step, but you can nest steps and load another design in the sub-step. Consider these two excerpts of designs:

```
data1:
    design:
        a: Alice
        b: *3
        c: Charles
        d: Daniel

data2:
    design:
        d: David
```

Let's use them in these steps:

```
1:
    data: {source: data1}
    description: "`{{a}} {{c}} {{d}}`"
1:
    data: {source: data2}
    description: "`{{a}} {{c}} {{d}}`"
```

The descriptions should be expanded as follows:

1.description: "Alice Charles Daniel" 1.1.description: "Alice Charles David"

In 1.1, "\$\$b" does not exist, but "\$a" and "\$c" still do. That is to say: column data from a previous data directive are not carried into sub-steps with a new data directive, but the values that were the same for all columns remain in scope.