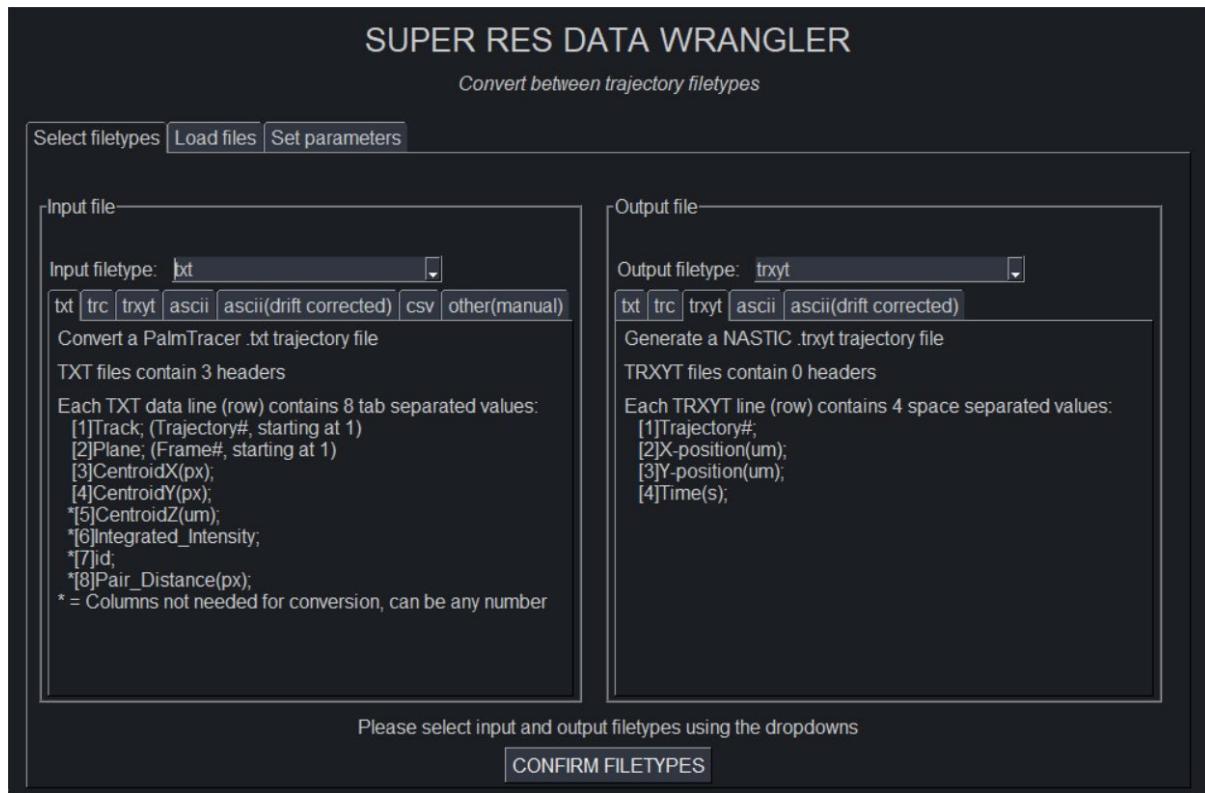


SUPER RES DATA WRANGLER (GUI)

USER MANUAL

This user manual is for the graphical user interface (GUI) version.

For information on how to use the command line (CLI) version, please refer to the Super Res Data Wrangler (CLI) User Manual.



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Introduction

Meunier lab super resolution data analysis pipeline:

Super resolution data analysis often requires the sequential use of different analysis software, with each performing a different role.

Our lab uses either PalmTracer or TrackMate to first locate single particle centroids in each frame (localisation) and subsequently connect these centroids together to form trajectories (tracking), prior to drift correction in SharpViSu and cluster analysis in NASTIC, segNASTIC or BOOSH, followed by meta-analysis of the clustering results in NASTIC Wrangler.

Each of these steps in the super resolution analysis pipeline requires different input filetypes and produce different output filetypes.

Table 1: Analysis software that make up the super-resolution analysis pipeline used in the Meunier lab, with input and output filetypes shown for each.

Analysis software	Input filetype	Output filetype
Step 1: Localisation and Tracking		
PalmTracer (Metamorph plugin)	Mutliframe time-lapse acquisition (e.g., .czi, .tif)	.txt .trc
TrackMate (FIJI plugin)	Mutliframe time-lapse acquisition (e.g., .czi, .tif)	.csv
Step 2: Drift correction		
SharpViSu	.ascii .id (uncorrected)	.ascii .id (drift corrected)
Step 3: Cluster analysis		
NASTIC, segNASTIC and BOOSH	.trxyt	metrics.tsv
Step 4: Meta analysis of clustering data		
NASTIC Wrangler	metrics.tsv	processed_metrics.tsv

Super Res Data Wrangler GUI:

The purpose of the Super Res Data Wrangler GUI is to bridge the gaps between the software used in this super-resolution analysis pipeline by enabling the conversion between the different trajectory filetypes.

Input filetypes that can be converted:

There are currently 6 different input filetypes (using preset input filetype parameters) to select from:

- .txt (PalmTracer)
- .trc (PalmTracer)
- .trxyt (NASTIC, segNASTIC, BOOSH)
- .ascii (SharpViSu)
- .ascii (drift corrected) (SharpViSu)
- .csv (TrackMate) (TrackMate)

Additionally, there is an option to manually set the parameters of the input file in order to convert from a much wider range of trajectory filetypes:

- Other (manual input) (Trajectory files produced by other software)

Output filetypes that can be generated:

Each of the above input filetypes can be converted to following 5 output filetypes:

- .txt (PalmTracer)
- .trc (PalmTracer)
- .trxyt (NASTIC, segNASTIC, BOOSH)
- .ascii (SharpViSu)
- .ascii (drift corrected) (SharpViSu)

See Appendix 1 for detailed information on each trajectory filetype.

Parameters

The Super Res Data Wrangler GUI uses several parameters to convert files from one filetype to another filetype. See Appendix 2 for detailed information on each parameter.

Table 2: parameters used by the Super Res Data Wrangler GUI.

Parameter	Description	Options / user input
Spatial and temporal information		
X,Y units	Spatial units of the trajectory x,y co-ordinates	px (pixels) um (micrometers) nm (nanometers)
Pixel size (px/um)	Used to convert between different spatial units	Numerical input by user (appears if required)
Time units	Temporal units of the trajectory data	Frames (frame number) s (seconds)
Acquisition frequency (Hz)	Used to convert between different time units	Numerical input by user (appears if required)
File structure		
Number of headers	Number of headers (rows) before the data rows start	Number between 0 and 10
Delimiter	Character that separates the data into columns	Comma, tab, 1 space, 2 spaces, 3 spaces, 4 spaces, semicolon
Column numbering		
Trajectory col	Number of the column that contains Trajectory # data	Number between 1 and 30
X-position col	Number of the column that contains X-position data	Number between 1 and 30
Y-position col	Number of the column that contains Y-position data	Number between 1 and 30
Frame/Time col	Number of the column that contains Time data	Number between 1 and 30
Starting frame	Number of first Frame	0 or 1 (appears if required)

Computer requirements

The NASTIC suite (which includes the Super Res Data Wrangler GUI) consists of Python scripts that require Python 3.8 or later, and a number of Python modules to run. Python is available for most computer platforms so you can run it on Windows, Linux and Mac. It will not run on the older version of Python 2.7 which is still lingering on a lot of computer systems. You are strongly encouraged to either visit <https://www.python.org> and download and install the latest version. You will also need to install a number of Python modules, which is simple to do from a command line:

```
python -m pip install freesimplegui colorama scipy numpy scikit-learn pillow
```

```
C:\Users\uqamcc11>python -m pip install freesimplegui colorama scipy numpy scikit-learn pillow
```

At the time of writing, we used the below Python module versions:

freesimplegui	v5.2.0.post1
colorama	v0.4.6
scipy	v1.13.1
numpy	v1.23.2
scikit-learn	v1.1.2
pillow	v9.2.0

If you are having problems, you can try installing the specific versions that we used. To do this, open a new instance of the command line and copy-paste in the following:

```
python -m pip install freesimplegui==5.2.0.post1 colorama==0.4.6 scipy==1.13.1 numpy==1.23.2 scikit-learn==1.1.2 pillow==9.2.0
```

```
C:\Users\uqamcc11>python -m pip install freesimplegui==5.2.0.post1 colorama==0.4.6 scipy==1.13.1 numpy==1.23.2 scikit-learn==1.1.2 pillow==9.2.0
```

Updates

The Super Res Data Wrangler GUI along with other NASTIC family members is periodically updated with new functionalities.

Check the GitHub for updates using this link:

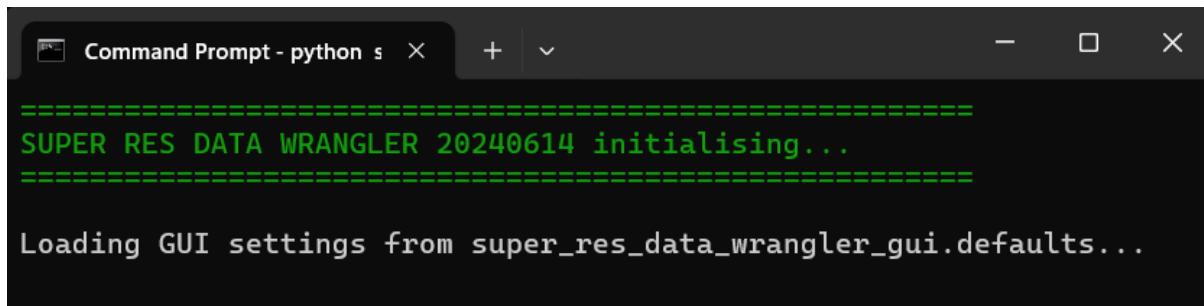
https://github.com/tristanwallis/smlm_clustering/releases

Running the Super Res Data Wrangler GUI

Step 1 – run the script

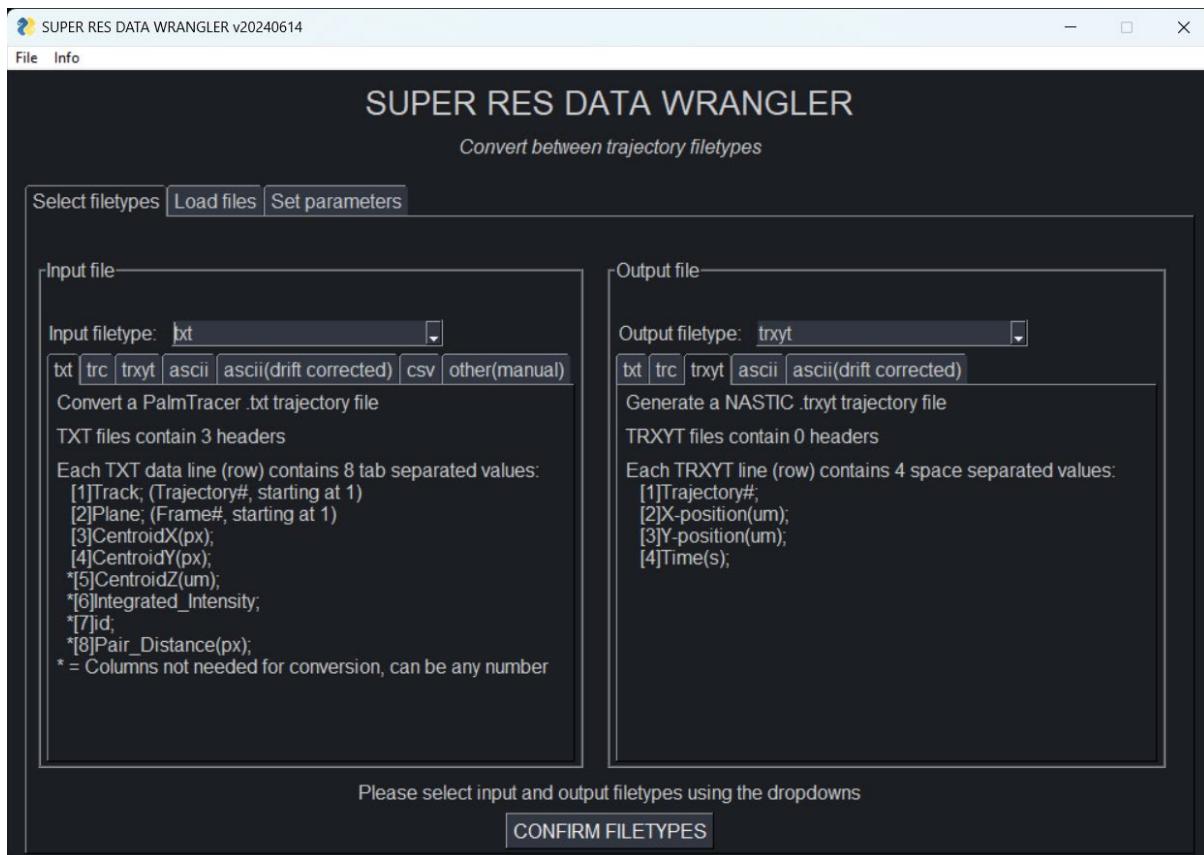
If all is installed properly then double clicking the super_res_data_wrangler_GUI.py icon will launch a console, followed shortly after by the GUI.

Console:



```
Command Prompt - python s  X  +  ▾
=====
SUPER RES DATA WRANGLER 20240614 initialising...
=====
Loading GUI settings from super_res_data_wrangler_gui.defaults...
```

Graphical user interface (GUI):



Alternatively, the Super Res Data Wrangler GUI can be opened using the command line by navigating to the location of the Super_Res_Data_Wrangler_GUI.py script and typing the below followed by the return key:

```
python super_res_data_wrangler_gui.py
```

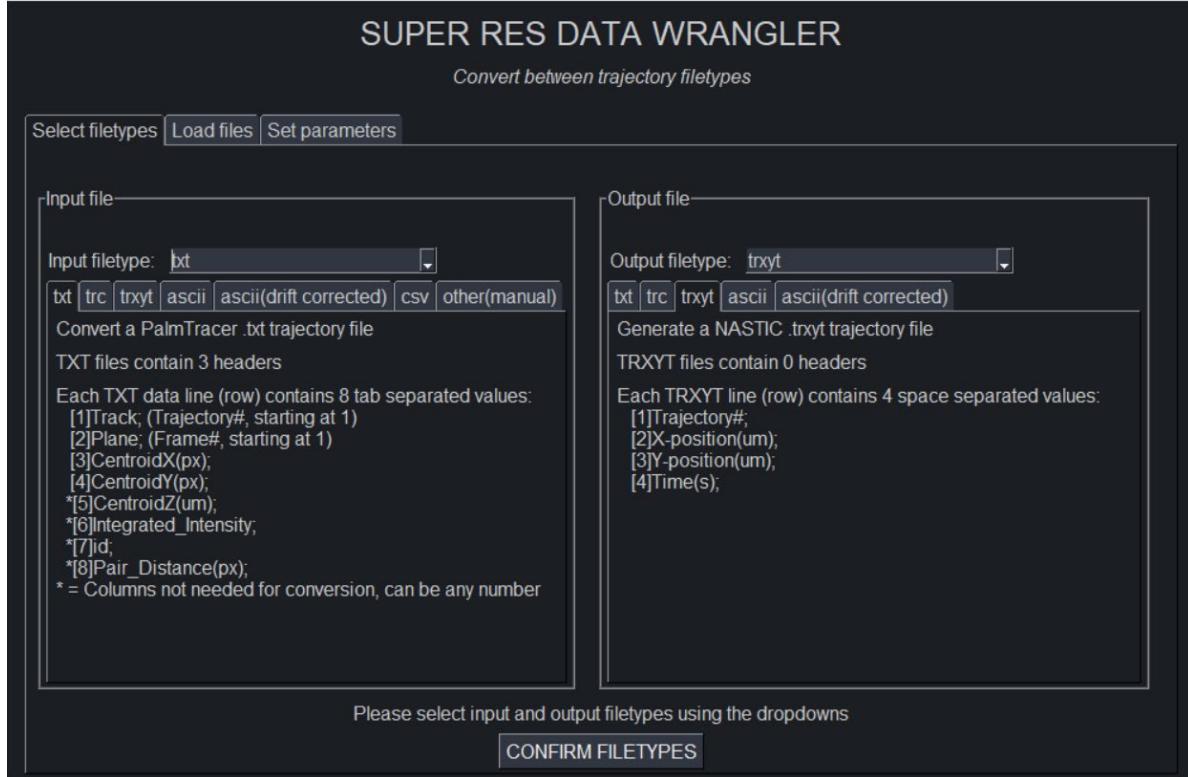
The GUI is divided into three functional tabs, which it will automatically switch to as appropriate:

- **Select filetypes:** select the filetype that you wish to convert from (input file), and the filetype that you wish to convert to (output file).
- **Load files:** search for and select a single file to convert, or search for a folder containing multiple files and select which ones to include in the file conversion.
- **Set parameters:** select the parameters corresponding to the input file.

Select filetypes Tab

This tab enables the user to select the filetype they wish to convert FROM (input filetype), and the filetype they wish to convert TO (output filetype).

