PULsE v1.5_07

Processing Unit for Laser flash Experiments
Quick start guide

February 5, 2020

This short guide contains information on installation, running, and basic functionality of PULsE v1.5_07. It does not contain extensive description of the numerical algorithms or techniques, which are detailed in the reference papers.

Contents

1 Installation

(a) Download and unzip the PULsE package, which should include the runnable .jar file and a folder with external libraries. Do not rename these files.

(b) PULsE requires Java 11 to run.

This can be downloaded at the Oracle website. You can use PULsE on any operating system that has support for JDK 11, including 64-bit Windows, Linux, MacOS, and potentially Solaris. Note that because Oracle does not offer support to 32-bit architecture starting from Java 9, you cannot run PULsE currently on a 32-bit operating system.

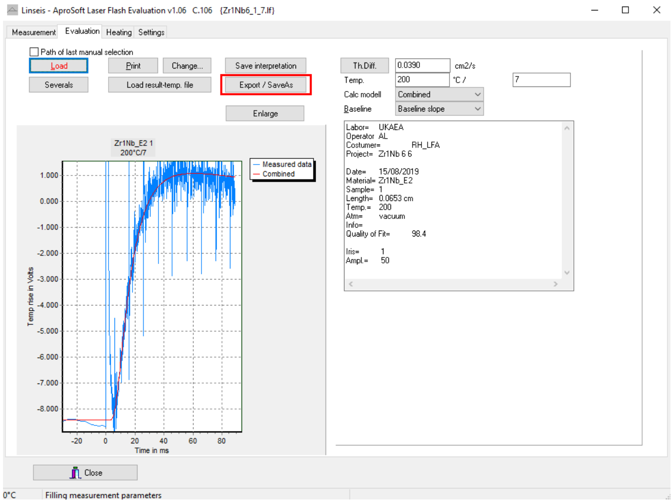
Terminal solution for Linux:

```
sudo add-apt-repository ppa:openjdk-r/ppa
sudo apt-get update
sudo apt-get install openjdk-11-jre
```

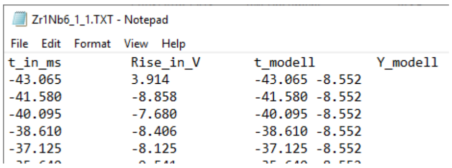
(c) Ensure the PULsE.jar is runnable.

Terminal solution for Linux: To allow the program to execute, open a terminal in the same folder as PULSE.jar, and into this type:

```
chmod +x PULsE.jar
```



(a) AproSoft Evaluation screen with the export button highlighted in red



(b) Exported .txt file example

Figure 1: Exporting in Linseis Aprosoft

2 Input file formats

2.1 LFR format

PULsE currently accepts the formats of files output by Linseis LFA systems. Note that by default the measurement results are stored in a binary (.lfi) format, but it is possible to export those curves in ASCII following the procedure below.

(a) After performing a shot, clicking "Export/Save As" in the Linseis AproSoft program (Fig. 1a) will export the data for the heating curve recorded as a .txt file (Fig. 1b). This should be done for any shot or curve you wish to analyse in PULsE.

(b) After all data has been recorded, click "Severals" in the Linseis analysis window (Fig. 1a) and select all exported heating curve .txt files for the experiment.

(c) Clicking "Ok" and "Save" on the following windows will create a .lfr file with file locations and data for all the heating curves (Fig. 2). Save this in the same folder as the .txt files.

MasterSheet_E2.lfr - Notepad

File Edit Format View Help

```
        Interval=5      Curve idx=0
Nr      File     Sample Temp in °C       Th.Diff. in cm2/s                Cp in J/gK      Density in g/cm3       Th.Cond in W/mK
1       Zr1Nb6_1_1.lf   \1       200.0   0.0351          0.000   0.000   0.000   Combined        98.8    0.106   C:\LFE\data\RH_LFA\Zr1Nb\Zr1Nb_E2\6
2       Zr1Nb6_1_2.lf   \1       200.0   0.0398          0.000   0.000   0.000   Combined        98.5    0.107   C:\LFE\data\RH_LFA\Zr1Nb\Zr1Nb_E2\6
3       Zr1Nb6_1_3.lf   \1       200.0   0.0356          0.000   0.000   0.000   Combined        99.2    0.108   C:\LFE\data\RH_LFA\Zr1Nb\Zr1Nb_E2\6
4       Zr1Nb6_1_4.lf   \1       200.0   0.0386          0.000   0.000   0.000   Combined        99.2    0.107   C:\LFE\data\RH_LFA\Zr1Nb\Zr1Nb_E2\6
5       Zr1Nb6_1_5.lf   \1       200.0   0.0415          0.000   0.000   0.000   Combined        99.1    0.105   C:\LFE\data\RH_LFA\Zr1Nb\Zr1Nb_E2\6
```

