McStasScript

Mads Bertelsen

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1 Introduction

This document serves as the documentation for the McStasScript scripting language for python. Its purpose is to generate McStas instrument files from python which is simply another way of writing an instrument file. The main advantages is the possibility of using for-loops and that it can be used directly from a python terminal. The simulation described by the instrument can be executed from the scripting language and the data can be manipulated before plotting.

2 Installation and configuration

Download all files from github to a directory. The configuration file is called "configuration.yaml" and needs to be updated with the paths to the local McStas installation. It is also possible to set a maximum number of characters per line used in terminal output. Below is an example of my configuration file.

```
---
paths:
    # path to mcrun, example for OS X
    mcrun_path: "/Applications/McStas-2.5.app/Contents/Resources/mcstas/2.5/bin/"
    # path to mcstas directory, example for OS X
    # the mcstas directory should contain the component folders, sources, optics, ...
    mcstas_path: "/Applications/McStas-2.5.app/Contents/Resources/mcstas/2.5/"
other:
    # limit characters per line in terminal output
    characters_per_line: 117
```

3 Importing the package

The code is structured as a python package where the classes and functions meant for the user is to be imported to the python file. In order to import the package, the downloaded directory which contains the package must be added to the path. The important classes and functions are contained in the interface package, and are called instr, plotter and functions.

```
import sys
sys.path.append('/Users/madsbertelsen/PaNOSC/McStasScript') # Path to package
from mcstasscript.interface import instr, plotter, functions
```

4 Documentation

This section describes the classes and their methods.

class McStas_instr

Holds methods for creating a McStas instrument file

Initiating an instance of the class requires a name to be given as the first argument and two optional keyword arguments currently supported, allowing information on the author an origin of the code. In the table below the positional arguments are above the dotted line and the keyword arguments are below.

input	type	explanation
first argument	string	name of the instrument
author	string	name of the author
origin	string	origin of the work
mcrun_path	string	path to local mcrun (overwrites default from config file)
mcstas_path	string	path to mcstas directory (overwrites default from config file)

Below an instance called detector will contain an instrument called "LOKI_detector" while the instance named example has a instrument named test with a specified author.

```
detector = instr.McStas_instr("LOKI_detector")
example = instr.McStas_instr("test",author="Mads Bertelsen")
```

McStas_instr method add_parameter

Adds input parameter to instrument, uses class parameter_variable

input	type	explanation
first argument (optional)	string	variable type
second argument	string	name of the parameter
value	any	default value for the parameter
comment	string	comment that will be displayed with the variable

Here four different parameters are added to the instrument file using the different allowed keywords.

```
detector.add_parameter("wavelength")
detector.add_parameter("double","height", value=1.0, comment="Height in [m]")
detector.add_parameter("string","reflection_filename", comment="Stored reflections")
detector.add_parameter("string","data_filename", value="\"data.dat\"", comment="Data")
```

The two first variables called *wavelength* and *height* are of the default type because no type was given. In McStas the default type is a double. The *height* variable was given a default value and a comment. The *refelction_filename* and *data_filename* are both specified to be strings and the latter was given a default value, note the \" needed to insert the quotation marks into strings.

McStas_instr method show_parameters

Shows currently defined parameters in the instrument

This method is useful when running the simulation to get an overview of the available instrument parameters.

```
detector.show_parameters()
        wavelength
double  height                  =  1.0          // Height in [m]
string  reflection_filename                     // Stored reflections
string  data_filename           =  "data.dat"   // Data
```

McStas_instr method add_declare_var

Adds declared variable to the instrument file

input	type	explanation
first argument	string	variable type
second argument	string	name of the parameter
value	any	value for the parameter (can be array)
array	int	length of array
comment	string	comment that will be displayed with the variable

Here four different variables are added to the instrument file using some of the different allowed keywords.

```
detector.add_declare_var("double", "energy")
detector.add_declare_var("int", "flag")
detector.add_declare_var("double", "tube_radius", value=0.013)
detector.add_declare_var("double", "displacements", array=7)
detector.add_declare_var("double", "t_array", array=4, value=[0.65E-6, 0.65E-6, 1E-6])
```

When declaring an array the array keyword must be used even when setting the values. The values are given as a python array as shown in the last example. The declared variables will appear in the declare section of the instrument file.