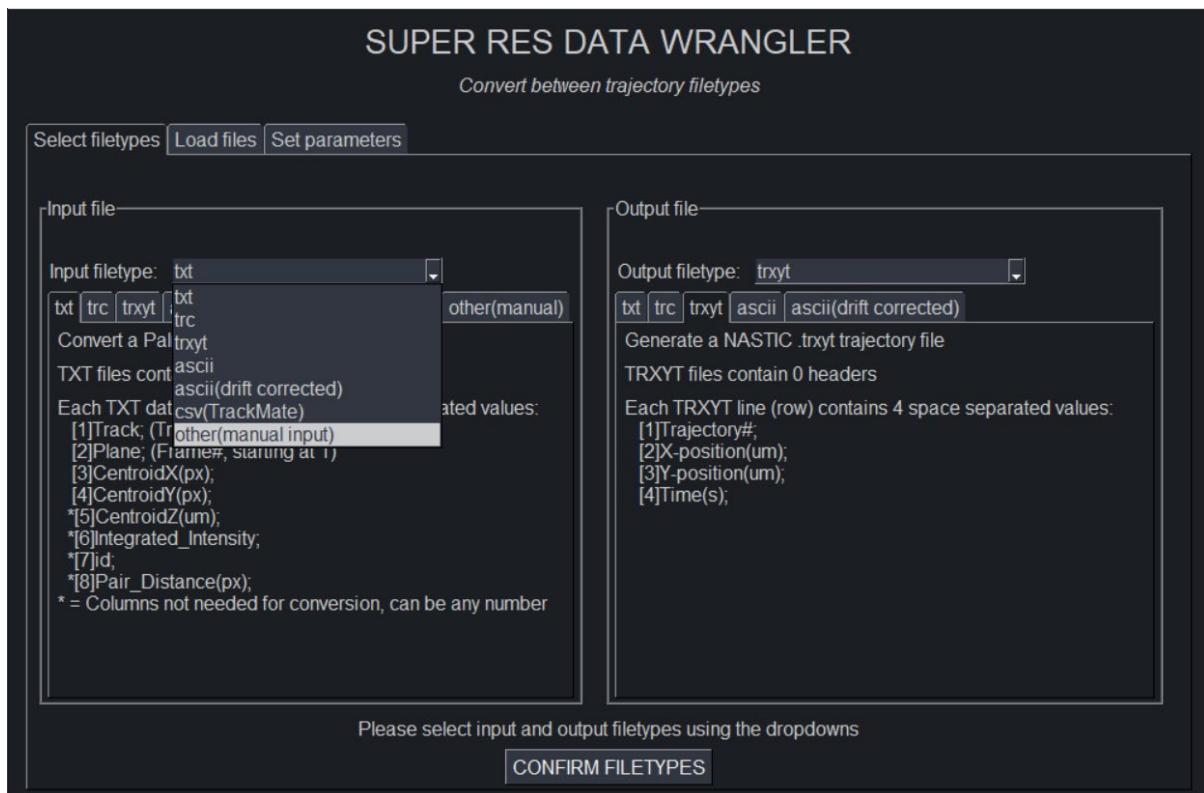
Upon launching the program, the ‘Select filetypes’ tab will be displayed:



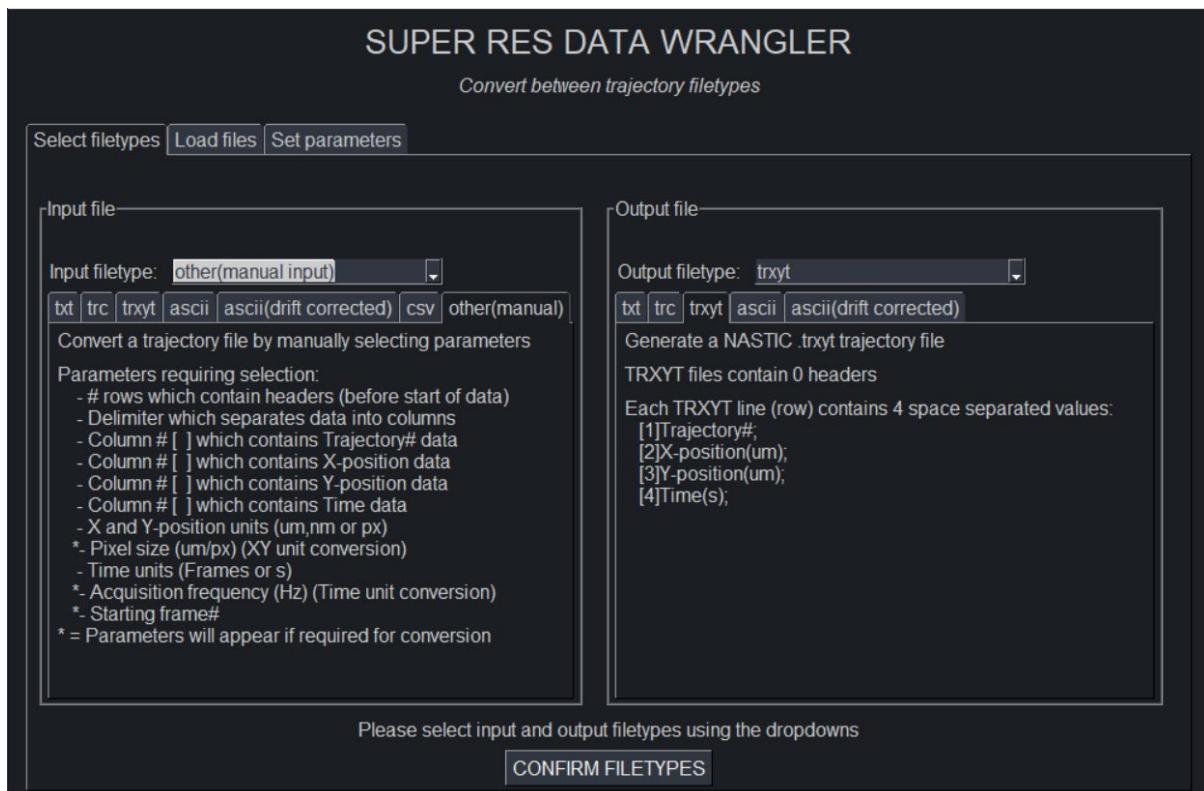
It is divided into two main sections, ‘Input file’ on the left, and ‘Output file’ on the right. Within each of these two sections are subtabs containing information for each of the filetypes that can be selected (e.g., ‘txt’, ‘trc’, ‘trxyt’, ‘ascii’, ‘ascii(drift corrected)’, ‘csv’ and ‘other(manual)’). This allows the user to easily see the requirements of the selected input file on the left, and the format of the output file that will be generated on the right.

Step 2 – select the input filetype:

To change the input filetype, click on the downward arrow of the dropdown box next to “Input filetype:” and select the desired filetype you wish to convert FROM:

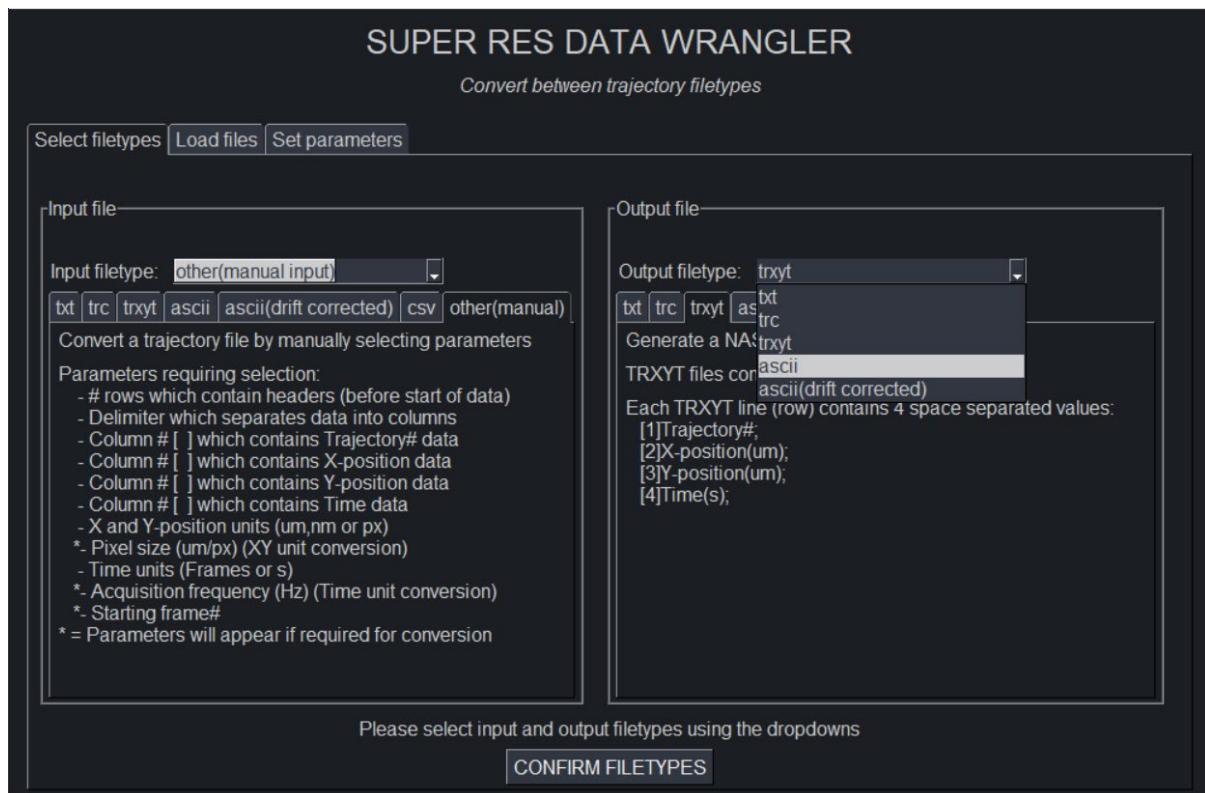


This will automatically swap to the selected input filetype subtab and display the information about that filetype:

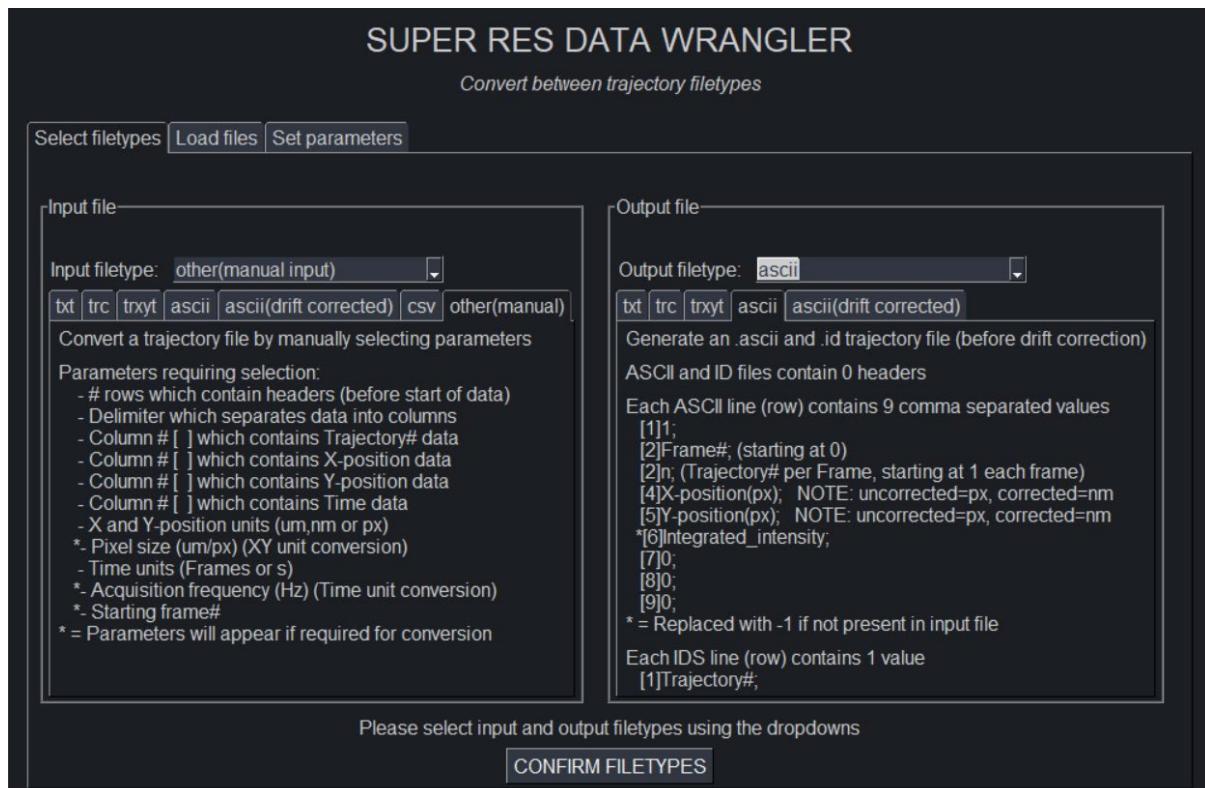


Step 3 – select the output filetype:

To change the output filetype, click on the dropdown box next to “Output filetype:” and select the desired filetype you wish to convert TO:

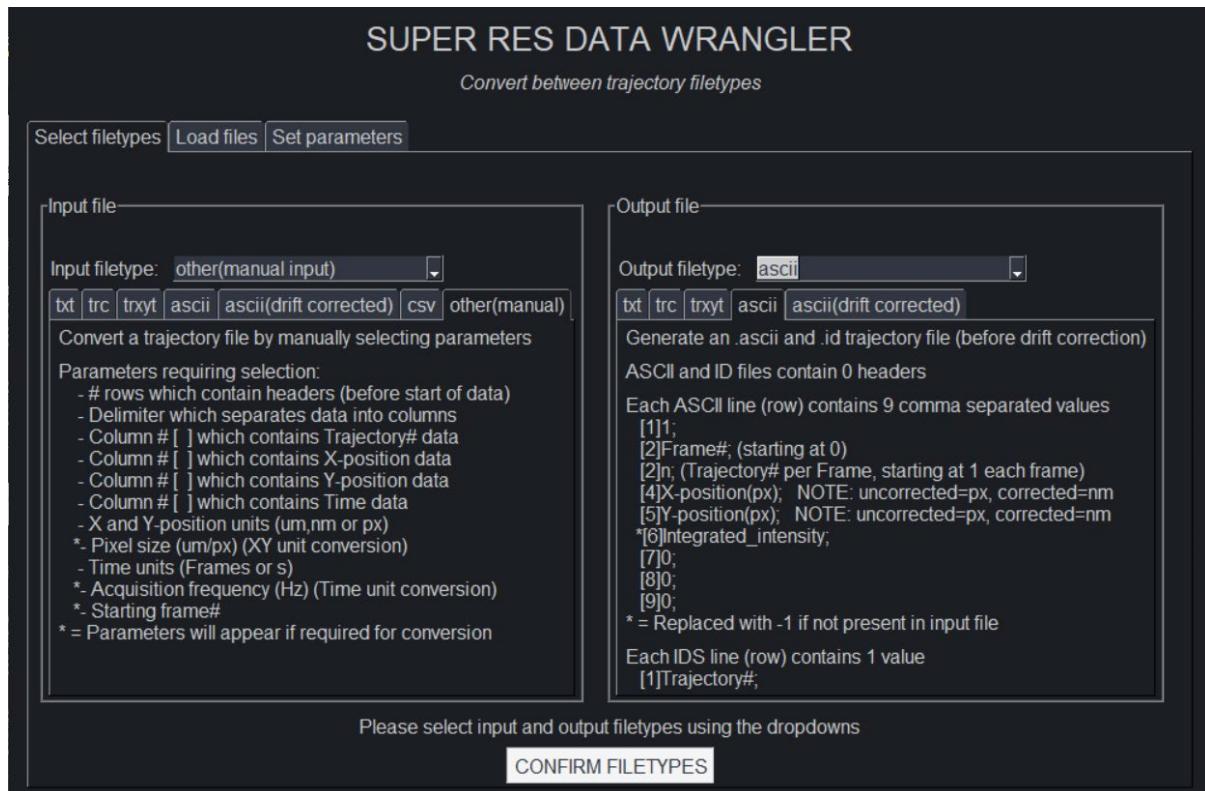


This will automatically swap to the selected output filetype subtab showing information about that filetype:



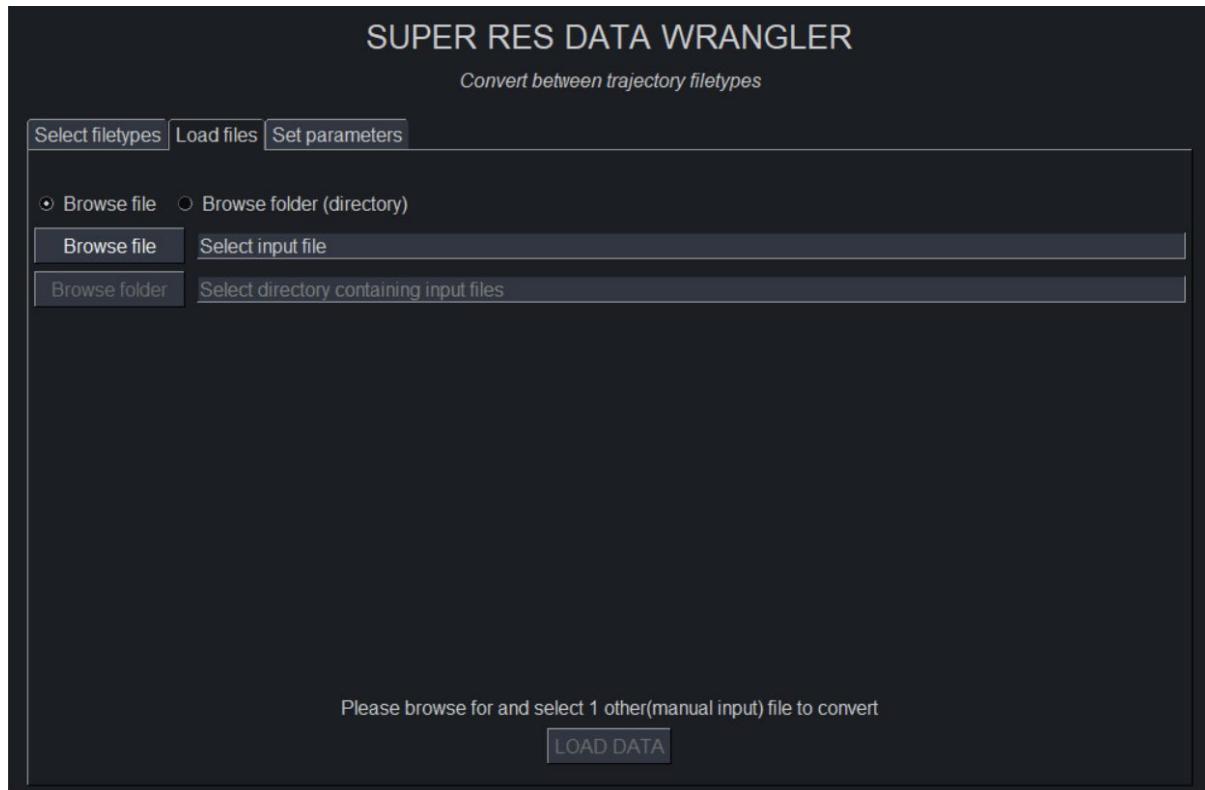
Step 4 – confirm filetype selection

Once the desired input and output filetypes have been selected, press the ‘CONFIRM FILETYPES’ button at the bottom on the GUI. If the selected input and output filetypes are different, this will automatically swap the GUI to the next tab (‘Load files’ tab). Otherwise, an error message will be displayed asking the user to make sure that the input filetype is different to the output filetype.



Load files Tab

This tab enables the user to browse for and select either a single trajectory file, or a folder containing multiple trajectory files to convert.