Figure 2: Example .lfr file generated from "Severals"

2.2 DAT format

PULsE also accepts ASCII data for individual shots in a .dat format, where the first row gives the temperature (in degrees Celsius), with a two or three column table below, with columns of time (in seconds) and sample-furnace temperature difference (in degrees Celsius) respectively:

```
587.863
0.0000000   -0.01227   5.99260742187500E+0002
0.0002720   -0.04987   5.99349670410156E+0002
0.0005440    0.25281   5.99201477050781E+0002
0.0008160    0.24573   5.99171752929688E+0002
0.0010880    0.17072   5.99260742187500E+0002
0.0013600    0.13086   5.99245910644531E+0002
0.0016320    0.12146   5.99216247558594E+0002
0.0019040    0.12384   5.99334838867188E+0002
0.0021760    0.11682   5.99320007324219E+0002
0.0024480    0.12854   5.99260742187500E+0002
...             ...                ...
```

2.3 Metadata

Ideally, metadata for each shot should be recorded during the experiment in a tab delimited ASCII format, with a .met file suffix (Fig. 3).

(a) Constant data should be recorded in tab-separated pairs at the top of the file, such as Sample_Name, Thickness (of the sample, in mm), Diameter (of the sample, in mm), Spot_Diameter (diameter of laser spot, in mm), PulseShape (in capitals; e.g. TRAPEZOIDAL, RECTANGULAR) and Detector_Iris;

(b) Two line breaks below, a tab-delimited table with headers for variables should contain variable data for each shot. These variables should include ID (which should relate to the final number of the file name for each shot), Test_Temperature (in °C), Pulse_Width (the time width of the laser pulse, in ms), Absorbed_Energy (the energy transmitted by the laser, in J), and Detector_Gain (gain of the detector). If any of the "constants" listed above are variable, then they should be included in the variable table, and vice versa.

```
Zr1Nb_E2_200_to_850_Metadata.met - Notepad
File  Edit  Format  View  Help
Sample_Name     Zr1Nb_E2
Thickness       0.653
Diameter        10
Spot_Diameter   2
PulseShape      TRAPEZOIDAL
Detector_Iris   1

ID      Test_Temperature        Pulse_Width     Absorbed_Energy Detector_Gain
1       200     1.2     9.83    50
2       200     1.2     9.83    50
3       200     2       15.68   50
4       200     1.8     14.22   50
5       200     1.8     14.22   50
```

Figure 3: Example metadata .met file

2.4 Specific heat (C_p) and density (ρ) file formats

Specific heat and density at different temperatures can be read as ASCII files with a .tbl suffix (Fig. 4), where the first column is temperature (in °C) and the second column is the specific heat capacity (in $J \times kg^{-1} \times K^{-1}$) or density (in $kg \times m^{-3}$).

```
UO2_Specific_Heat.tbl ...
File  Edit  Format  View  Help
-273    0.0
0       218.2648368
50      239.0325626
100     253.2270824
150     263.2550148
200     270.5584236
250     276.0222064
300     280.2062572
350     283.4759085
400     286.0764962
450     288.1771373
```

(a) Example specific heat capacity .tbl file

```
UO2_Density.tbl - Notepad
File  Edit  Format  View  Help
-273    11000.00
0       10959.84
50      10943.82
100     10927.80
150     10911.77
200     10895.73
250     10879.67
300     10863.56
350     10847.41
400     10831.21
450     10814.93
```

(b) Example density .tbl file

Figure 4: Example .tbl input files

3 Basic use and loading curves

3.1 Opening and quitting PULsE

Open PULsE by clicking the PULSE.jar file. If this does not work, please run the software manually by typing the followings commands in the terminal/console (assuming PULsE.jar is in your current working directory, otherwise change directory):

```
java -jar PULsE.jar
```

PULsE can be quit by clicking the cross in the top right corner, which will prompt a confirmation. You may want to save any results or export your data (see "Save

Results", section ??) and export your fits (see "Export and Export All", section ??) before quitting.