McStas_instr method append_initialize

Adds line of code to initialize section

This methods adds a line of text to the initialize section of the McStas file and has no keyword arguments. A similar method called append_initialize_no_new_line exists for adding to the same line with multiple calls.

```
detector.append_initialize("energy=pow(2*PI/wavelength*K2V,2)*VS2E;")
```

McStas_instr method show_components

Shows currently available McStas components

Before adding components to our instrument, it is nice to get an overview of the available components. The method show_components can be called without arguments, and will show the available categories of McStas components such as sources, optics and samples.

input	type	explanation
first argument	string	name of category to show components in

By specifying a category, the components in that category is shown.

```
detector.show_components("samples")
```

```
Here are all components in the samples category.
 Incoherent        Phonon_simple    Res_sample        Single_crystal
 Isotropic_Sqw     Powder1          Sans_spheres      TOFRes_sample
 Magnon_bcc        PowderN          SasView_model     Tunneling_sample
```

McStas_instr method component_help

Shows parameters, their defaults and an explanation for given component

input	type	explanation
first argument	string	name of component

The text is shown with some additional formatting highlighting which parameters are required and optional, along with what the default values are. This information is loaded directly from the local component file, and any component in the work directory will take priority over the standard version.

```
detector.component_help("Phonon_simple")
```

```
 ___ Help Phonon_simple ____________________________________________________
radius [m] // Outer radius of sample in (x,z) plane
yheight [m] // Height of sample in y direction
sigma_abs [barns] // Absorption cross section at 2200 m/s per atom
sigma_inc [barns] // Incoherent scattering cross section per atom
a [AA] // fcc Lattice constant
b [fm] // Scattering length
M [a.u.] // Atomic mass
c [meV/AA^(-1)] // Velocity of sound
DW [1] // Debye-Waller factor
T [K] // Temperature
target_x = 0 [m] // position of target to focus at . Transverse coordinate
target_y = 0 [m] // position of target to focus at. Vertical coordinate
target_z = 0 [m] // position of target to focus at. Straight ahead.
target_index = 0 [1] // relative index of component to focus at, e.g. next is +1
focus_r = 0 [m] // Radius of sphere containing target.
focus_xw = 0 [m] // horiz. dimension of a rectangular area
focus_yh = 0 [m] // vert.  dimension of a rectangular area
focus_aw = 0 [deg] // horiz. angular dimension of a rectangular area
focus_ah = 0 [deg] // vert.  angular dimension of a rectangular area
gap = 0 [meV] // Bandgap energy (unphysical)
_____________________________________________________________________________
```

McStas_instr method add_component

Method for adding a new component to the instrument file

A McStas component describes a part of the instrument including its position and rotation in space. When adding a new component in McStasScript the name and type must be specified. The add_component method returns the appropriate component object that can be manipulated directly, but it is also possible to manipulate through methods in McStas_Instr. Most commonly a component is added to the end of an instrument file, but the keyword arguments *before* or *after* can be used to place the component before/after a previously specified component. All component classes are dynamically generated based on components in your local McStas installation and in the python work directory, and in this way have all input parameters as class atributes.

input	type	explanation
first argument	string	name of the component instance
second argument	string	name of the component to use
AT	float list[3]	position in (x,y,z)
AT_RELATIVE	string	name of earlier component used as reference for position
ROTATED	float list[3]	rotation around (x,y,z)
ROTATED_RELATIVE	string	name of earlier component used as reference for rotation
RELATIVE	string	name of earlier component used as reference
before	string	name of component this component should be before
after	string	name of component this component should be after
WHEN	string	WHEN statement (McStas keyword)
EXTEND	string	EXTEND c code (McStas keyword)
GROUP	string	GROUP name (McStas keyword)
JUMP	string	JUMP string (McStas keyword)
comment	string	comment that will be displayed with the variable

A component in McStas needs a name, which is the first argument. The second argument select what component should be used from the component library. Below are some examples of simple use.

```
detector.add_component("Origin","Arm")
src = detector.add_component("source", "Source_simple", RELATIVE="Origin")
detector.add_component("beam_extraction", "Guide_gravity",
                       AT=[0,0,2], RELATIVE="source")
```

Here src would by a python object that can be modified to change the source. If one wishes to insert another component between the source and beam_extraction it can be done with the *before* or *after* keyword.

```
detector.add_component("pre_guide_slit", "Slit", before="beam_extraction",
                       AT=[0,0,1], RELATIVE="source", comment="Slit before the guide")
```