Step 5 – Select the browse method:

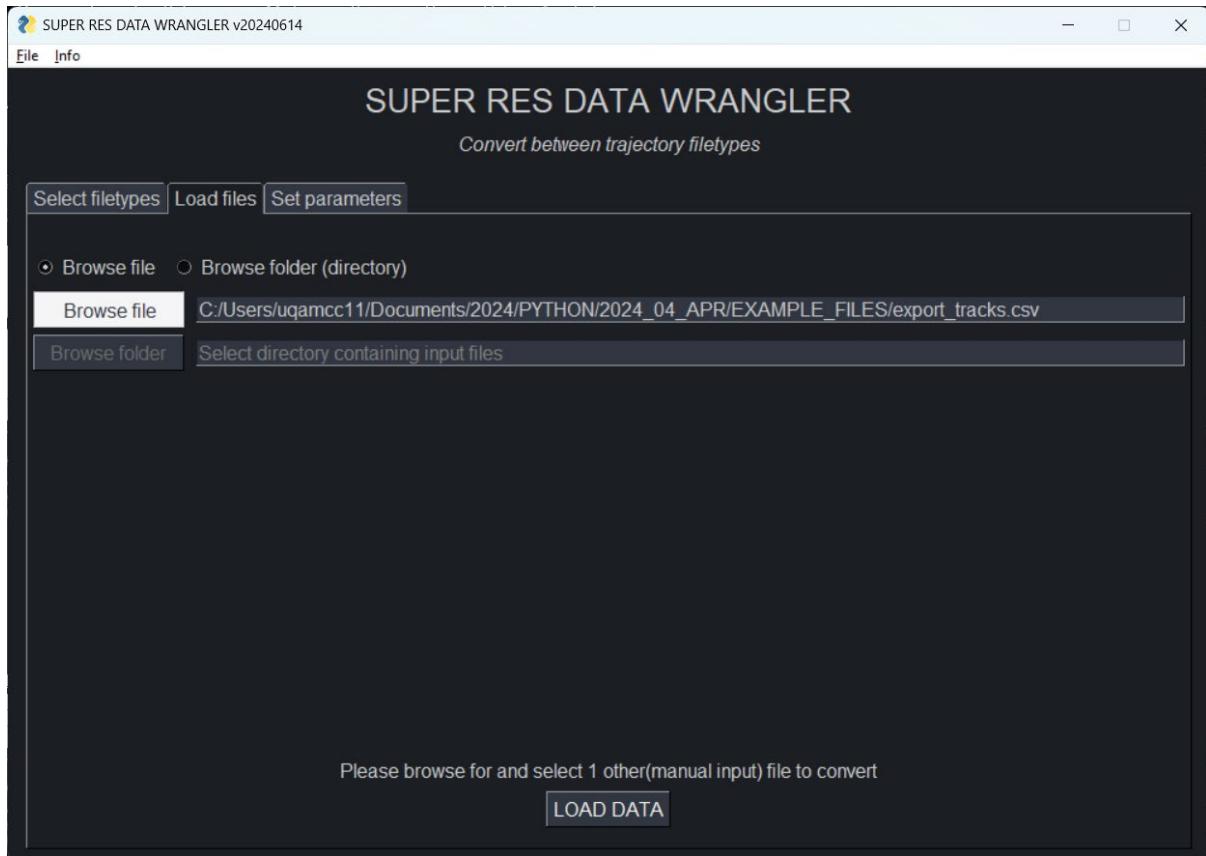
Select whether you wish to load a single trajectory file (click on the 'Browse file' radio option) or multiple files (click on the 'Browse folder (directory)' option).

Step 6 – Browse for the trajectory file/folder containing trajectory files:

Option 1 – 'Browse file' option:

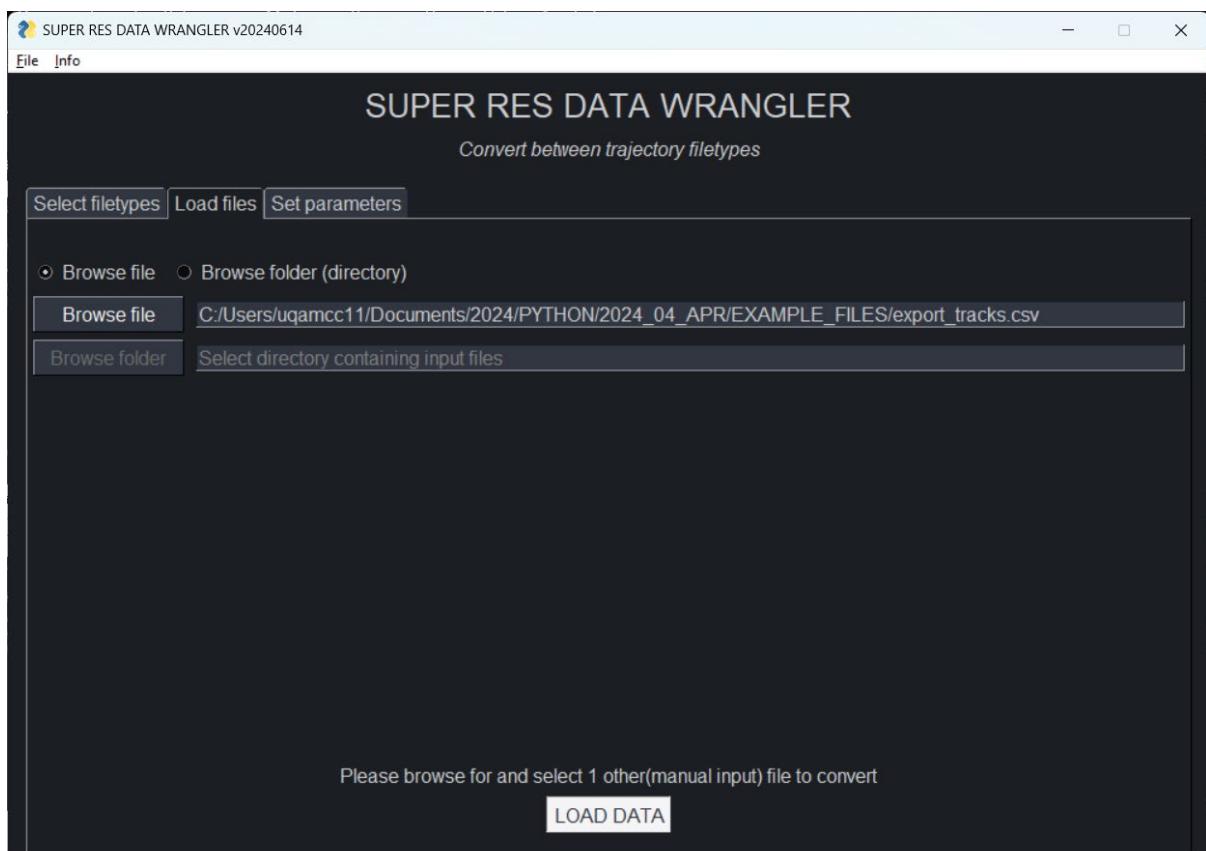
Step 6.1 – Browse for a single trajectory file:

Press the 'Browse file' button on the left of the 'Select input file' textbox to browse for and select the trajectory file that you wish to convert. This will open up a browse window showing the files (with the relevant extension) within the current directory. Click on the desired trajectory file to select it, then press the 'Open' button to confirm the selection.

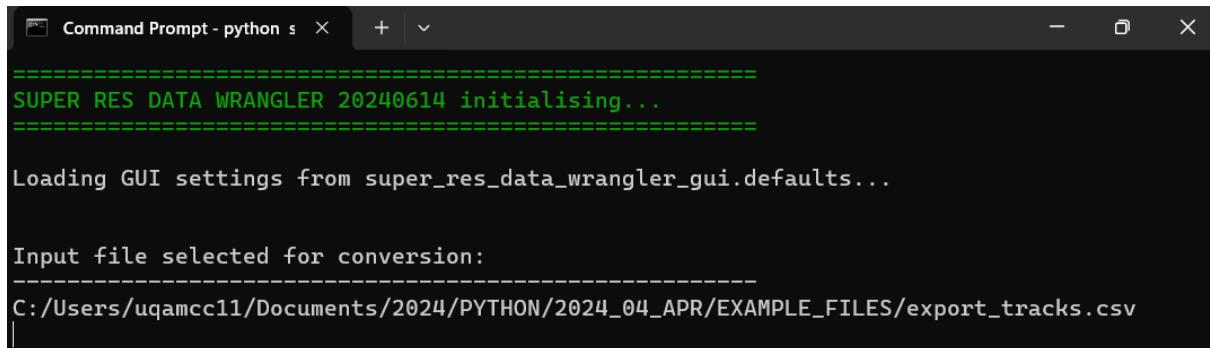


Step 6.2 – Confirm input file selection:

Press the 'LOAD DATA' button to confirm the file that was selected for conversion.



The filename of the file that was selected for conversion will be displayed in the text console, and the GUI will automatically swap the GUI to the 'Set parameters' tab.

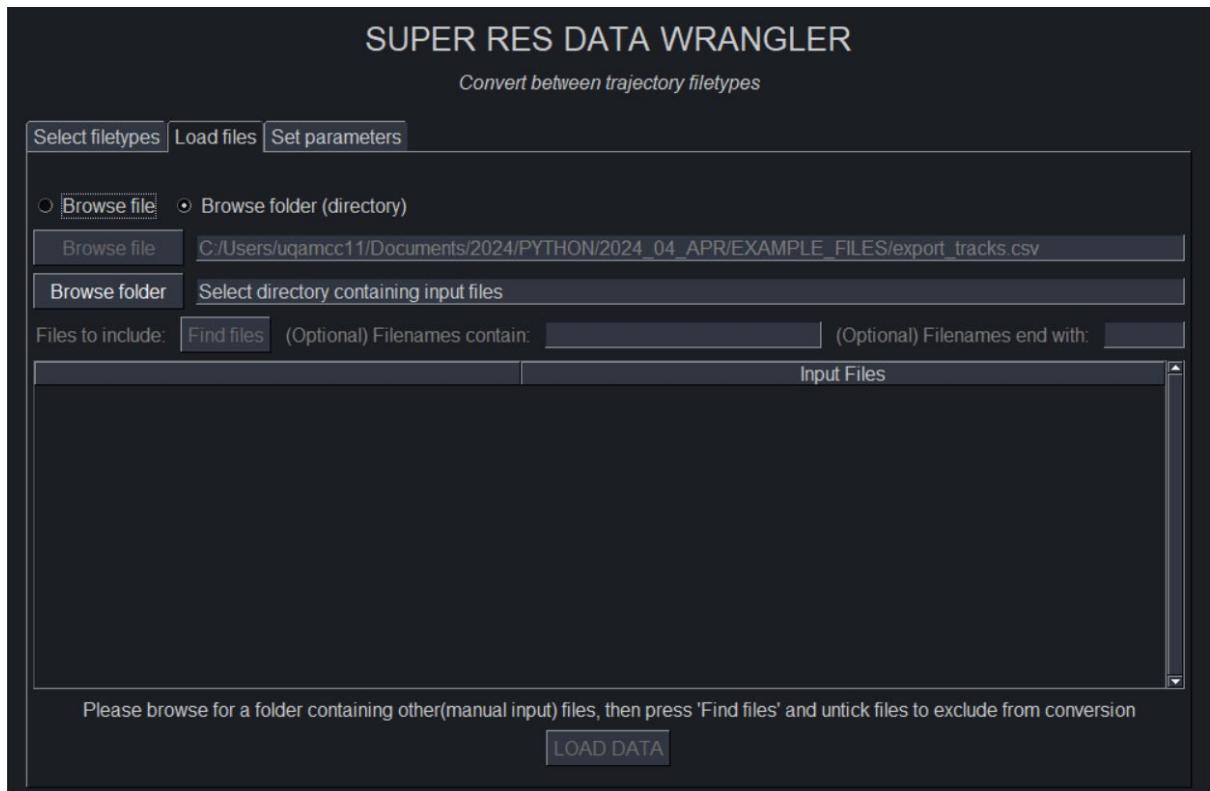


```
=====  
SUPER RES DATA WRANGLER 20240614 initialising...  
=====  
Loading GUI settings from super_res_data_wrangler_gui.defaults...  
  
Input file selected for conversion:  
-----  
C:/Users/uqamcc11/Documents/2024/PYTHON/2024_04_APRA/EXAMPLE_FILES/export_tracks.csv
```

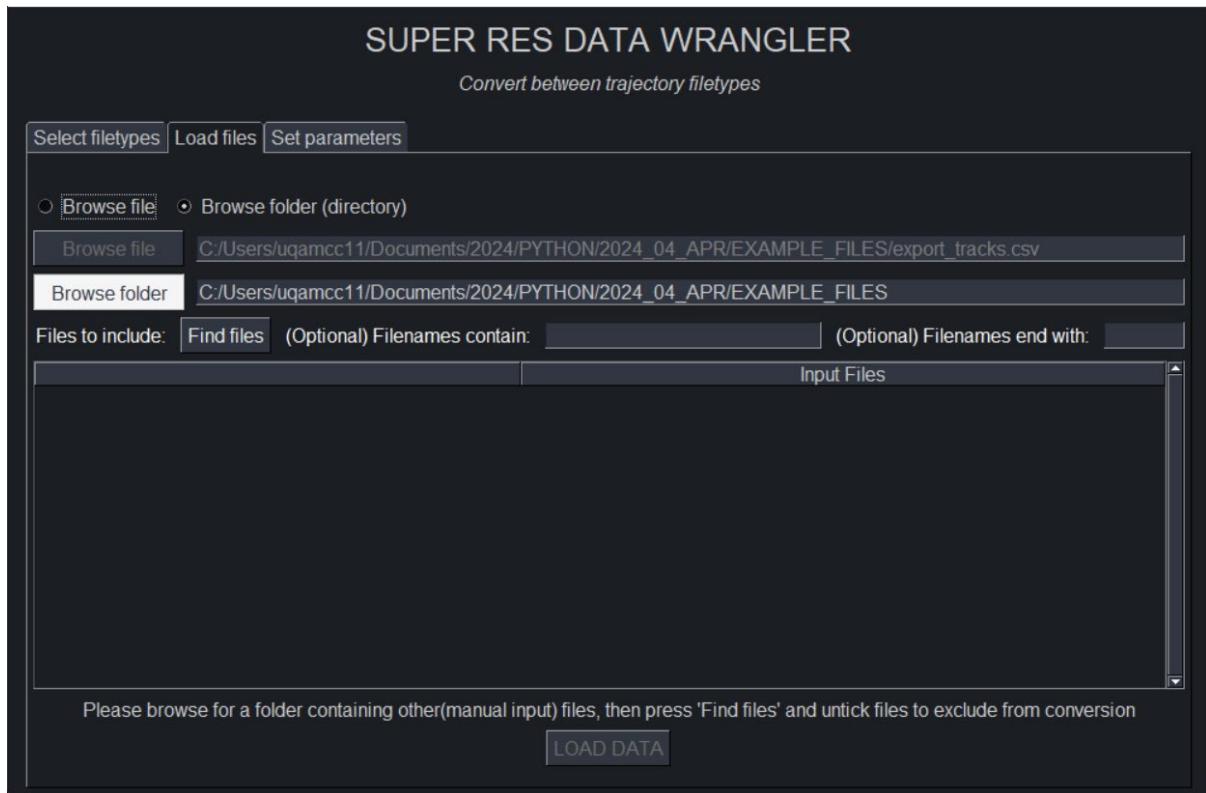
Option 2 – ‘Browse folder (directory)’ option:

Step 6.1 – Browse for a folder containing multiple trajectory files:

Clicking on the ‘Browse folder (directory)’ radio option will display additional fields:

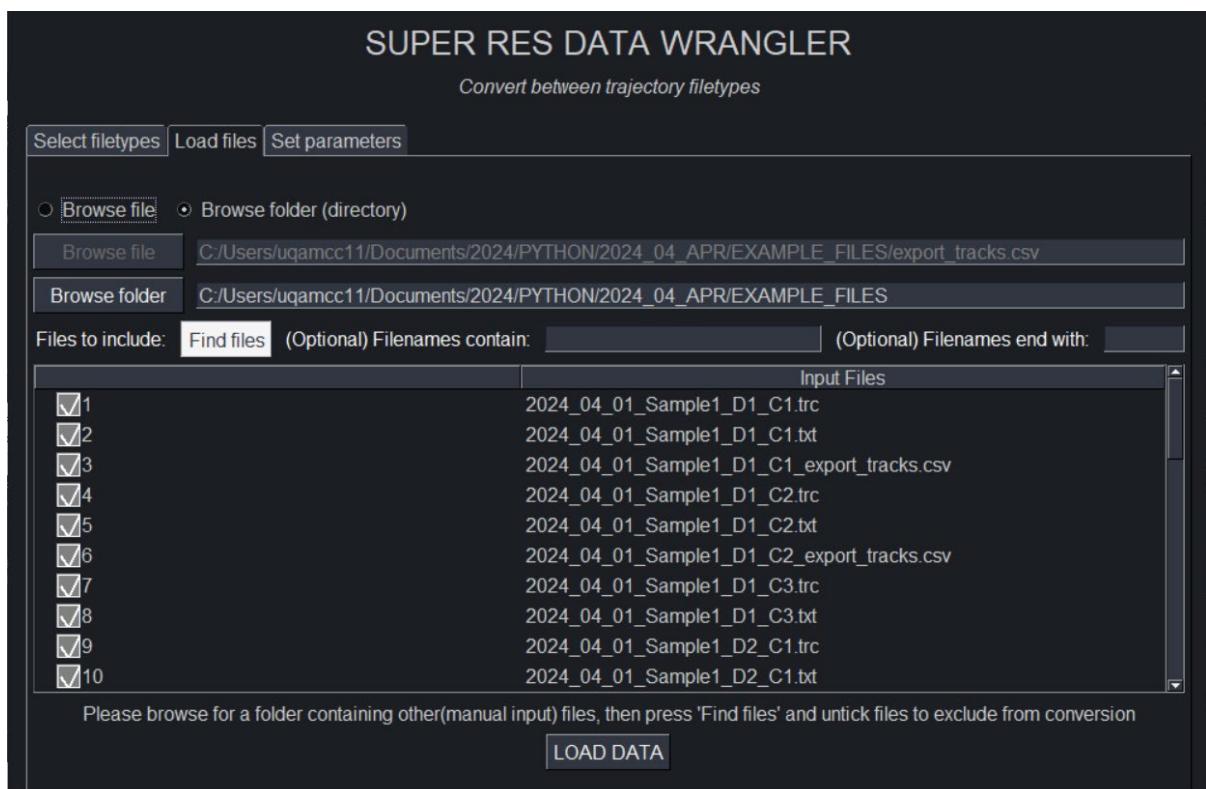


Press the 'Browse folder' button on the left of the 'Select directory containing input files' textbox to browse for and select a folder containing the trajectory files that you wish to convert. This will open up a browse window showing the folders present in the current directory. Click on the folder containing the trajectory files to select it, then press the 'Select Folder' button to confirm the selection.



Step 6.2 – Find files:

Press the ‘Find files’ button to populate the below table with files from the selected folder.



Note: the 'Input Files' field displaying the names of all of the files that were found can be expanded if needed (by clicking on the column divider at the top of the table and dragging it across to the left).