3.2 Loading heating curves and metadata

Launching PULsE should open a frame (Fig. 5).

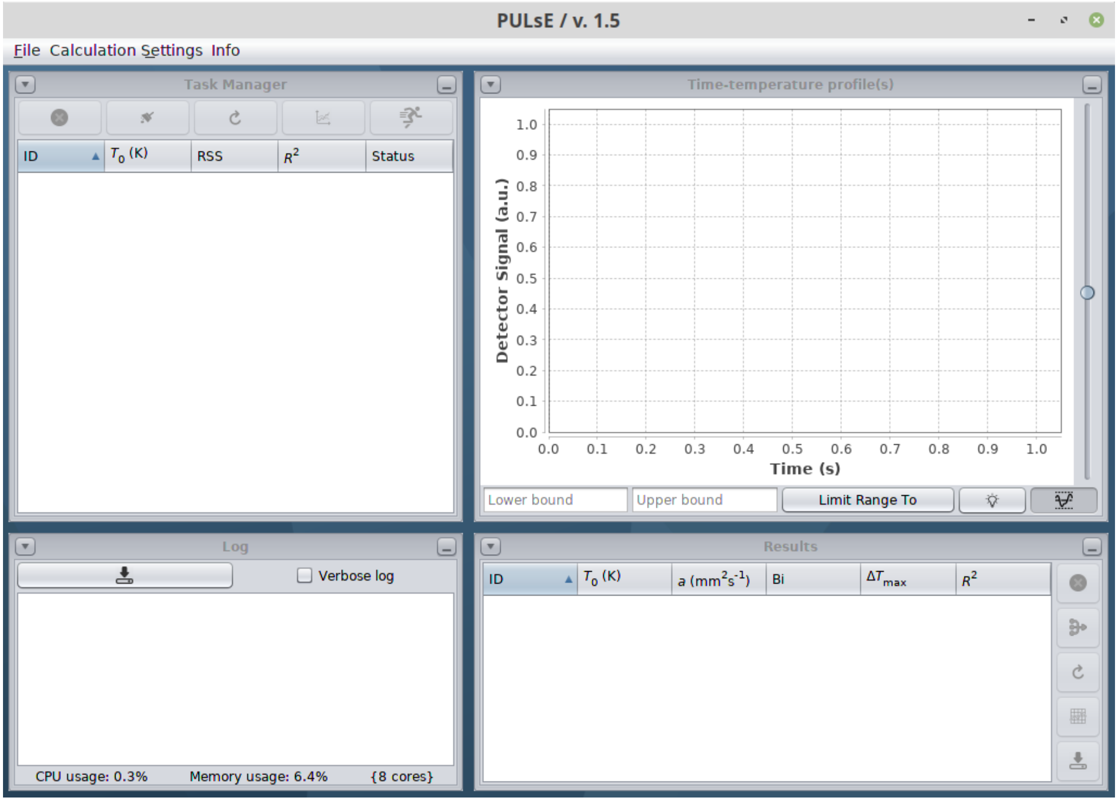


Figure 5: Main view.

(a) Loading data, changing calculation settings, exporting data and program information can be done using the menu bar at the top;

(b) The task pane is found on the left top quadrant. Going clockwise, you should see the following: the graph internal frame, the results table, and the log pane.

(c) At the top left, select "File - Load Data" and then "Load Heating Curve(s)...". Select the files (either .lfr or .dat) containing the data measured by the machine. Separate tasks will be assigned to each heating curve, appearing in the task table (Fig. 6).

(d) Clicking "File - Load Metadata..." and selecting your metadata file for this dataset will fill in the experimental parameters for each task.