McStas_instr method print_components

Method for printing current list of components to the terminal

To check that the components defined in the documentation so far are in the expected order, the print_components method is demonstrated. Data on the rotation of components is normally included but is omited here. This method has no arguments.

```
detector.print_components()
Origin              Arm              AT  [0, 0, 0]    ABSOLUTE
source              Source_simple    AT  [0, 0, 0]    RELATIVE Origin
pre_guide_slit      Slit             AT  [0, 0, 1]    RELATIVE Origin
beam_extraction     Guide_gravity    AT  [0, 0, 2]    RELATIVE source
```

McStas_instr method set_component_parameter

Method for setting parameters of a component using a dictionary

This methods sets the parameters of a defined component using a python dictionary.

input	type	explanation
first argument	string	name of the component instance to modify
second argument	dict	dictionary with parameter names and values

It is possible to add several parameters in one call, and new calls add further parameters.

```
detector.set_component_parameter("source", {"xwidth" : 0.12, "E0" : "energy"})
detector.set_component_parameter("source", {"yheight" : 0.12})
```

An error will occur if the given parameter name does not match a parameter in the component type.

McStas_instr method print_component

Method for printing information contained in defined component

This method takes the name of a component and prints the current information. We can check that the parameters and position of a component has been registered correctly.

```
detector.print_component("source")

COMPONENT source = Source_simple
  yheight = 0.12 [m]
  xwidth = 0.12 [m]
  E0 = energy [meV]
AT [0, 0, 0] RELATIVE Origin
ROTATED [0, 0, 0] RELATIVE Origin
```

This is not intended for copy-pasting into McStas instruments as the syntax is not correct. Generation of the instrument file is covered later in the documentation. The units are collected from the header file of the component definition. If a required parameter has not yet been specified, the user will be reminded when using this method.

McStas_instr method set_component_AT

Method for updating position of a component

There are a range of methods for updating information on a component after it has been defined. The syntax is similar to the original call for add_component in all cases.

input	type	explanation
first argument	string	name of component to modify
first argument	float list[3]	position in (x,y,z)
RELATIVE	string	name of earlier component used as reference for position

```
detector.set_component_AT("source", [0.01,0,0])
```

McStas_instr method set_component_ROTATED

Method for updating rotation of a component

input	type	explanation
first argument	string	name of component to modify
first argument	float list[3]	rotation around (x,y,z)
RELATIVE	string	name of earlier component used as reference for rotation

```
detector.set_component_ROTATED("beam_extraction", [0,2.0,0], RELATIVE="Origin")
```

McStas_instr method set_component_RELATIVE

Method for updating RELATIVE reference for both position and rotation

This method will override both positional relative and rotational relative. It has no keyword arguments.

```
detector.set_component_RELATIVE("beam_extraction", "pre_guide_slit")
```

After these updates the output from print_components is shown again to see the changes.

```
Origin              Arm              AT   [0, 0, 0]          ABSOLUTE
source              Source_simple    AT   [0.01, 0, 0]       RELATIVE Origin
pre_guide_slit      Slit             AT   [0, 0, 1]          RELATIVE Origin
beam_extraction     Guide_gravity    AT   [0, 0, 2]          RELATIVE pre_guide_slit
```

```
Origin              Arm              ROTATED  [0, 0, 0]          ABSOLUTE
source              Source_simple    ROTATED  [0, 0, 0]          RELATIVE Origin
pre_guide_slit      Slit             ROTATED  [0, 0, 0]          RELATIVE Origin
beam_extraction     Guide_gravity    ROTATED  [0, 2.0, 0]        RELATIVE pre_guide_slit
```

McStas_instr method set_component_WHEN

Method for setting WHEN condition on component

The input for this method is a string, which should be a c logical expression involving variables defined in declare and the state parameters of the neutron.

```
detector.set_component_WHEN("beam_extraction", "vx > 0")
```

McStas_instr method append_component_EXTEND

Method for adding a line to the extend section of a component

The EXTEND section adds additional code to a McStas component and its scope includes variables declared in the instrument file and the component. The number of scattering events in a component can for example be saved to an external parameter using the SCATTERED keyword. Two events are subtracted since entering and leaving the guide counts as a scattering event.

```
detector.append_component_EXTEND("beam_extraction", "n_scattering = SCATTERED - 2")
```

McStas_instr method set_component_GROUP

Method for setting GROUP name of a component

The GROUP keyword is used to make a number of components parallel in the execution, however the order still matters. Could for example be used if several guides were simulated after the source, and each of these would be in the same group.

```
detector.set_component_GROUP("beam_extraction", "guides")
```

McStas_instr method set_component_JUMP

Method for setting JUMP statement of a component

The JUMP keyword is an advanced feature of McStas that is similar to a goto. The string given to the method should contain everything after JUMP in the McStas keyword line, so for example with the syntax below. Here there is no point in iterating over a guide, and merly shows the syntax.

```
detector.set_component_JUMP("beam_extraction", "myself iterate 3")
```

McStas_instr method set_component_comment

Method for updating the comment on a component

It is also possible to add a comment to a component after it was defined.