SUPER RES DATA WRANGLER

Convert between trajectory filetypes

[Select filetypes](#) [Load files](#) [Set parameters](#)

Browse file Browse folder (directory)

Browse file: C:/Users/uqamcc11/Documents/2024/PYTHON/2024_04_AP/EXAMPLE_FILES/export_tracks.csv

Browse folder: C:/Users/uqamcc11/Documents/2024/PYTHON/2024_04_AP/EXAMPLE_FILES

Files to include: [Find files](#) (Optional) Filenames contain: (Optional) Filenames end with:

Input Files
<input checked="" type="checkbox"/> 1 2024_04_01_Sample1_D1_C1.trc
<input checked="" type="checkbox"/> 2 2024_04_01_Sample1_D1_C1.txt
<input checked="" type="checkbox"/> 3 2024_04_01_Sample1_D1_C1_export_tracks.csv
<input checked="" type="checkbox"/> 4 2024_04_01_Sample1_D1_C2.trc
<input checked="" type="checkbox"/> 5 2024_04_01_Sample1_D1_C2.txt
<input checked="" type="checkbox"/> 6 2024_04_01_Sample1_D1_C2_export_tracks.csv
<input checked="" type="checkbox"/> 7 2024_04_01_Sample1_D1_C3.trc
<input checked="" type="checkbox"/> 8 2024_04_01_Sample1_D1_C3.txt
<input checked="" type="checkbox"/> 9 2024_04_01_Sample1_D2_C1.trc
<input checked="" type="checkbox"/> 10 2024_04_01_Sample1_D2_C1.txt

Please browse for a folder containing other(manual input) files, then press 'Find files' and untick files to exclude from conversion

[LOAD DATA](#)

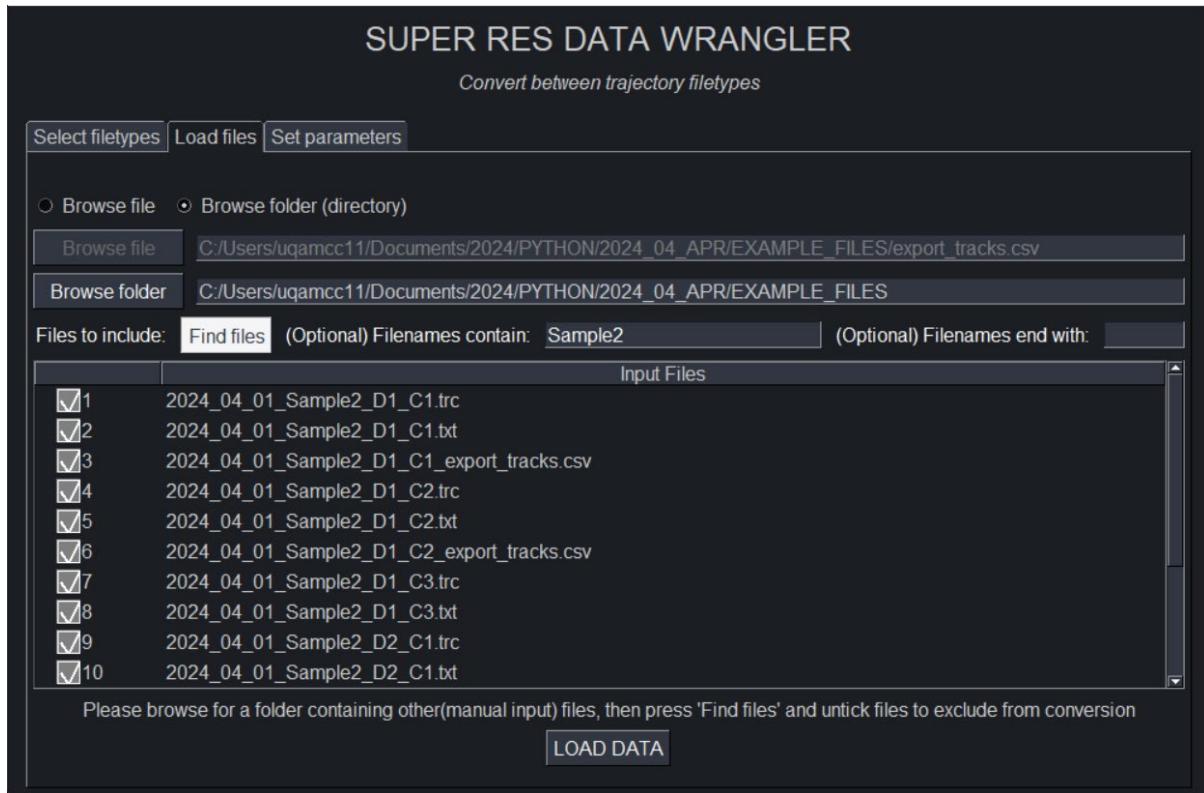
Files that are found in the selected folder/directory will also be shown in the console:

```
Input files found in selected directory: (33 files)
-----
File 1 C:/Users/uqamcc11/Documents/2024/PYTHON/2024_04_AP/EXAMPLE_FILES/2024_04_01_Sample1_D1_C1.trc
File 2 C:/Users/uqamcc11/Documents/2024/PYTHON/2024_04_AP/EXAMPLE_FILES/2024_04_01_Sample1_D1_C1.txt
File 3 C:/Users/uqamcc11/Documents/2024/PYTHON/2024_04_AP/EXAMPLE_FILES/2024_04_01_Sample1_D1_C1_export_tracks.csv
File 4 C:/Users/uqamcc11/Documents/2024/PYTHON/2024_04_AP/EXAMPLE_FILES/2024_04_01_Sample1_D1_C2.trc
File 5 C:/Users/uqamcc11/Documents/2024/PYTHON/2024_04_AP/EXAMPLE_FILES/2024_04_01_Sample1_D1_C2.txt
File 6 C:/Users/uqamcc11/Documents/2024/PYTHON/2024_04_AP/EXAMPLE_FILES/2024_04_01_Sample1_D1_C2_export_tracks.csv
File 7 C:/Users/uqamcc11/Documents/2024/PYTHON/2024_04_AP/EXAMPLE_FILES/2024_04_01_Sample1_D1_C3.trc
File 8 C:/Users/uqamcc11/Documents/2024/PYTHON/2024_04_AP/EXAMPLE_FILES/2024_04_01_Sample1_D1_C3.txt
File 9 C:/Users/uqamcc11/Documents/2024/PYTHON/2024_04_AP/EXAMPLE_FILES/2024_04_01_Sample1_D2_C1.trc
File 10 C:/Users/uqamcc11/Documents/2024/PYTHON/2024_04_AP/EXAMPLE_FILES/2024_04_01_Sample1_D2_C1.txt
```

Step 6.3 – (Optional) Filter files by filename:

Optional: to only find files that contain a certain phrase within the filename, enter that phrase in the '(Optional) Filenames contain:' text box on the right of the 'Find files' button before pressing the 'Find files' button to display the filtered list of files. Leave this text box blank to find all files.

In this example, only files containing the name “Sample2” will be included in the list:



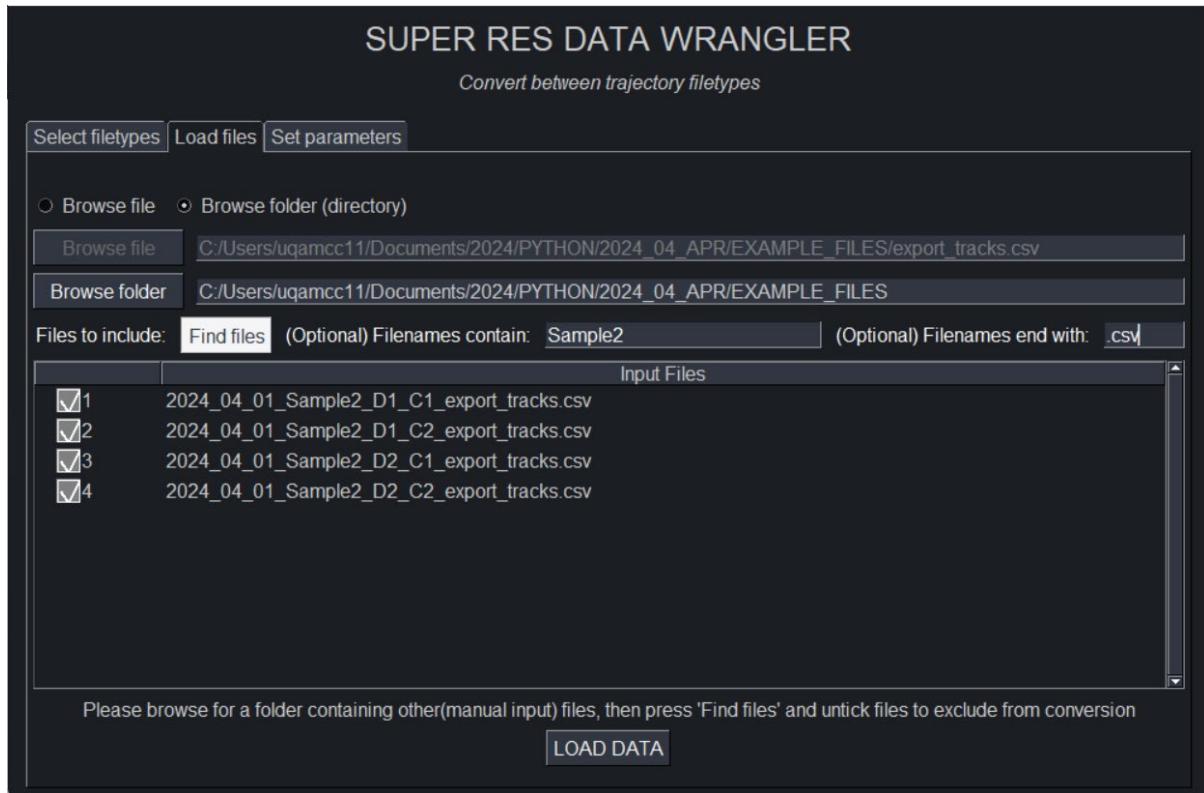
This will also update the list of files that were found in the console:

```
Input files found in selected directory: (16 files)
-----
File 1 C:/Users/uqamcc11/Documents/2024/PYTHON/2024_04_AP/EXAMPLE_FILES/2024_04_01_Sample2_D1_C1.trc
File 2 C:/Users/uqamcc11/Documents/2024/PYTHON/2024_04_AP/EXAMPLE_FILES/2024_04_01_Sample2_D1_C1.txt
File 3 C:/Users/uqamcc11/Documents/2024/PYTHON/2024_04_AP/EXAMPLE_FILES/2024_04_01_Sample2_D1_C1_export_tracks.csv
File 4 C:/Users/uqamcc11/Documents/2024/PYTHON/2024_04_AP/EXAMPLE_FILES/2024_04_01_Sample2_D1_C2.trc
File 5 C:/Users/uqamcc11/Documents/2024/PYTHON/2024_04_AP/EXAMPLE_FILES/2024_04_01_Sample2_D1_C2.txt
File 6 C:/Users/uqamcc11/Documents/2024/PYTHON/2024_04_AP/EXAMPLE_FILES/2024_04_01_Sample2_D1_C2_export_tracks.csv
File 7 C:/Users/uqamcc11/Documents/2024/PYTHON/2024_04_AP/EXAMPLE_FILES/2024_04_01_Sample2_D1_C3.trc
File 8 C:/Users/uqamcc11/Documents/2024/PYTHON/2024_04_AP/EXAMPLE_FILES/2024_04_01_Sample2_D1_C3.txt
File 9 C:/Users/uqamcc11/Documents/2024/PYTHON/2024_04_AP/EXAMPLE_FILES/2024_04_01_Sample2_D2_C1.trc
File 10 C:/Users/uqamcc11/Documents/2024/PYTHON/2024_04_AP/EXAMPLE_FILES/2024_04_01_Sample2_D2_C1.txt
```

Step 6.4 – (Optional) Filter files by extension:

Optional (other(manual input) files only): to only find files of a particular filetype (extension), enter the extension in the '(Optional) Filenames end with:' text box to the right of the '(Optional) Filenames contain:' text box, before pressing the 'Find files' button to display the filtered list of files. Leave this text box blank to find all filetypes.

In this example, only files with the extension “.csv” will be shown in the list:



This will also update the list in the console:

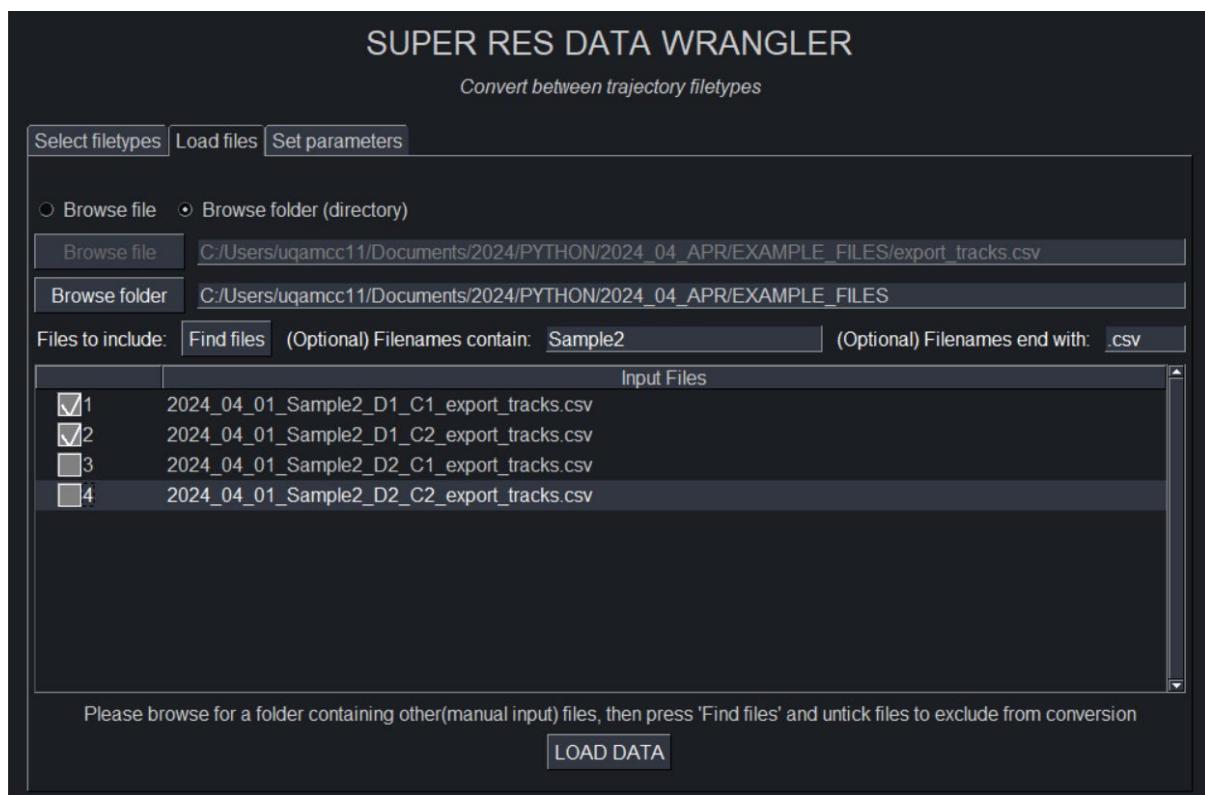
```
Input files found in selected directory: (4 files)
-----
File 1 C:/Users/uqamcc11/Documents/2024/PYTHON/2024_04_AP/EXAMPLE_FILES/2024_04_01_Sample2_D1_C1_export_tracks.csv
File 2 C:/Users/uqamcc11/Documents/2024/PYTHON/2024_04_AP/EXAMPLE_FILES/2024_04_01_Sample2_D1_C2_export_tracks.csv
File 3 C:/Users/uqamcc11/Documents/2024/PYTHON/2024_04_AP/EXAMPLE_FILES/2024_04_01_Sample2_D2_C1_export_tracks.csv
File 4 C:/Users/uqamcc11/Documents/2024/PYTHON/2024_04_AP/EXAMPLE_FILES/2024_04_01_Sample2_D2_C2_export_tracks.csv
```

Step 6.5 – (Optional) Select which files to include:

Tick/untick files that you wish to include/exclude from conversion.

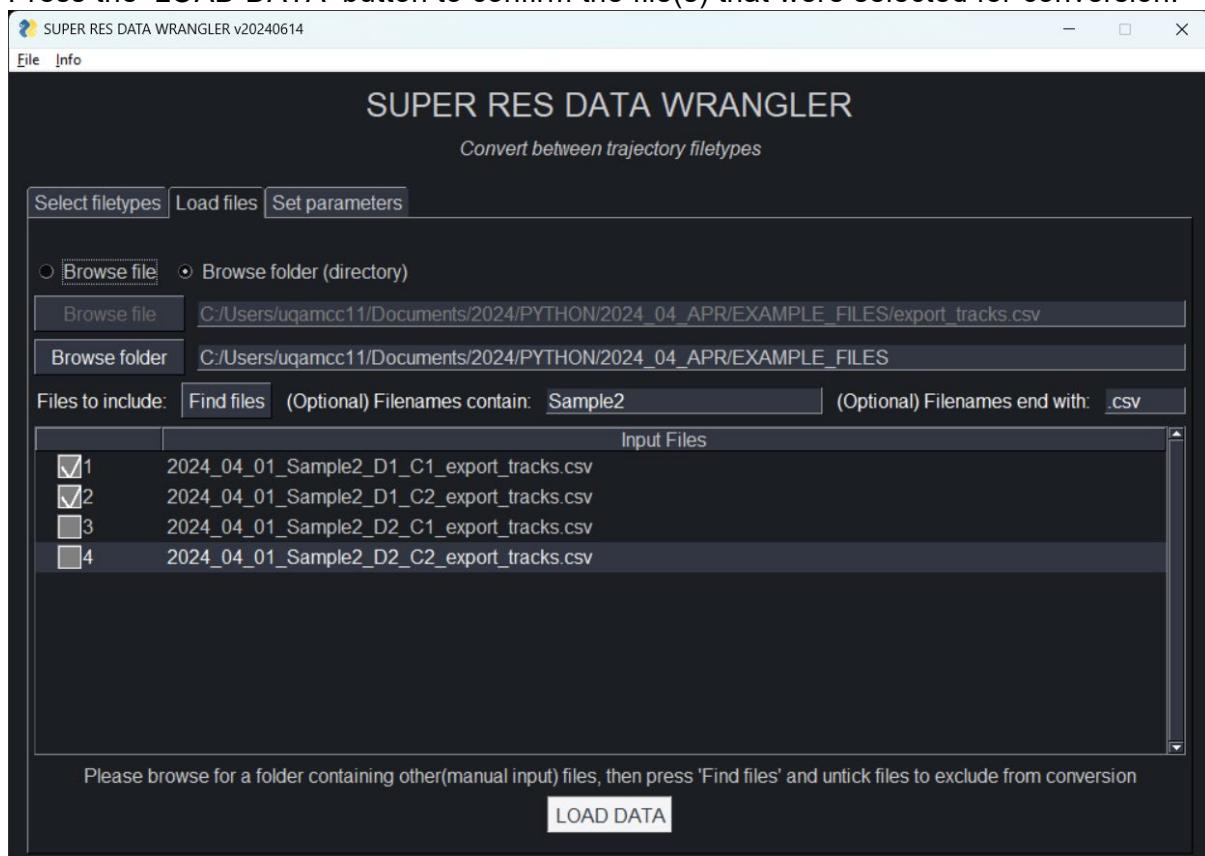
Note: You may need to wait ~1s between clicks for the checkbox to register the change.

In this example, only files #1 and #2 will be included in the conversion:



Step 6.6 – Confirm input file selection:

Press the 'LOAD DATA' button to confirm the file(s) that were selected for conversion.



The filename of the files that were selected for conversion will be displayed in the text console, and the GUI will automatically swap the GUI to the ‘Set parameters’ tab.

```
Input files selected for conversion: (2 files)
-----
File 1 C:/Users/uqamcc11/Documents/2024/PYTHON/2024_04_AP/R/EXAMPLE_FILES/2024_04_01_Sample2_D1_C1_export_tracks.csv
File 2 C:/Users/uqamcc11/Documents/2024/PYTHON/2024_04_AP/R/EXAMPLE_FILES/2024_04_01_Sample2_D1_C2_export_tracks.csv
```

Set parameters Tab

This tab enables the user to select the parameters of the input file.

The screenshot shows the 'SUPER RES DATA WRANGLER' software interface with the 'Set parameters' tab selected. The interface is divided into two main sections: 'Input csv parameters' on the left and 'Output ascii parameters' on the right. Both sections contain fields for defining spatial and temporal information, file structure, and trajectory data selection. A message at the bottom left says 'Please enter input file parameters' and a 'CONVERT' button is at the bottom center.