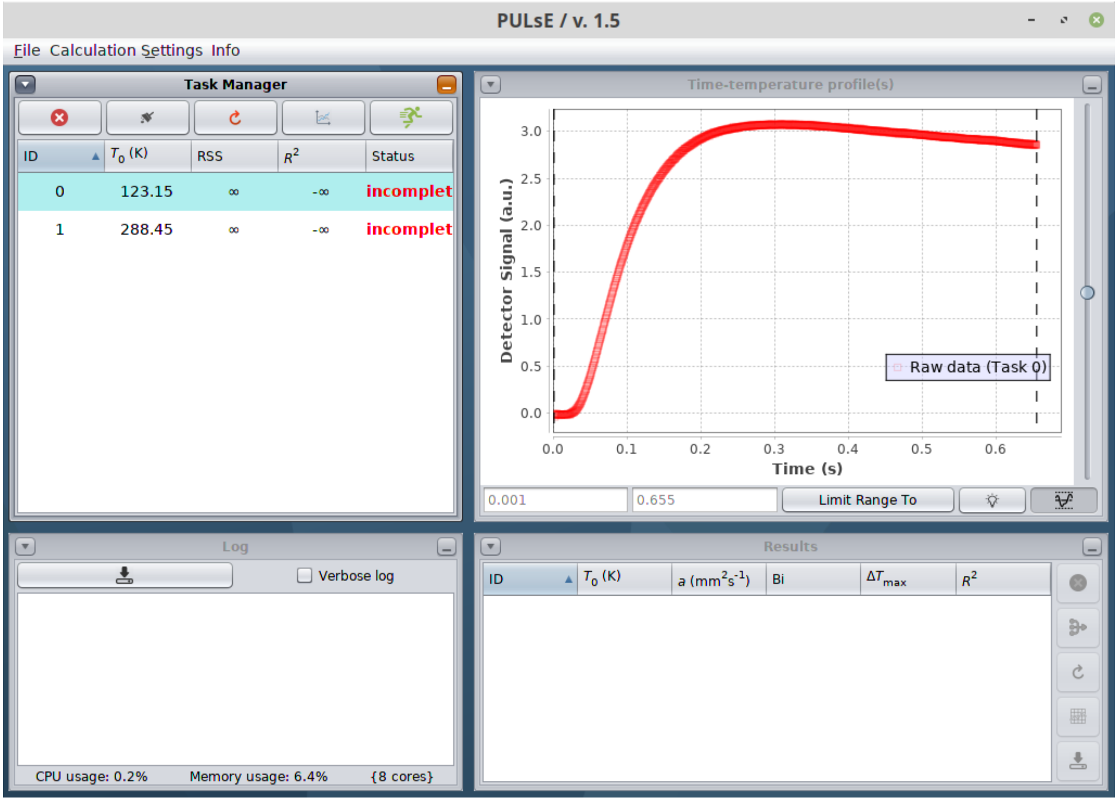


Figure 6: After loading the heating curves.

(e) A message about data truncation may appear. If the acquisition time for any heating curves is deemed to be too long, PULsE can automatically truncate data if you click "Truncate". This will generally aid accuracy of results, as otherwise the model estimates might be biased.

3.3 Managing tasks

(a) The task table shows the task ID for each (an internal value, not necessarily related to the ID of the shot's metadata), the ambient temperature at the time of shot T_0 (in Kelvin), the residual sum of squares, the coefficient of determination R^2 value of the minimisation procedure (if started), and the Status of each task.

(b) These columns can be sorted by clicking the corresponding header of the table. Click the same header again to reverse the sorting direction.

(c) Right-clicking on a selected task will bring up a menu, with the following options:

"Metadata" shows the metadata for the selected task. The units here are SI (distances in metres, energy in Joules, temperature in Kelvin) so may differ from the values in the metadata file;

"What is missing?" shows any outstanding actions before the tasks can be run;

"Show basic $T(t > 0)$ profile" shows a graph excluding the baseline data prior to the laser being shot;

"Show extended $T(t)$ profile" shows the complete time-temperature profile;

"Reset" will reset the task to its original state when loadedl

"Generate result now" will quickly calculate an estimated solution for the selected heating curve, either using the Parker's solution (if the task has not yet been executed) or using the most recent parameter values (if it has been executed). The result will be found in the results table;

"Execute" will execute a full calculation for the selected task only. The result will be found in the results table.

(d) The toolbar above the task table lets you manage all tasks at once, by removing or resetting all of them, removing only a specific tasks, and submitting all tasks to execution.