McStas_instr method set_component_comment

Method for updating the comment on a component

It is also possible to add a comment to a component after it was defined.

```
detector.set_component_comment("beam_extraction", "Simulating severe misalignment")
detector.print_component("beam_extraction")
// Simulating severe misalignment
COMPONENT beam_extraction = Guide_gravity
AT [0, 0, 2] RELATIVE pre_guide_slit
ROTATED [0, 2.0, 0] RELATIVE pre_guide_slit
```

McStas_instr method write_c_files

Methods for writing c files to folder named generated_includes

This method will write c files describing the declare, initialize and trace sections of the generated instrument.

```
detector.write_c_files()
```

These can then be included in another McStas file. This is useful as this python tool is most often used to generate large repeating part of an instrument that can then be included in a regular instrument file. The instrument file can include them using the %include keyword from McStas as shown below.

```
DECLARE
%{
// include parameters declared from generate_LOKI_parts.py
%include "generated_includes/LOKI_detector_declare.c"
%}

INITIALIZE
%{
// include initialization code from generate_LOKI_parts.py
%include "generated_includes/LOKI_detector_initialize.c"
%}

TRACE
// include components from generate_LOKI_parts.py
%include "generated_includes/LOKI_detector_component_trace.c"
```

McStas_instr method write_full_instrument

Writes the full instrument file with name defined in original McStas_instr call

This method instead writes the entire instrument file using the provided information.

```
detector.write_full_instrument()
```

McStas_instr method run_full_instrument

Runs McStas simulation of defined instrument and returns array of McStasData objects

This methods runs the simulation using the mcrun commands of the system and returns the resulting data as a array of McStasData objects. Normally an error will occur if the fodldername already exists, but using the increment_folder_name keyword parameter the foldername can be updated automatically to avoid this.

input	type	explanation
foldername	string	name of folder that will be created for data
parameters	dict	dictionary with input parameters and their values
ncount	int	number of rays to simulate
mpi	int	number of mpi threads to use for simulation
custom_flags	string	custom mcstas flags added to mcrun launch command
mcrun_path	string	absolute path to mcrun (overwrites path from config file)
increment_folder_name	bool	if true, increments data folder name automatically

```
data = detector.run_full_instrument(foldername="data1",
                                    parameters= {"wavelength":5.1},
                                    ncount=1E7, mpi=2)
```

class McStasData

Holds a single McStas data set in either 1D or 2D

A class to handle data from McStas simulations in a transparent way which provides easy access to manipulation of the data. The included data is located in the following variables

variable	type	explanation
Intensity	float array	numpy array containing intensity
Error	float array	numpy array containing error on intensity
Ncount	int array	numpy array containing number of rays in each pixel
xaxis	float array	numpy array of xaxis if data is one dimensional
metadata	metadata class	contains necessary meta data
plot_options	plot_options class	preferences for plotting the data

McStasData method set_xlabel

Sets the xlabel of a data set

Method for setting xlabel on a data set, similar methods exists for ylabel and title with same syntax.

```
data[0].set_xlabel("custom xlabel [m]")
```

McStasData method set_plot_options

Sets plotting preferences for data set

Plotting options are associated with the data set instead of being given during the plotting. All plot options are given as a dictionary input. Currently the following are available.

name	type	explanation
log	bool or int	plot on logarithmic scale
orders_of_mag	float	maximum orders of magnitude for colorscale
colormap	string	name of colormap to be used
cut_max	float	cut top of data, 1 is all data
cut_min	float	cut bottom of data, 1 is all data
left_lim	float	lower limit of plot
right_lim	float	higher limit of plot
top_lim	float	top limit (Only 2D)
bottom_lim	float	bottom limit (Only 2D)
x_axis_multiplier	float	Multiplier for xaxis, for example change unit
y_axis_multiplier	float	Multiplier for yaxis, for example change unit

```
data[0].set_plot_options(log=True, colormap="hot")
```