Input csv parameters

Define spatial and temporal information:
X,Y units: px ▾
Time units: Frames ▾

Define file structure:
Number of headers: 3 ▾
Delimiter: tab ▾

Select which columns contain trajectory data:
Trajectory col: 1 ▾
X-position col: 3 ▾
Y-position col: 4 ▾
Frame col: 2 ▾ Starting frame: 1 ▾

Output ascii parameters

Define spatial and temporal information:
X,Y units: px ▾
Time units: Frames ▾

Define file structure:
Number of headers: 0 ▾
Delimiter: comma ▾

Select which columns contain trajectory data:
Trajectory col: ID ▾
X-position col: 3 ▾
Y-position col: 4 ▾
Frame col: 2 ▾ Starting frame: 0 ▾

Please enter input file parameters
CONVERT

See Appendix 1 for detailed information on each file format, and Appendix 2 for detailed information on each parameter.

Step 8 - Select input file parameters:

Parameters that require input will be visible, with white text and dropdown boxes/text boxes enabled.

Parameters that do not require input will either be invisible, or have greyed out text and dropdown boxes/text boxes disabled.

'Define spatial and temporal information' parameter inputs:

Step 8.1 – Select the X,Y units:

If applicable (white text, dropdown box enabled): click on the downward arrow of the dropdown box next to 'X,Y units:' and select the spatial units of the input file.

SUPER RES DATA WRANGLER

Convert between trajectory filetypes

Select filetypes Load files Set parameters

Input csv parameters

Define spatial and temporal information:

X,Y units: px
px
um
Time units: nm ns

Define file structure:

Number of headers: 3
Delimiter: tab

Select which columns contain trajectory data:

Trajectory col: 1
X-position col: 3
Y-position col: 4
Frame col: 2 Starting frame: 1

Output ascii parameters

Define spatial and temporal information:

X,Y units: px

Time units: Frames

Define file structure:

Number of headers: 0
Delimiter: comma

Select which columns contain trajectory data:

Trajectory col: ID
X-position col: 3
Y-position col: 4
Frame col: 2 Starting frame: 0

Please enter input file parameters

CONVERT

In this example, as the X,Y units of the input file are different to that of the output file, the 'Pixel size (um/px)' parameter will become visible:

SUPER RES DATA WRANGLER

Convert between trajectory filetypes

Select filetypes Load files Set parameters

Input csv parameters

Define spatial and temporal information:

X,Y units: um
Pixel size (um/px): 0.106
Time units: Frames

Define file structure:

Number of headers: 3
Delimiter: tab

Select which columns contain trajectory data:

Trajectory col: 1
X-position col: 3
Y-position col: 4
Frame col: 2 Starting frame: 1

Output ascii parameters

Define spatial and temporal information:

X,Y units: px

Time units: Frames

Define file structure:

Number of headers: 0
Delimiter: comma

Select which columns contain trajectory data:

Trajectory col: ID
X-position col: 3
Y-position col: 4
Frame col: 2 Starting frame: 0

Please enter input file parameters

CONVERT

Step 8.2 – Define the Pixel size (um/px):

If applicable (becomes visible): click on the textbox next to ‘Pixel size (um/px):’ to begin typing, and type in the correct pixel size.

SUPER RES DATA WRANGLER
Convert between trajectory filetypes

Select filetypes | Load files | Set parameters

Input csv parameters

Define spatial and temporal information:

X,Y units: **um** ↗
Pixel size (um/px): **0.1**
Time units: **Frames** ↗

Define file structure:

Number of headers: **3** ↗
Delimiter: **tab** ↗

Select which columns contain trajectory data:

Trajectory col: **1** ↗
X-position col: **3** ↗
Y-position col: **4** ↗
Frame col: **2** ↗ Starting frame: **1** ↗

Output ascii parameters

Define spatial and temporal information:

X,Y units: **px** ↗
Time units: **Frames** ↗

Define file structure:

Number of headers: **0** ↗
Delimiter: **comma** ↗

Select which columns contain trajectory data:

Trajectory col: **ID** ↗
X-position col: **3** ↗
Y-position col: **4** ↗
Frame col: **2** ↗ Starting frame: **0** ↗

Please enter input file parameters

CONVERT

Step 8.3 – Select the Time units:

If applicable (white text, dropdown box enabled): click on the downward arrow of the dropdown box next to ‘Time units.’ and select the temporal units of the input file.

SUPER RES DATA WRANGLER

Convert between trajectory filetypes

Select filetypes | Load files | Set parameters

Input csv parameters Define spatial and temporal information: X,Y units: um <input type="button" value="px"/> Pixel size (um/px): 0.1 <input type="button" value="mm"/> Time units: Frames <input type="button" value="s"/> s Define file structure: Number of headers: 3 <input type="button" value="0"/> Delimiter: tab <input type="button" value="comma"/> Select which columns contain trajectory data: Trajectory col: 1 <input type="button" value="ID"/> X-position col: 3 <input type="button" value="X-position"/> Y-position col: 4 <input type="button" value="Y-position"/> Frame col: 2 <input type="button" value="Frame"/> Starting frame: 1 <input type="button" value="0"/>	Output ascii parameters Define spatial and temporal information: X,Y units: px <input type="button" value="um"/> Time units: Frames <input type="button" value="s"/> Define file structure: Number of headers: 0 <input type="button" value="3"/> Delimiter: comma <input type="button" value="tab"/> Select which columns contain trajectory data: Trajectory col: ID <input type="button" value="1"/> X-position col: 3 <input type="button" value="X-position"/> Y-position col: 4 <input type="button" value="Y-position"/> Frame col: 2 <input type="button" value="Frame"/> Starting frame: 0 <input type="button" value="1"/>
Please enter input file parameters	
<input type="button" value="CONVERT"/>	

In this example, as the Time units of the input file are different to that of the output file, the 'Acquisition frequency (Hz)' parameter becomes visible:

SUPER RES DATA WRANGLER

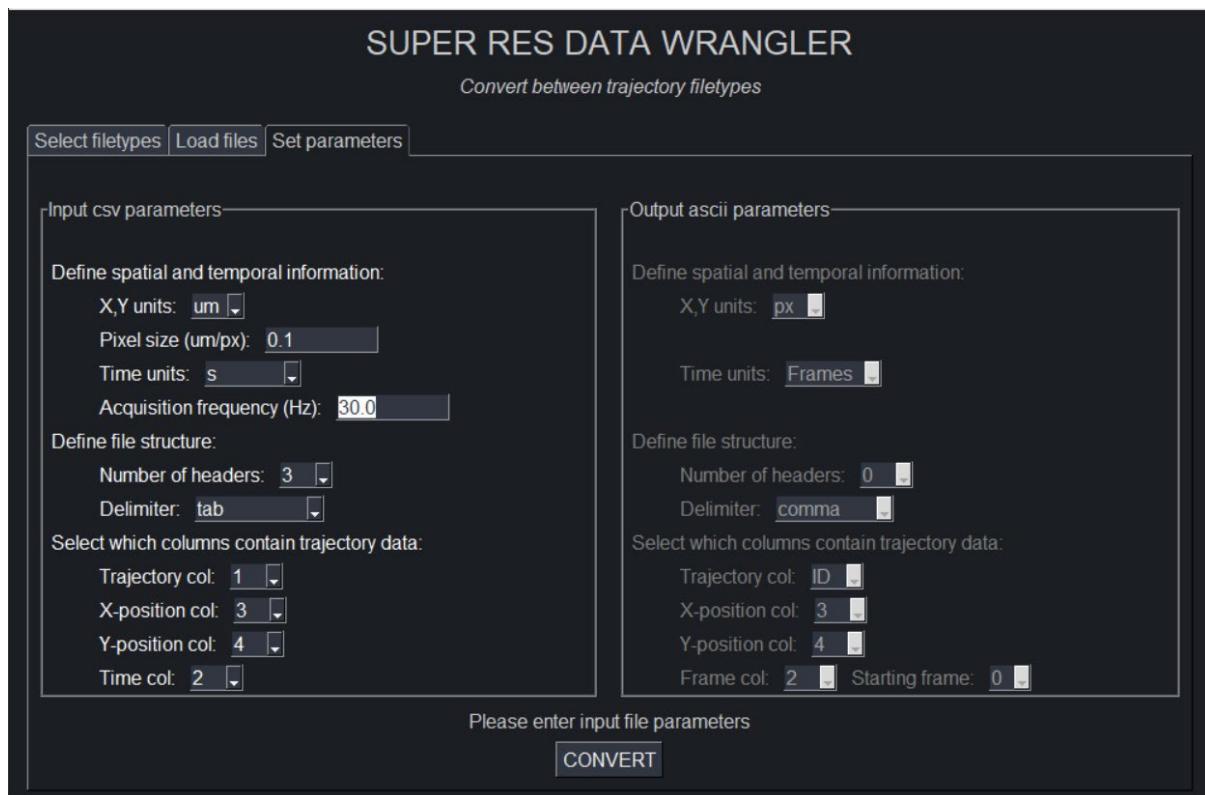
Convert between trajectory filetypes

Select filetypes | Load files | Set parameters

Input csv parameters Define spatial and temporal information: X,Y units: um <input type="button" value="px"/> Pixel size (um/px): 0.1 <input type="button" value="mm"/> Time units: s <input type="button" value="Frames"/> Acquisition frequency (Hz): 50.0 <input type="button" value="Hz"/> Define file structure: Number of headers: 3 <input type="button" value="0"/> Delimiter: tab <input type="button" value="comma"/> Select which columns contain trajectory data: Trajectory col: 1 <input type="button" value="ID"/> X-position col: 3 <input type="button" value="X-position"/> Y-position col: 4 <input type="button" value="Y-position"/> Time col: 2 <input type="button" value="Time"/>	Output ascii parameters Define spatial and temporal information: X,Y units: px <input type="button" value="um"/> Time units: Frames <input type="button" value="s"/> Define file structure: Number of headers: 0 <input type="button" value="3"/> Delimiter: comma <input type="button" value="tab"/> Select which columns contain trajectory data: Trajectory col: ID <input type="button" value="1"/> X-position col: 3 <input type="button" value="X-position"/> Y-position col: 4 <input type="button" value="Y-position"/> Frame col: 2 <input type="button" value="Frame"/> Starting frame: 0 <input type="button" value="1"/>
Please enter input file parameters	
<input type="button" value="CONVERT"/>	

Step 8.4 – Define the Acquisition frequency (Hz):

If applicable (becomes visible): click on the textbox next to ‘Acquisition frequency (Hz):’ to begin typing, and type in the correct acquisition frequency.



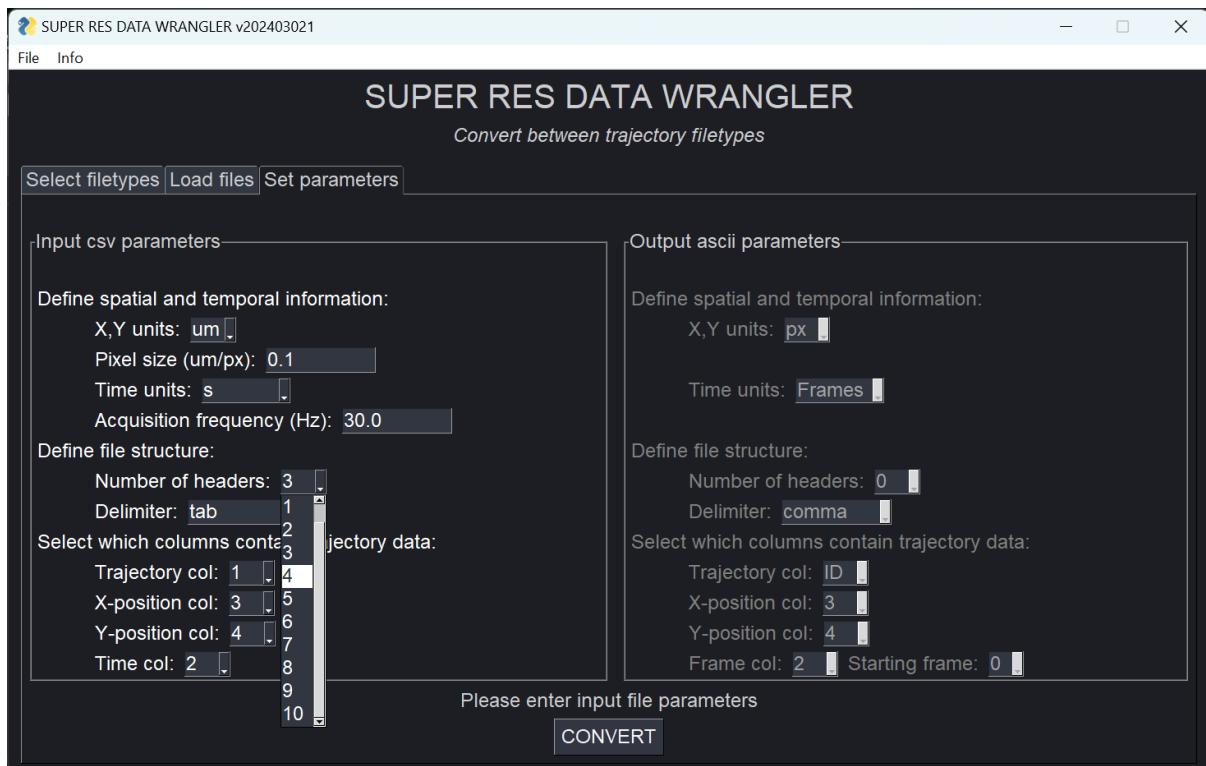
‘Define file structure’ parameter inputs:

Step 8.5 – Select the number of headers:

If applicable (white text, dropdown box enabled): click on the downward arrow of the dropdown box next to ‘Number of headers.’ and select the number of headers present in the input file.

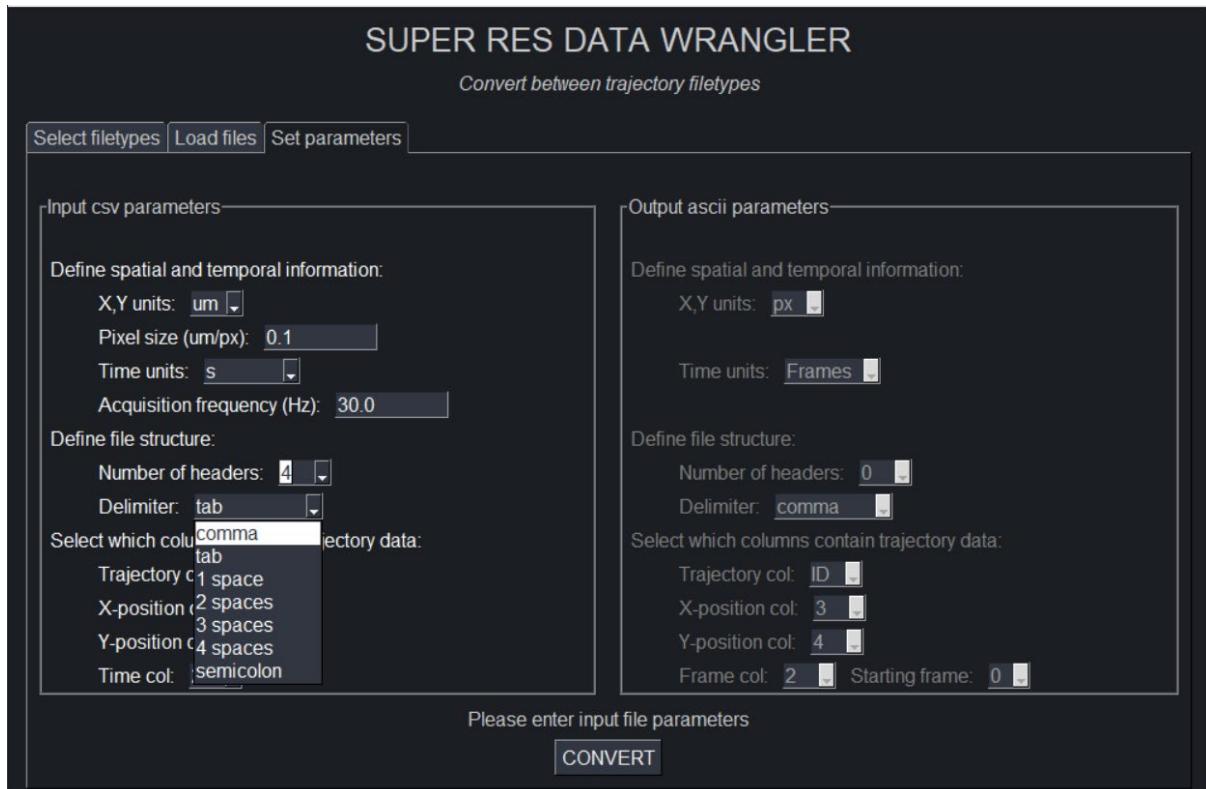
In the below example trajectory file, the number of headers is 4:

	A	B	C	D	E	F	G	H	I
1	LABEL	ID	TRACK_ID	QUALITY	POSITION_X	POSITION_Y	POSITION_Z	POSITION_T	FRAME
2	Label	Spot ID	Track ID	Quality	X	Y	Z	T	Frame
3	Label	Spot ID	Track ID	Quality	X	Y	Z	T	Frame
4			(quality)	(micron)	(micron)	(micron)	(micron)	(sec)	
5	ID282628	282628	2	298.08950	21.768646719687094	36.30233107255382	0	55.178712483495474	1723
6	ID200706	200706	2	609.30944	21.773257041958786	36.38438244742006	0	7.621899925172329	238
7	ID192512	192512	2	640.43560	21.761712355504102	36.40632485447212	0	4.419420965015888	138
8	ID229377	229377	2	579.67681	21.762051124116294	36.42347658376698	0	20.912187609821558	653
9	ID270343	270343	2	181.92572	21.733771126644143	36.28705446667755	0	45.41115165501833	1418
10	ID286722	286722	2	156.44577	21.760403180353105	36.35765508	0	58.63738976046443	1831



Step 8.6 – Select the delimiter:

If applicable (white text, dropdown box enabled): click on the downward arrow for the dropdown box next to 'Delimiter:' and select the character in the input file that separates the data into columns.