It is often simpler to access the data using the name of the monitor rather than the index, which can be done using the function name_search.

```
PSD_sample = functions.name_search("PSD_sample", data)
PSD_sample.set_plot_options(log=True, colormap="hot")
```

Since setting the plot options will be a very frequent operation, a function is provided for this particular operation.

```
functions.name_plot_options("PSD_sample", data, log=True, colormap="hot")
```

In most circumstances McStasData objects will be returned from simulations performed with McStasScript, but it is possible to load a data folder that contains a mccode.sim file and the associated data. The returned data is a list of McStasData objects.

```
data = functions.load_data("data_folder_name")
```

class make_plot

plots single McStasData object or an array of these

Class for simple plotting of McStasData objects. Will be expanded over time to contain more control over the resulting plots. Currently only the initialization is done so the returned object has no useful methods.

input	type	explanation
first argument	McStasData array	data to be plotted

Here all data in the array data is plotted according to the preferences stored in the plot_options class of each data set.

```
plot = plotter.make_plot(data)
```

class make_sub_plot

plots single McStasData object or an array of these as subplots

Class for simple plotting of McStasData objects in one window. Will be expanded over time to contain more control over the resulting plots. Currently only the initialization is done so the returned object has no useful methods.

input	type	explanation
first argument	McStasData array	data to be plotted

Here all data in the array data is plotted according to the preferences stored in the plot_options class of each data set.

```
plot = plotter.make_sub_plot(data, log=[1,0,1], max_orders_of_mag=[10,2,4])
```

4.1 Advanced use

The parts of the api covered by the documentation so far is the simplest way of using the API, but some additional methods in the McStas_instr are useful for experienced python users that want more direct access to the underlying classes.

McStas_instr method get_component

Returns the component class instance of a selected component

It is possible to get direct access to the component instances inside the McStas_instr instance for direct manipulation. This can make the syntax a bit shorter in some cases.

```
guide_piece = detector.get_component("beam_extraction")
```

McStas_instr method get_last_component

Returns the component class instance of the last component in the component sequence

Same as *get_component* but no argument is needed when returning the last component of the sequence.

```
guide_piece = detector.get_last_component()
```

class component

Holds information on a component and methods for updates and writing to file

The component class is used as a superclass for each component type added to the instrument. The subclass for a specific component type also includes attributes for each parameter of the component, and these can be changed directly. The class is frozen after initialize so no new attributes can be created, and in this way misspelled parameter names are caught on user input. Most of the methods contain in the component class are just passed directly to the McStas_instr and thus does not require further explanation, they are however listed here for completeness.

component method show_parameters

Equivalent to component_help in McStas_instr, also shows changed parameters

component method show_parameters_simple

Same information as show_parameters, but without use of ANSI colors

component method set_AT

Equivalent to set_component_AT in McStas_instr

component method set_ROTATED

Equivalent to set_component_ROTATED in McStas_instr

component method set_RELATIVE

Equivalent to set_component_RELATIVE in McStas_instr

component method set_parameters

Equivalent to set_component_parameter in McStas_instr

component method set_comment

Equivalent to set_component_comment in McStas_instr

component method _freeze

Freezes the object, an error will occur if new attributes are added

component method _unfreeze

Unfreezes the object, new attributes can be added

component method write_component

Writes the component to file

input	type	explanation
first argument	file identifier	file identifier ready for writing

component method print_long

Prints information on the component to the terminal

5 Discussion

This section contains discussion on the python module.

5.1 Possible improvements / requests

Features that are still missing and should be added. Also keeps track of user requests.

5.1.1 Add code to trace

It should be possible to add code directly to trace, for example include statements. The position of this code should be relative to components.

5.1.2 FINALLY

Should be possible to add code to the FINALLY section which is ignored so far.

5.1.3 Limits on parameters

Allow user to easily set limits on parameters and generate appropriate input sanitation for instrument file with error message.

5.1.4 Methods for removing parameters / variables / components

When using the software from a terminal it could be useful to remove components. Might also be useful to be able to move a component to another location in the sequence.

5.2 Jupyter notebook experience

It is entirely possible to write an instrument file from a jupyter notebook using this tool, but at this point it behaves more like a script, and thus there is no inherent benefit. The main issue is that rerunning a cell will cause errors because the same components are added again, and they recognize the names are not unique. Should instead allow to update components when the same name is used, but this adds a severe risk of users replacing an earlier component instead of creating a new.

Another issue is the lack of feedback beyond printing all added components. A simple improvement would be to have a method that prints all changes since last print was executed, which would be a natural end of each cell.