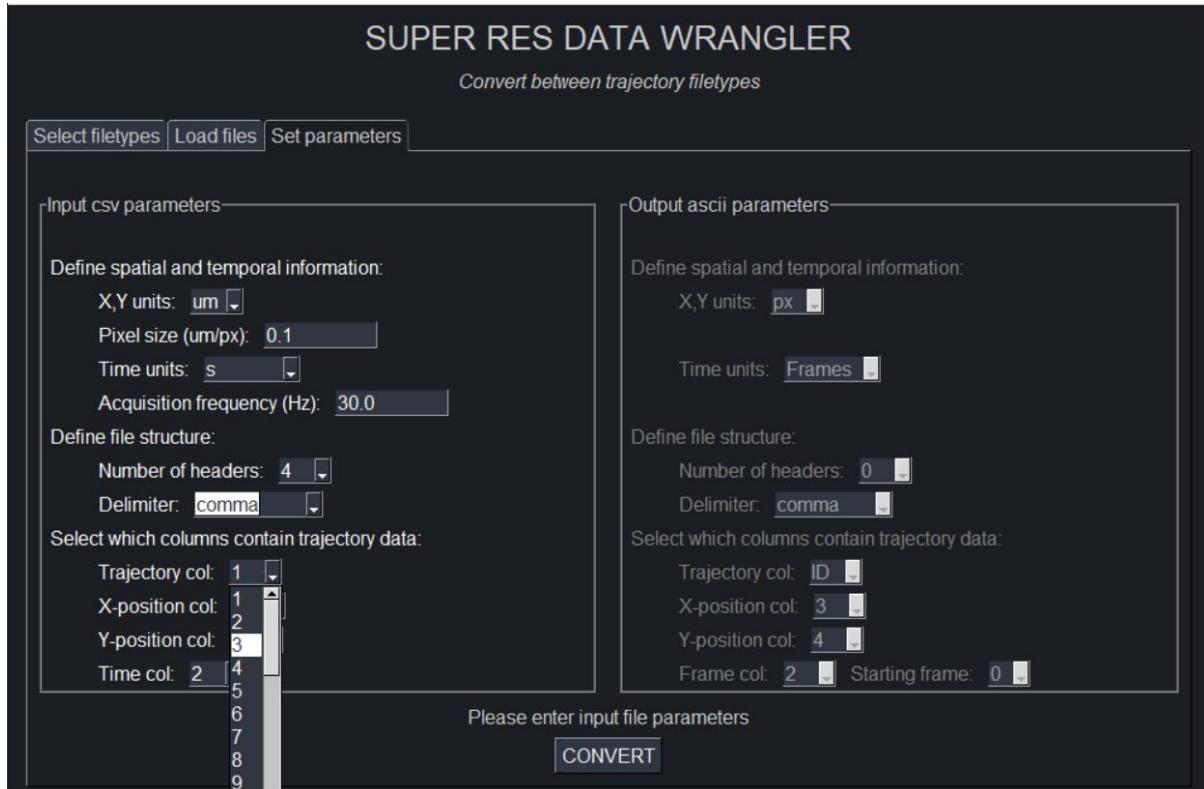
'Select which columns contain trajectory data' parameter inputs:

Step 8.7 – Select the column containing trajectory # information:

If applicable (white text, dropdown box enabled): click on the downward arrow for the dropdown box next to 'Trajectory col:' and select the number of the column that contains the trajectory # / trajectory ID information.

In the below example trajectory file, the column containing the trajectory ID information 'TRACK_ID' is column #3:

	A	B	C	D	E	F	G	H	I
1	LABEL	ID	TRACK_ID	QUALITY	POSITION_X	POSITION_Y	POSITION_Z	POSITION_T	FRAME
2	Label	Spot ID	Track ID	Quality	X	Y	Z	T	Frame
3	Label	Spot ID	Track ID	Quality (quality)	X (micron)	Y (micron)	Z (micron)	T (sec)	Frame
5	ID282628	282628	2	298.08950	21.768646719687094	36.30233107255382	0	55.178712483495474	1723
6	ID200706	200706	2	609.30944	21.773257041958786	36.38438244742006	0	7.621899925172329	238
7	ID192512	192512	2	640.43560	21.761712355504102	36.40632485447212	0	4.419420965015888	138
8	ID229377	229377	2	579.67681	21.762051124116294	36.42347658376698	0	20.912187609821558	653
9	ID270343	270343	2	181.92572	21.733771126644143	36.28705446667755	0	45.41115165501833	1418
10	ID286722	286722	2	156.44577	21.760403180353105	36.35765508	0	58.63738976046443	1831



Step 8.8 – Select the column containing X-position information:

If applicable (white text, dropdown box enabled): click on the downward arrow for the dropdown box next to 'X-position col:' and select the number of the column that contains the X-position / X-centroid information.

In the below example trajectory file, the column containing the X-position of the trajectory centroids 'POSITION_X' is column #5:

	A	B	C	D	E	F	G	H	I
1	LABEL	ID	TRACK_ID	QUALITY	POSITION_X	POSITION_Y	POSITION_Z	POSITION_T	FRAME
2	Label	Spot ID	Track ID	Quality	X	Y	Z	T	Frame
3	Label	Spot ID	Track ID	Quality	X	Y	Z	T	Frame
4				(quality)	(micron)	(micron)	(micron)	(sec)	
5	ID282628	282628	2	298.08950	21.768646719687094	36.30233107255382	0	55.178712483495474	1723
6	ID200706	200706	2	609.30944	21.773257041958786	36.38438244742006	0	7.621899925172329	238
7	ID192512	192512	2	640.43560	21.761712355504102	36.40632485447212	0	4.419420965015888	138
8	ID229377	229377	2	579.67681	21.762051124116294	36.42347658376698	0	20.912187609821558	653
9	ID270343	270343	2	181.92572	21.733771126644143	36.28705446667755	0	45.41115165501833	1418
10	ID286722	286722	2	156.44577	21.760403180353105	36.35765508	0	58.63738976046443	1831

SUPER RES DATA WRANGLER

Convert between trajectory filetypes

Select filetypes

Input csv parameters

Define spatial and temporal information:

X,Y units:

Pixel size (um/px):

Time units:

Acquisition frequency (Hz):

Define file structure:

Number of headers:

Delimiter:

Select which columns contain trajectory data:

Trajectory col:	<input type="text" value="3"/> <input type="button" value="▼"/>
X-position col:	<input type="text" value="3"/> <input type="button" value="▼"/>
Y-position col:	<input type="text" value="3"/> <input type="button" value="▼"/>
Time col:	<input type="text" value="2"/> <input type="button" value="▼"/> <input type="text" value="5"/>

Output ascii parameters

Define spatial and temporal information:

X,Y units:

Time units:

Define file structure:

Number of headers:

Delimiter:

Select which columns contain trajectory data:

Trajectory col:	<input type="text" value="ID"/> <input type="button" value="▼"/>
X-position col:	<input type="text" value="3"/> <input type="button" value="▼"/>
Y-position col:	<input type="text" value="4"/> <input type="button" value="▼"/>
Frame col:	<input type="text" value="2"/> <input type="button" value="▼"/> Starting frame: <input type="text" value="0"/> <input type="button" value="▼"/>

Please enter input file parameters

Step 8.9 – Select the column containing Y-position information:

If applicable (white text, dropdown box enabled): click on the downward arrow for the dropdown box next to the 'Y-position col:' and select the number of the column that contains the Y-position / Y-centroid information.

In the below example trajectory file, the column containing the Y-position of the trajectory centroids 'POSITION_Y' is column #6:

	A	B	C	D	E	F	G	H	I
1	LABEL	ID	TRACK_ID	QUALITY	POSITION_X	POSITION_Y	POSITION_Z	POSITION_T	FRAME
2	Label	Spot ID	Track ID	Quality	X	Y	Z	T	Frame
3	Label	Spot ID	Track ID	Quality	X	Y	Z	T	Frame
4			(quality)	(micron)		(micron)	(micron)	(sec)	
5	ID282628	282628	2 298.0895021.768646719687094		36.30233107255382		0 55.178712483495474		1723
6	ID200706	200706	2 609.3094421.773257041958786		36.38438244742006		0 7.621899925172329		238
7	ID192512	192512	2 640.4356021.761712355504102		36.40632485447212		0 4.419420965015888		138
8	ID229377	229377	2 579.6768121.762051124116294		36.42347658376698		0 20.912187609821558		653
9	ID270343	270343	2 181.9257221.733771126644143		36.28705446667755		0 45.41115165501833		1418
10	ID286722	286722	2 156.4457721.760403180353105		36.35765508		0 58.63738976046443		1831

SUPER RES DATA WRANGLER

Convert between trajectory filetypes

[Select filetypes](#) [Load files](#) [Set parameters](#)

Input csv parameters

Define spatial and temporal information:

X,Y units: ↗
 Pixel size (um/px):
 Time units: ↗
 Acquisition frequency (Hz):

Define file structure:

Number of headers: ↗
 Delimiter: ↗

Select which columns contain trajectory data:

Trajectory col: ↗
 X-position col: ↗
 Y-position col: ↗
 Time col: ↗
 ↗
 ↗
 ↗
 ↗
 ↗
 ↗

Output ascii parameters

Define spatial and temporal information:

X,Y units: ↗
 Time units: ↗

Define file structure:

Number of headers: ↗
 Delimiter: ↗

Select which columns contain trajectory data:

Trajectory col: ↗
 X-position col: ↗
 Y-position col: ↗
 Frame col: ↗ Starting frame: ↗

Please enter input file parameters

CONVERT

Step 8.10 – Select the column containing Time information:

If applicable (white text, dropdown box enabled): click on the downward arrow for the dropdown box next to 'Frame col:' or 'Time col:' and select the number of the column that contains the Time information.

In the below example trajectory file, there are two columns containing time information.

'POSITION T' in column #8 which contains time information in seconds:

	A	B	C	D	E	F	G	H	I
1	LABEL	ID	TRACK_ID	QUALITY	POSITION_X	POSITION_Y	POSITION_Z	POSITION_T	FRAME
2	Label	Spot ID	Track ID	Quality	X	Y	Z	T	Frame
3	Label	Spot ID	Track ID	Quality	X	Y	Z	T	Frame
4			(quality)	(micron)		(micron)	(micron)	(sec)	
5	ID282628	282628	298.0895021.768646719687094	36.30233107255382		0	55.178712483495474	1723	
6	ID200706	200706	2609.3094421.773257041958786	36.38438244742006		0	7.621899925172329	238	
7	ID192512	192512	2640.4356021.761712355504102	36.40632485447212		0	4.419420965015888	138	
8	ID229377	229377	2579.6768121.762051124116294	36.42347658376698		0	20.912187609821558	653	
9	ID270343	270343	2181.9257221.733771126644143	36.28705446667755		0	45.41115165501833	1418	
10	ID286722	286722	2156.4457721.760403180353105	36.35765508		0	58.63738976046443	1831	

'FRAME' in column #9 which contains time information in frames:

	A	B	C	D	E	F	G	H	I
1	LABEL	ID	TRACK_ID	QUALITY	POSITION_X	POSITION_Y	POSITION_Z	POSITION_T	FRAME
2	Label	Spot ID	Track ID	Quality	X	Y	Z	T	Frame
3				(quality)	(micron)	(micron)	(micron)	(sec)	Frame
5	ID282628	282628	2	298.08950	21.768646719687094	36.30233107255382	0	55.178712483495474	1723
6	ID200706	200706	2	609.30944	21.773257041958786	36.38438244742006	0	7.621899925172329	238
7	ID192512	192512	2	640.43560	21.761712355504102	36.40632485447212	0	4.419420965015888	138
8	ID229377	229377	2	579.67681	21.762051124116294	36.42347658376698	0	20.912187609821558	653
9	ID270343	270343	2	181.92572	21.733771126644143	36.28705446667755	0	45.41115165501833	1418
10	ID286722	286722	2	156.44577	21.760403180353105	36.35765508	0	58.63738976046443	1831

SUPER RES DATA WRANGLER

Convert between trajectory filetypes

Select filetypes

Input csv parameters

Define spatial and temporal information:

X,Y units: Pixel size (um/px): Time units: Acquisition frequency (Hz):

Define file structure:

Number of headers: Delimiter:

Select which columns contain trajectory data:

Trajectory col: X-position col: Y-position col: Time col:

Output ascii parameters

Define spatial and temporal information:

X,Y units: Time units:

Define file structure:

Number of headers: Delimiter:

Select which columns contain trajectory data:

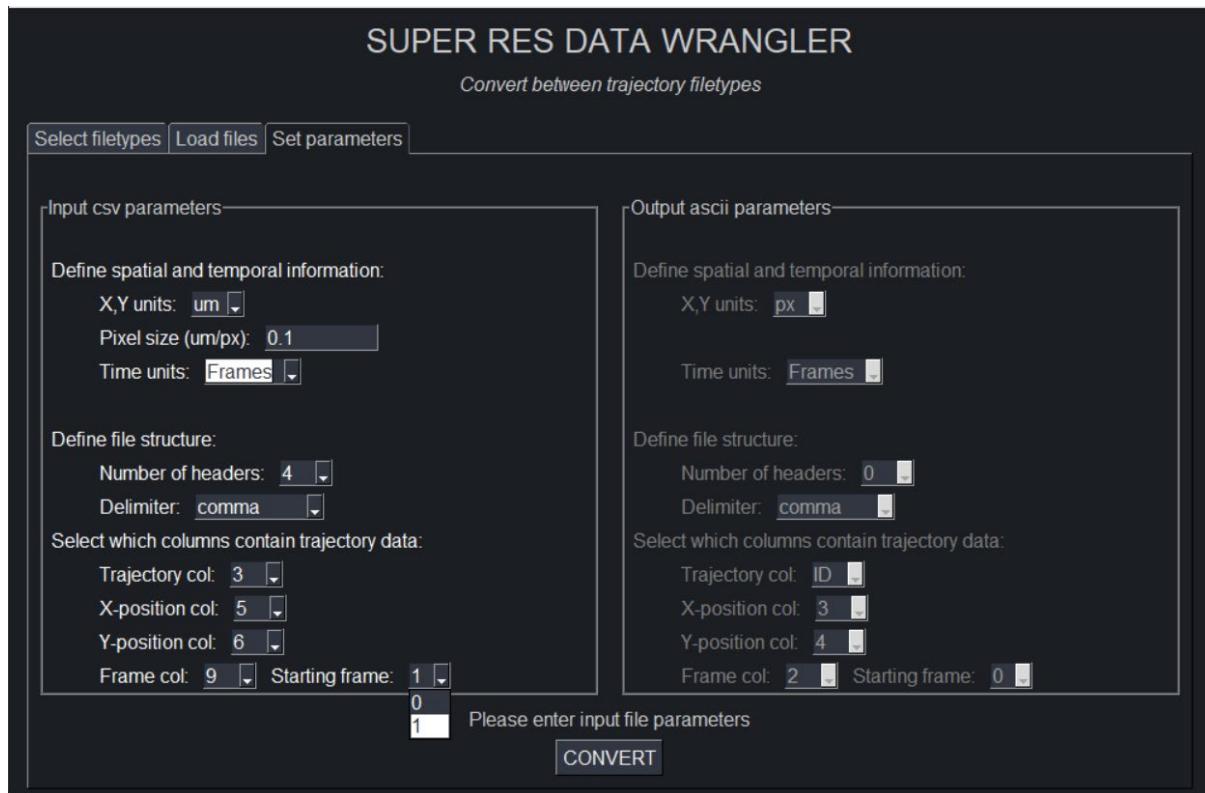
Trajectory col: X-position col: Y-position col: Frame col: Starting frame:

Please enter input file parameters

Step 8.11 – Select the starting frame:

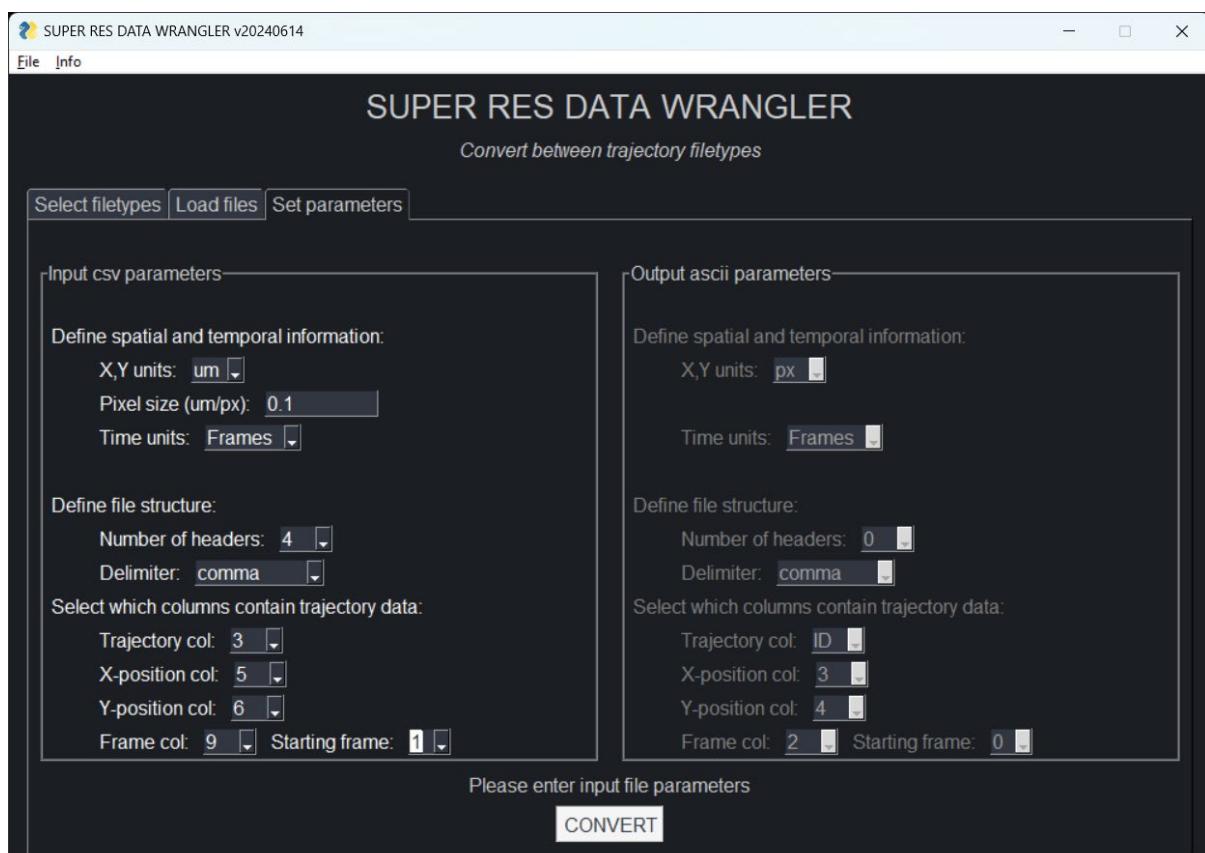
If the Time units are in Frames, the 'Starting frame' parameter will appear.

If applicable (visible): click on the downward arrow for the dropdown box next to 'Starting frame:' and select 0 for files that start counting frames from 0, or select 1 for files that start counting frames from 1.



Step 9 – Convert files:

Press the 'CONVERT' button to convert the input file(s) to the selected output file format.



Files will be converted and saved to the same place as the original file, with the appropriate suffix and a date stamp.

The console will display each input file that was read and each output file that was written:

```
Converting File 1:
-----
Reading C:/Users/uqamcc11/Documents/2024/PYTHON/2024_04_AP/EXAMPLE_FILES/2024_04_01_Sample2_D1_C1_export_tracks.csv...
86914 lines read

Writing C:/Users/uqamcc11/Documents/2024/PYTHON/2024_04_AP/EXAMPLE_FILES/2024_04_01_Sample2_D1_C1_export_tracks-20240416-125746.ascii...
86914 lines written

Writing C:/Users/uqamcc11/Documents/2024/PYTHON/2024_04_AP/EXAMPLE_FILES/2024_04_01_Sample2_D1_C1_export_tracks-20240416-125746.id...
86914 lines written

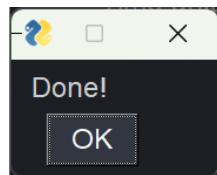
Converting File 2:
-----
Reading C:/Users/uqamcc11/Documents/2024/PYTHON/2024_04_AP/EXAMPLE_FILES/2024_04_01_Sample2_D1_C2_export_tracks.csv...
86914 lines read

Writing C:/Users/uqamcc11/Documents/2024/PYTHON/2024_04_AP/EXAMPLE_FILES/2024_04_01_Sample2_D1_C2_export_tracks-20240416-125746.ascii...
86914 lines written

Writing C:/Users/uqamcc11/Documents/2024/PYTHON/2024_04_AP/EXAMPLE_FILES/2024_04_01_Sample2_D1_C2_export_tracks-20240416-125746.id...
86914 lines written

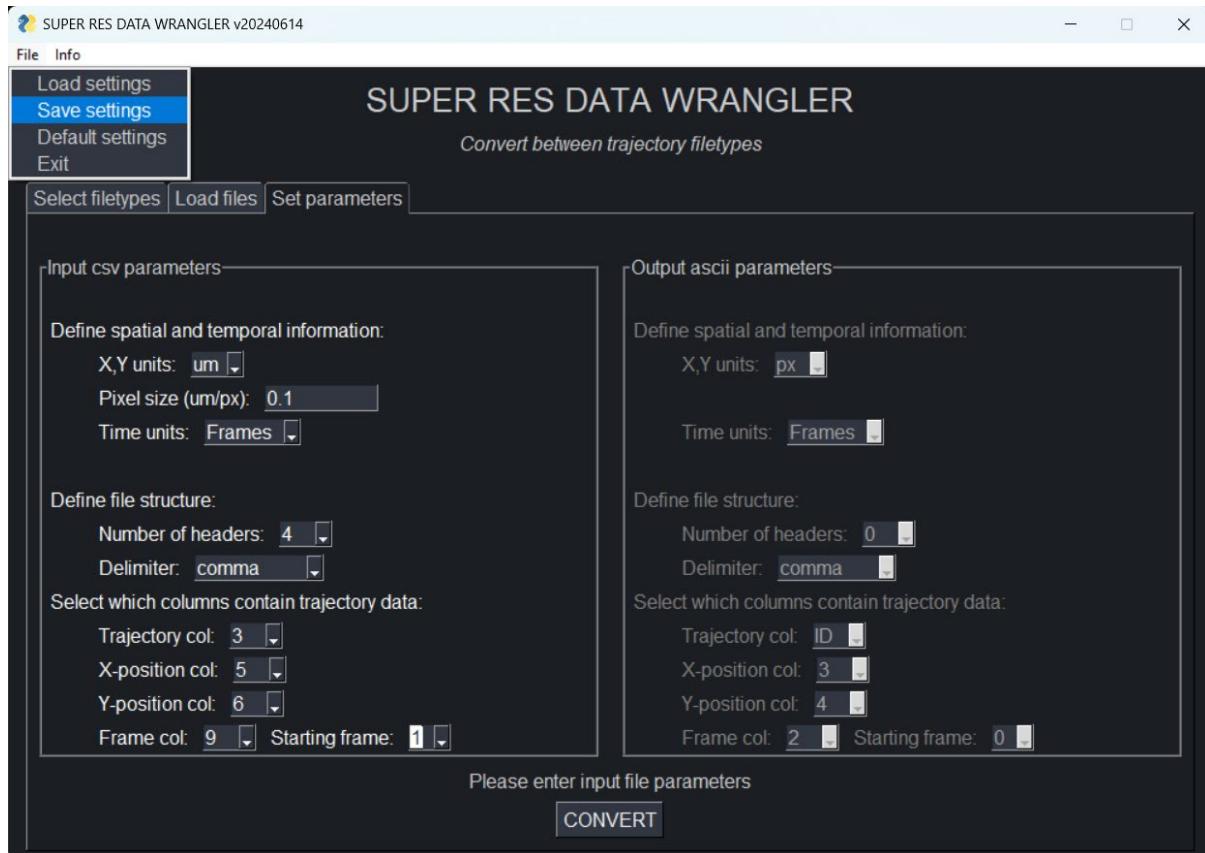
Done!
```

A 'Done!' popup will show once the GUI has finished converting the files:



Save settings

If you will be doing a lot of file conversions using the same parameters, first select the parameters that will be used again in the future, and then in the menu bar (top left hand corner of the GUI), click ‘File >> Save settings’ to save the changed values to the super_res_data_wrangler_gui.defaults file.



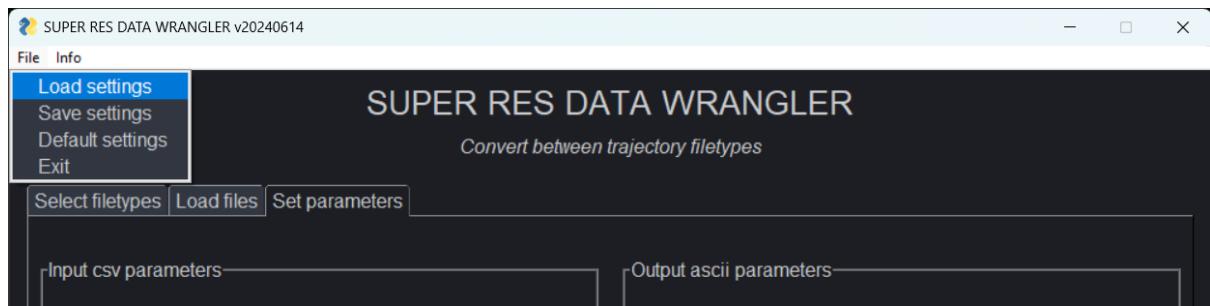
A message will display in the console:

```
Saving GUI settings to super_res_data_wrangler_gui.defaults...
```

Load settings

If you wish to load the previously saved settings, click ‘File >> Load settings’ in the menu bar.

Note: if the input filetype has changed, the GUI will automatically swap back to the first tab (‘Select filetypes’ tab), where the filetypes will have to be confirmed and the input file(s) will have to be reselected.



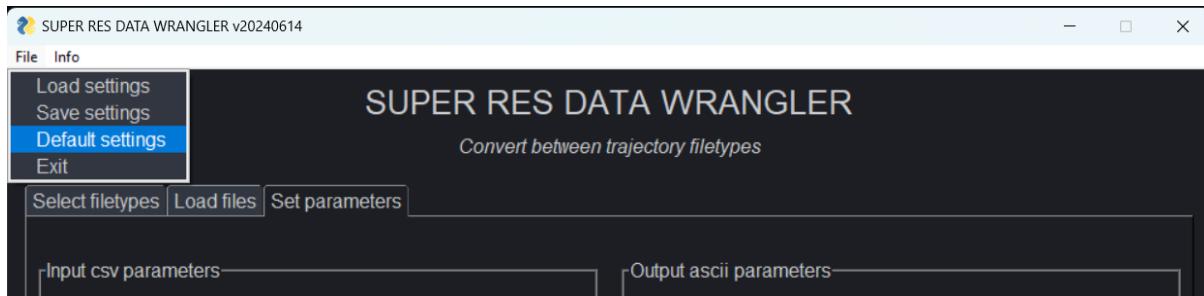
A message will display in the console:

```
| Loading GUI settings from super_res_data_wrangler_gui.defaults...|
```

Default settings

If you wish to restore values to the original default values, click ‘File >> Default settings’ in the menu bar. Subsequently click ‘File >> Save settings’ to save the original default values as the default settings.

Note: if the input filetype has changed, the GUI will automatically swap back to the first tab (‘Select filetypes’ tab), where the filetypes will have to be confirmed and the input file(s) will have to be reselected.



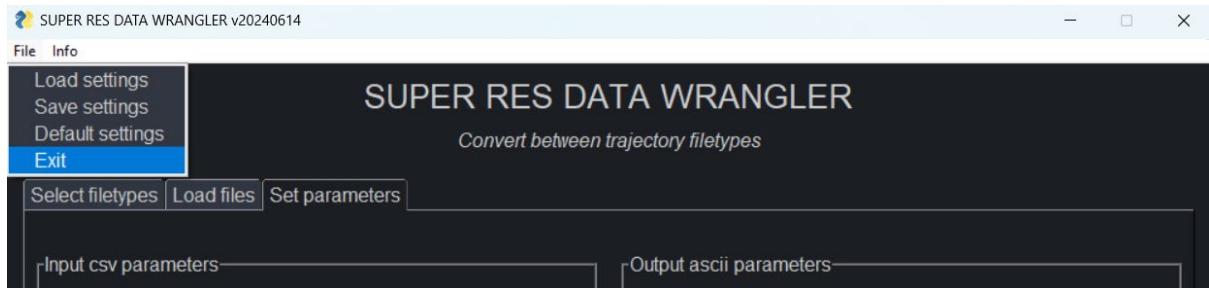
A message will display in the console:

```
Using default GUI settings...
```

IMPORTANT NOTE: Periodically the Super Res Data Wrangler GUI is updated with new functionality that requires a new super_res_data_wrangler_gui.defaults file. Newer versions of the Super Res Data Wrangler GUI may crash if loading an older defaults file. You are encouraged to delete your existing defaults file and run the new version of the Super Res Data Wrangler GUI to recreate the correct file with default settings.

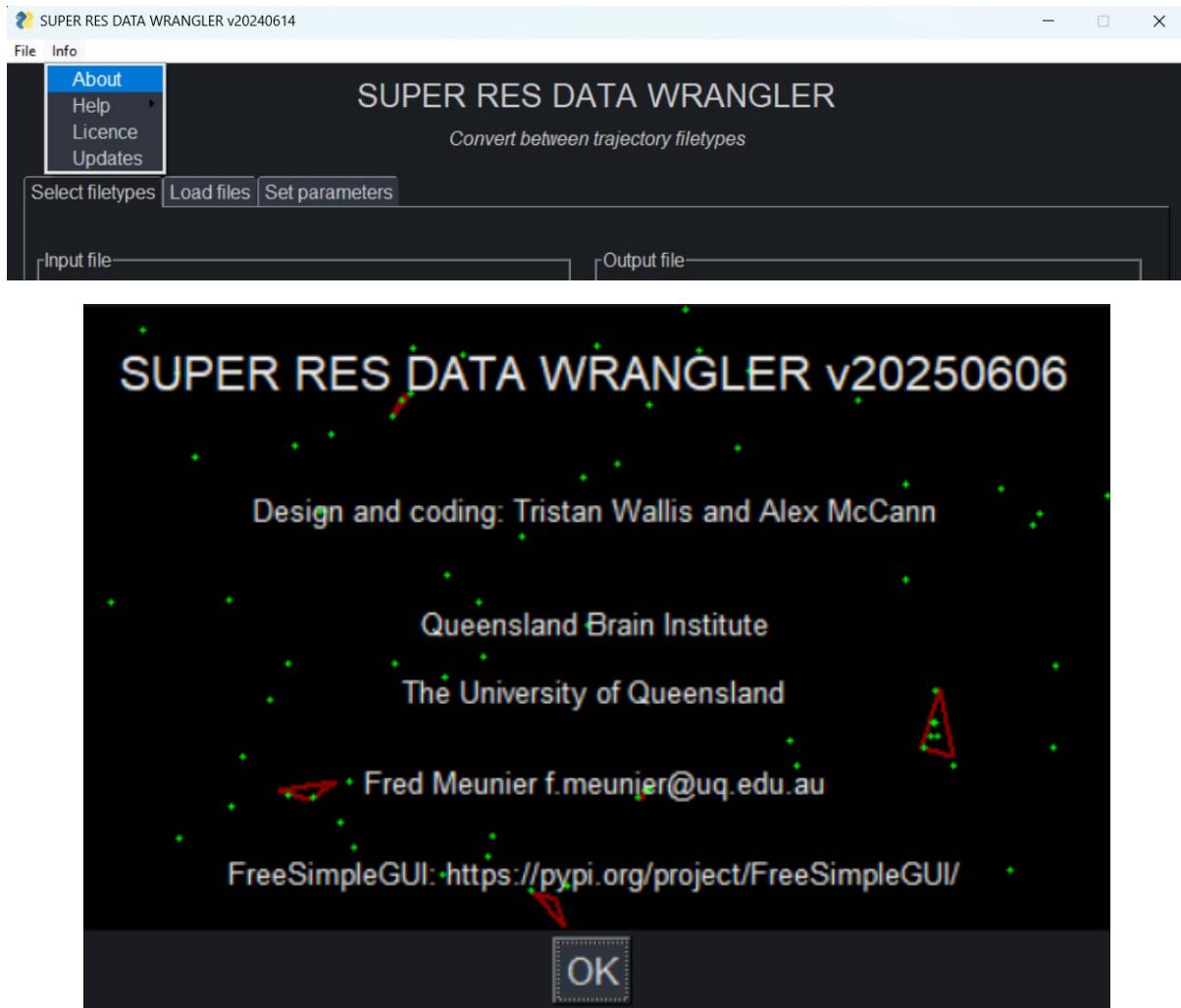
Exiting the program

The program can be exited either by clicking 'File >> Exit' in the menu bar, clicking the 'x' in the top right corner of the window, or by typing Ctrl + C in the terminal.



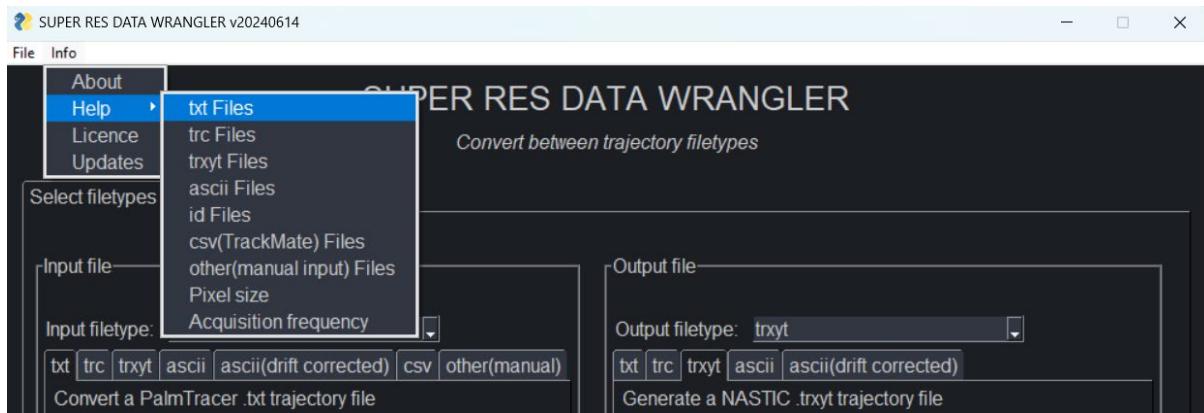
About

Clicking 'Info >> About' in the menu bar brings up a splash screen showing the about information for the GUI.



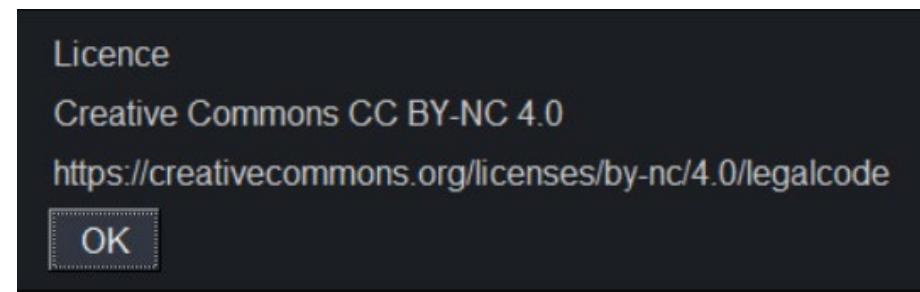
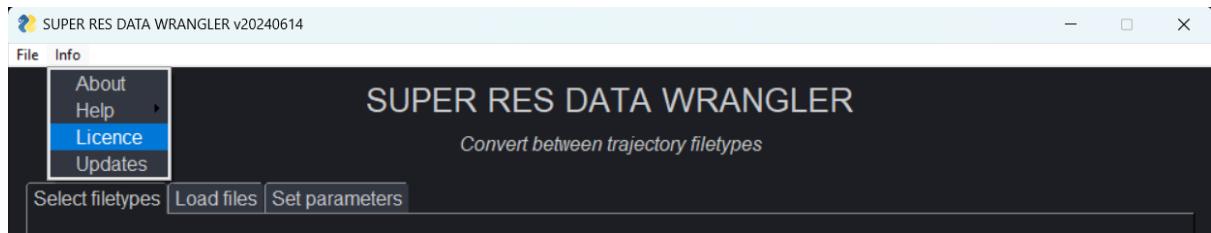
Help

Detailed information about each trajectory filetype, as well as the pixel size and acquisition frequency parameters can be viewed by clicking 'Info >> Help' in the menu bar of the GUI.



Licence

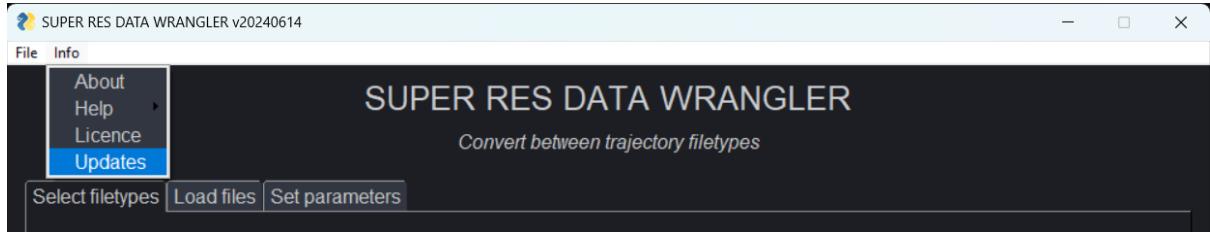
Clicking 'Info >> Licence' in the menu bar brings up the licence information.



Updates

The Super Res Data Wrangler GUI along with other NASTIC family members is periodically updated with new functionalities.

Clicking 'Info >> Updates' will open a webpage for the GitHub.



A screenshot of a GitHub releases page. The URL is https://github.com/tristanwallis/smlm_clustering/releases. The page shows a single release titled "NASTIC v1.0.7" released on Dec 13, 2023 by user "tristanwallis". The release notes state: "A suite of Python GUIs for spatiotemporal analysis of super resolution microscopy data. This release contains single threaded versions of NASTIC and derivatives, which will run on virtual servers, and which can be compiled to standalone executables using PyInstaller. The release now includes command line versions of NASTIC and derivatives for potential batch processing workflows, and additional tools for file conversion between different super resolution data formats." Below the release notes is a section for "Assets" containing three items: "NASTICv1_0_7.zip" (4.36 MB, Dec 13, 2023), "Source code (zip)" (Dec 13, 2023), and "Source code (tar.gz)" (Dec 13, 2023). The GitHub interface includes standard navigation bars like "Code", "Issues", "Pull requests", "Actions", "Projects", "Security", and "Insights".

Appendix 1: Trajectory filetypes

PalmTracer .txt file format:

Contain 3 headers (number of rows before data rows starts).

Each data line (row) contains 8 tab separated values (columns):

- [1] Track; (Trajectory #, counting up from 1)
- [2] Plane; (Temporal information, Frame #, counting up from 1)
- [3] CentroidX(px); (Spatial information, X-position, pixels)
- [4] CentroidY(px); (Spatial information, Y-position, pixels)
- *[5] CentroidZ(um);
- *[6] Integrated_Intensity;
- *[7] id;
- *[8] Pair-Distance(px);

* = Columns not needed for conversion, can be any number. If converting from another filetype, columns 5, 7 and 8 will be replaced with a 0, and column 6 will be replaced with -1 if the input filetype does not contain integrated intensity information.

Example:

Width	Height	nb_Planes	nb_Tracks	Pixel_Size(um)	Frame_Duration(s)	Gaussian_Fit	Spectral
329	158	8000	8081	0.106	0.02	None	False
Track	Plane	CentroidX(px)	CentroidY(px)	CentroidZ(um)	Integrated_Intensity	id	Pair_Distance(px)
1	1	276.269572830706	47.0805395577243	0	13089.1528320313	43	0
1	2	274.303133516352	48.2782523520935	0	7672.34887695313	76	0
1	3	274.891970316922	47.5279810094224	0	9931.11743164063	146	0
1	4	273.669614996879	47.8070693296009	0	5767.41088867188	236	0
1	5	275.414575953906	47.397724656005	0	7558.37377929688	291	0
1	6	275.93406753494	46.6645400960479	0	6259.39013671875	308	0
1	7	275.840465835188	46.1239353282329	0	3471.96459960938	416	0
1	8	275.438006269573	46.2149241717978	0	2029.81518554688	440	0
1	9	274.791478789354	45.8095767231888	0	9122.86352539063	524	0

PalmTracer .trc file format:

Contain 0 headers.

Each data line (row) consists of 6 tab separated values (columns):

- [1] Trajectory#;
- [2] Frame#;
- [3] X-position(px);
- [4] Y-position(px);
- *[5] -1;
- *[6] Integrated_Intensity;

* = Columns not needed for conversion, can be any number. Column 6 will be replaced with -1 if the input filetype does not contain integrated intensity information.

Example:

1	1	276.269572723821	47.080539615183	-1	13089.1525878906
1	2	274.303133599286	48.2782523061602	-1	7672.34838867188
1	3	274.891970360777	47.5279809124645	-1	9931.11694335938
1	4	273.669614968534	47.8070693377678	-1	5767.4111328125
1	5	275.414575972816	47.3977246431582	-1	7558.3740234375
1	6	275.93406753494	46.664540057044	-1	6259.39013671875
1	7	275.840465753652	46.12393526663	-1	3471.96435546875
1	8	275.43800630337	46.2149242190112	-1	2029.81530761719
1	9	274.791478757012	45.809576798377	-1	9122.86328125
1	1	275.824958927795	46.5723829447615	-1	8954.314453125
2	2	58.6367908782501	101.742870799136	-1	12686.4106445313
2	3	58.361849347087	102.198444512936	-1	10684.8942871094
2	4	58.3014790906691	102.042988140333	-1	16990.9973144531
2	5	58.3724221575284	101.936737912003	-1	15367.7707519531

NASTIC/segNASTIC/BOOSH .trxyt file format:

Contain 0 headers.

Each data line (row) consists of 4 space separated values (columns):

- [1] Trajectory #; (trajectory number)
- [2] X-position(um); (spatial information, microns)
- [3] Y-position(um); (spatial information, microns)
- [4] Time(s); (temporal information, seconds)

Example:

```
1 29.284574708725025 4.990537199209398 0.02
1 29.076132161524317 5.117494744452981 0.04
1 29.138548858242363 5.037965976721237 0.06
1 29.008979186664604 5.067549349803387 0.08
1 29.193945053118497 5.024158812174769 0.1
1 29.24901115870364 4.946441246046664 0.12
1 29.23908936988711 4.88913713826278 0.14
1 29.19642866815722 4.8987819672151875 0.16
1 29.12789674824327 4.855815140627962 0.18
1 29.23744564634627 4.936672592144719 0.2
2 6.215499833094511 10.784744304708415 0.02
2 6.186356030791222 10.833035118371216 0.04
2 6.179956783610924 10.816556742875298 0.06
2 6.18747674869801 10.805294218672318 0.08
```

SharpViSu .ascii file format:

.ascii files contain 0 headers

Each ascii data line (row) consists of 9 comma separated values (columns):

*[1] 1;
[2] Frame #;
[3] n;
[4] X-position; (Pixels (px))
[5] Y-position; (Pixels (px))
*[6] Integrated_intensity;
*[7] 0;
*[8] 0;
*[9] 0;

* = Columns not needed for conversion, can be any number

NOTE: If converting from PalmTracer, the X,Y units are in pixels. If converting from TrackMate, the X,Y units are either in pixels or microns, depending on how FIJI interpreted the microscope metadata (pixels if FIJI was unable to read the metadata) and whether or not this was subsequently changed by the user.

Example:

```
1,0,1,12.144466281714381,16.719987550850586,7627.04278564453,0,0,0  
1,0,2,21.380060175448545,7.56700319416653,3152.89190673828,0,0,0  
1,0,3,13.336731143401561,15.698784374751062,2915.20043945313,0,0,0  
1,0,4,17.45391412842103,11.668108966769635,2463.55096435547,0,0,0  
1,0,5,16.36251646438727,13.082774724648425,2459.45245361328,0,0,0  
1,0,6,14.997891859239918,14.165645956501866,2051.84259033203,0,0,0  
1,0,7,8.574230579986414,20.73708293209756,1937.65270996094,0,0,0  
1,0,8,15.630849608989978,13.848777888406932,1683.87921142578,0,0,0  
1,0,9,14.904775879085415,14.559877912338266,1505.90997314453,0,0,0  
1,0,10,8.150807399969825,21.237625625700968,1455.61853027344,0,0,0
```

NOTE: SharpViSu assumes pixel size is 0.100um/px (hardcoded value = 100). For acquisition files with other pixel sizes (e.g., 0.106um/px), navigate to the SharpViSu folder downloaded onto your computer, open the adjustformat.m script, adjust the '100' value in line 15 and 16 to the appropriate pixel size, and save. For example, if using a pixel size of 0.106: change line 15 from 'A(:,4:5) = A(:,4:5) * 100 % x, y in nm' to 'A(:,4:5) * 106 % x, y in nm' and change line 16 from 'A(:,8:9) = A(:,8:9) * 100; % sigmas in nm' to 'A(:,8:9) = A(:,8:9) * 106; % sigmas in nm'.

NOTE: when generating .ascii files, a trajectory .id file containing the Trajectory ID (Trajectory#) of each .ascii data line (row) is generated (with the same name and in the same folder as the .ascii), which is then used to convert back from the .ascii file format to other formats.

Each id data line (row) contains 1 value (column):

[1] Trajectory#;

Example:

1
2
3
4
5
6
7
8
9
10

SharpViSu .ascii (drift corrected) file format:

.ascii (drift corrected) files contain 0 headers

Each ascii data line (row) consists of 9 comma separated values (columns):

*[1] 1;
[2] Frame #;
[3] n;
[4] X-position; (nanometers (nm))
[5] Y-position; (nanometers (nm))
*[6] Integrated_intensity;
*[7] 0;
*[8] 0;
*[9] 0;

* = Columns not needed for conversion, can be any number

Example:

```
1,0,1, 209045.592443744, 142834.293217347, 50870.0478515625,0,0,0
1,0,2, 208435.743897142, 63666.8300319305, 10899.9936523438,0,0,0
1,0,3, 240230.942584511, 64285.0805918474, 8377.55151367188,0,0,0
1,0,4, 282032.840365532, 57774.6372087263, 6812.4140625,0,0,0
1,0,5, 127394.518568774, 86333.3469009349, 4333.64733886719,0,0,0
1,0,6, 286850.200721154, 38867.410435638, 2464.98876953125,0,0,0
1,1,1, 209045.196432015, 142698.726294003, 43768.1682128906,0,0,0
1,1,2, 208493.705895093, 63104.1156726907, 4010.64306640625,0,0,0
1,1,3, 240629.923029567, 64106.8561613844, 9554.67211914063,0,0,0
1,1,4, 281878.790360555, 57749.7140474961, 6441.98608398438,0,0,0
1,1,5, 125282.625184993, 89023.4809920917, 2805.40869140625,0,0,0
1,1,6, 283664.077863468, 38413.2870736027, 3613.64709472656,0,0,0
1,1,7, 58150.0695109681, 53421.1913628692, 9916.34057617188,0,0,0
```

NOTE: when generating .ascii files, a trajectory .id file containing the Trajectory ID (Trajectory#) of each .ascii data line (row) is generated (with the same name and in the same folder as the .ascii), which is then used to convert back from the .ascii file format to other formats.

Each id data line (row) contains 1 value (column):

[1] Trajectory#;

Example:

1
2
3
4
5
6
7
8
9
10

TrackMate .csv file format:

The number of headers can vary (requires manual selection in the 'Set parameters' tab).

Each line (row) contains several comma separated columns, 4 of which must contain the following information:

- [] Trajectory #; (e.g., TRACK_ID)
- [] X-position; (e.g., POSITION_X)
- [] Y-position; (e.g., POSITION_Y)
- [] Time(s); (e.g., FRAME or POSITION_T)

The X,Y units for TrackMate files depends on how FIJI interpreted the microscope metadata. If FIJI was unable to read the metadata, the units will be set to pixels. It is highly recommended that the user adjusts the units in TrackMate to microns prior to conversion. The X,Y units will need to be manually selected in the 'Set parameters' tab.

The Time units for TrackMate files can vary depending on which column containing temporal information is used (e.g., columns with the heading 'FRAME' are in Frames and columns with the headering 'POSITION_T' are in seconds). The Time units will need to be manually selected in the 'Set parameters' tab.

The number and order of data columns can vary. As such, the number of the columns that contain Trajectory # information (e.g., TRACK_ID), X-position information (e.g., POSITION_X), Y-position information (e.g., POSITION_Y) and Time information (e.g., FRAME or POSITION_T) will need to be manually selected in the 'Set parameters' tab.

Example:

	A	B	C	D	E	F	G	H	I
1	LABEL	ID	TRACK_ID	QUALITY	POSITION_X	POSITION_Y	POSITION_Z	POSITION_T	FRAME
2	Label	Spot ID	Track ID	Quality	X	Y	Z	T	Frame
3	Label	Spot ID	Track ID	Quality	X	Y	Z	T	Frame
4				(quality)	(micron)	(micron)	(micron)	(sec)	
5	ID282628	282628	2	298.08950	21.768646719	36.30233107	0	55.17871248	1723
6	ID200706	200706	2	609.30944	21.773257041	36.38438244	0	7.621899925	238
7	ID192512	192512	2	640.43560	21.761712355	36.40632485	0	4.419420965	138
8	ID229377	229377	2	579.67681	21.762051124	36.42347658	0	20.91218760	653
9	ID270343	270343	2	181.92572	21.733771126	36.28705446	0	45.41115165	1418
10	ID286722	286722	2	156.44577	21.760403180	36.3576551	0	58.63738976	1831
11	ID245770	245770	2	187.68449	21.725414183	36.37344346	0	29.91115348	934
12	ID204808	204808	2	791.29510	21.809109041	36.37986998	0	9.319213774	291
13	ID184334	184334	2	665.27423	21.767030449	36.50159964	0	1.313016373	41
14	ID237583	237583	2	200.45962	21.799884501	36.30813471	0	25.26755899	789
15	ID266260	266260	2	256.41061	21.717192211	36.36169707	0	42.68904453	1333

In the example above, there are 4 headers, the column containing Trajectory # information is column #3, the column containing X-position data is column #5, the

column containing Y-position data is column #6, and the column containing Time information can be either column #8 (using time in seconds) or column #9 (using time in Frames).

Other (manual input) file format:

To convert trajectory filetypes other than the ones described above, the ‘other(manual input)’ option can be selected as the input filetype. This enables the user to manually select the parameters corresponding to the input file.

See Appendix 2 for detailed information on each of the parameters that can be set.

Appendix 2: Parameters

X,Y units parameter:

The spatial units of each trajectory centroid (pixels (px), microns (um) and nanometers (nm)) depend on the filetype.

Table 3: X,Y units for each trajectory filetype used in the Super Res Data Wrangler GUI.

Filetype	X,Y units
.txt (PalmTracer)	Pixels (px)
.trc (PalmTracer)	Pixels (px)
.csv (TrackMate)	The units in TrackMate depend on how FIJI has interpreted the microscope data. May be in pixels (px) if FIJI is unable to obtain the length units from the microscope, or in microns (um) if the units have been obtained correctly. We strongly suggest that the units are set in TrackMate to microns (um).
.ascii (before drift correction) (SharpViSu)	Pixels (px)
.ascii (drift corrected) (SharpViSu)	Nanometers (nm)
.trxyt (NASTIC, segNASTIC, BOOSH)	Microns (um)
Other (manual input)	Pixels (px), microns (um) or nanometers (nm)

Pixel size (um/px) parameter:

Internally the Super Res Data Wrangler GUI works in microns (um). Filetypes that are in pixels (px) therefore need to be converted using the 'pixel size (um/px)' parameter, which works as a conversion factor (default value = 0.106 um/px). This parameter will appear as an option in the 'Set parameters' tab only when converting between pixels and either microns or nanometers (nm). This parameter is not needed when converting between

filetypes that are in nanometers and microns as X,Y coordinates are instead divided or multiplied by 1000 as needed.

Time units parameter:

The temporal units of each frame acquisition (seconds (s) or frame # (Frames)) depends on the filetype.

Table 4: Time units for each trajectory filetype used in the Super Res Data Wrangler GUI.

Filetype	Time units
.txt (PalmTracer)	Frames (Frame # counting up from 1)
.trc (PalmTracer)	Frames (Frame # counting up from 1)
.csv (TrackMate)	Frames (Frame #) if using a time column such as 'FRAME' Seconds (s) if using a time column such as 'POSITION_T'
.ascii (before drift correction) (SharpViSu)	Frames (Frame # counting up from 1)
.ascii (drift corrected) (SharpViSu)	Frames (Frame # counting up from 1)
.trxyt (NASTIC, segNASTIC, BOOSH)	Seconds (s)
Other (manual input)	Seconds (s) or Frames (Frame # counting up from either 0 or 1)

Acquisition frequency (Hz) parameter:

Internally, the Super Res Data Wrangler GUI works in seconds (s). Filetypes that are in Frames (Frame # counting up from either 0 or 1) therefore need to be converted using the 'acquisition frequency (Hz)' parameter, which works as a conversion factor (default value = 50 Hz). This parameter will appear as an option in the 'Set parameters' tab only when converting between Frames and seconds (s). To find the Acquisition frequency of a file, divide 1 by the Frame time (seconds): e.g., for a file where a frame is acquired every 0.02 seconds, $1/0.02 = 50\text{Hz}$.

Number of Headers parameter:

Headers refers to the number of rows at the top of the file that contain information (such as the data acquisition conditions and names of the data columns) before the start of the trajectory data.

Table 5: Number of headers in each trajectory file used in the Super Res Data Wrangler GUI.

Filetype	Number of headers
.txt (PalmTracer)	3
.trc (PalmTracer)	0
.csv (TrackMate)	The number of header rows in TrackMate files varies – this can be manually selected in the ‘Set parameters’ tab.
.ascii (before drift correction) (SharpViSu)	0
.ascii (drift corrected) (SharpViSu)	0
.trxyt (NASTIC, segNASTIC, BOOSH)	0
Other (manual input)	Manually select the number of header rows (between 0 and 10)

Delimiter parameter:

Delimiter refers to the character that separates the data into columns (e.g., comma, tab, 1 space, 2 spaces, 3 spaces, 4 spaces, semicolon).

Table 6: Delimiters separating data into columns for each trajectory file used in the Super Res Data Wrangler GUI.

Filetype	Delimiter / column number
.txt (PalmTracer)	8 tab separated columns
.trc (PalmTracer)	6 tab separated columns
.csv (TrackMate)	Columns are separated by commas. The number of columns varies – this can be manually selected in the ‘Set Parameters’ tab.
.ascii (before drift correction) (SharpViSu)	9 comma separated columns
.ascii (drift corrected) (SharpViSu)	9 comma separated columns
.id (SharpViSu)	1 column
.trxyt (NASTIC, segNASTIC, BOOSH)	4 space (1 space) separated columns
Other (manual input)	Manually select the delimiter type (comma, tab, 1 space, 2 spaces, 3 spaces, 4 spaces, semicolon)

Trajectory col parameter:

This refers to the number of the column that contains the trajectory ID / number (e.g., columns labelled with the heading 'Track', 'Trajectory #' or 'TRACK_ID'). Of note, for each line in a .ascii file, the ID of that trajectory is in a separate .id file that is generated at the same time as the .ascii file.

X-position col and Y-position col:

This refers to the number of the column that contains the X-position data and the number of the column that contains the Y-position data (e.g., columns labelled with the headings 'CentroidX(px)' and 'CentroidY(px)' or 'POSITION_X' and 'POSITION_Y').

Frame/Time col:

This refers to the number of the column that contains the Time data (in either seconds (s) or Frames) (e.g., columns labelled with the headings 'Plane', 'Frame#', 'Time(s)', 'FRAME' or 'POSITION_T'). This parameter will appear as 'Frame col' if the Time units are in Frames, and as 'Time col' if the Time units are in seconds.

Starting frame:

This parameter will appear if the Time units of the input file are in Frames. Some software starts numbering Frames from 0, whereas others start from 1.

Appendix 3: Defaults

Similarly to other GUIs in the NASTIC family of programs, the first time you run the Super Res Data Wrangler GUI, it will create a defaults file: `super_res_data_wrangler_gui.defaults`. This file contains the default values of the GUI. You can load it into a text editor or spreadsheet to view it if you'd like.

Screenshot of the `super_res_data_wrangler_gui.defaults` file when opened in Notepad:

```
Convert from filetype      txt
Convert to filetype        trxyt
Only find files with filenames that contain
Only find files with filenames that end with
XY units                  px
Pixel size (um/px)        0.106
Time units                 Frames
Acquisition frequency (Hz) 50.0
Number of headers          3
Delimiter separating columns tab
Column containing Trajectory# data      1
Column containing X-position data       3
Column containing Y-position data       4
Column containing Time data            2
Starting frame# 1
```

Table showing parameters saved in the default file, with the defaults values and potential options shown:

Parameter	Default value	Options
Convert from filetype	txt	txt, trc, trxyt, ascii, ascii(drift corrected), csv(TrackMate), other(manual input)
Convert to filetype	trxyt	txt, trc, trxyt, ascii, ascii(drift corrected)
Only find files with filenames that contain		Any text phrase that follows the rules for file naming (or left blank to find all files regardless of filename)
Only find files with filenames that end with		Any file extension (with or without phrase immediately preceding the file extension) (or left blank to find files of all file extensions)
XY units	px	px, um, nm

Pixel size (um/px)	0.106	Any decimal number (float) > 0
Time units	Frames	Frames, s
Acquisition frequency (Hz)	50.0	Any decimal number (float) > 1
Number of headers	3	Any whole number (integer) between 0 and 20
Delimiter separating columns	tab	tab, comma, 1 space, 2 spaces, 3 spaces, 4 spaces, semicolon
Column containing Trajectory# data	1	Any whole number (integer) between 0 and 20
Column containing X-position data	3	Any whole number (integer) between 0 and 20
Column containing Y-position data	4	Any whole number (integer) between 0 and 20
Column containing Time data	2	Any whole number (integer) between 0 and 20
Starting frame#	1	0 or 1