(e) The bottom of the frame shows the CPU and RAM usage and the available CPU cores. The corresponding labels will turn red if the CPU or RAM usage gets too high (above 75%) or amber (if above 50%).

4 Calculation Settings

To select or change the settings for the calculation, select the "Calculation Settings" menu in the top of the window.

4.1 Heat Problem: Statement & Solution

(a) Selecting this item opens an internal frame, allowing the user to choose the heat transfer model and specify any parameters that will be used for calculation (Fig 7). In addition to selecting a problem statement, the user must also select the difference scheme that will be applied to solve this problem;

(b) All values and settings can be edited by clicking on the text fields with their values. Note that by default all changes are made to all tasks. If the use wishes to edit only one task, the checkbox "Apply to all tasks" should be unticked. Conversely, if the user is interested in entering an expert mode, the checkbox "Keep it simple" should be unticked;

(c) C_p and ρ data tables can be loaded using the "Load C_p" and "Load ρ" buttons at the bottom of this window, allowing calculation of thermal conductivity. This is not necessary for thermal diffusivity calculation.

(d) Click the cross in the top right of the menu to return to the task view.

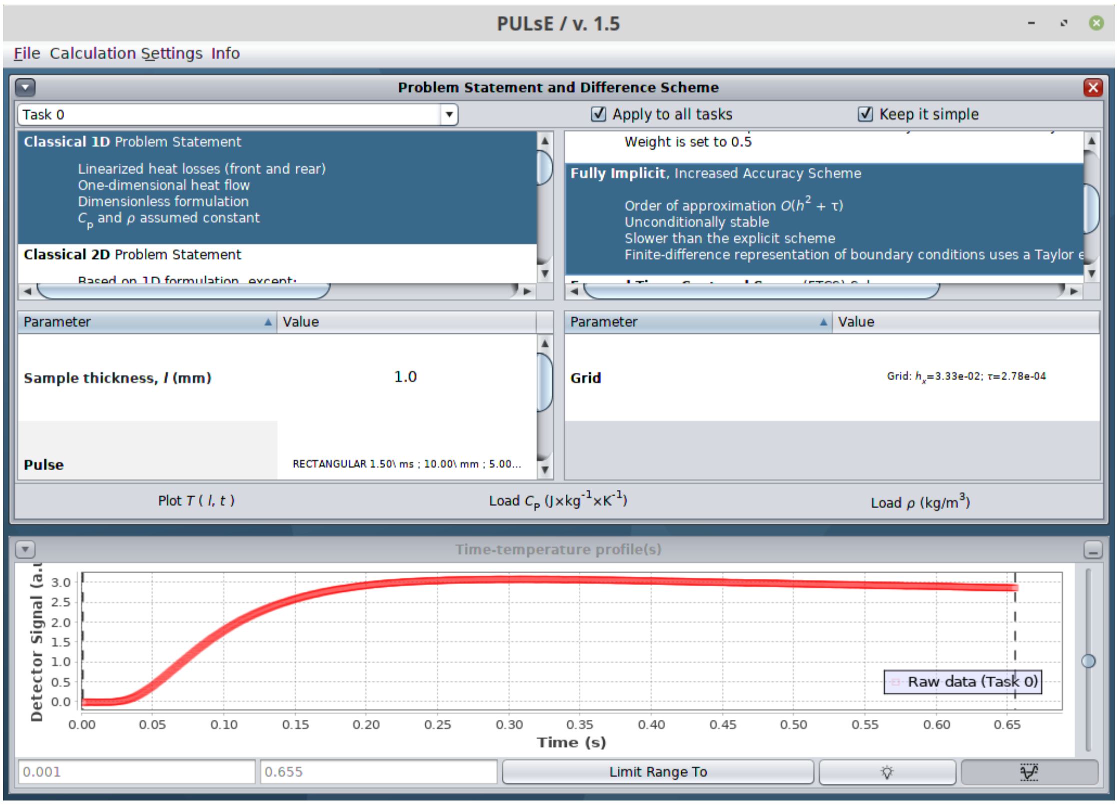


Figure 7: Choosing the heat transfer model and parameters.

4.2 Parameter Estimation: Methods & Settings

(a) This will show up an internal frame where the user is required to select the search algorithms, the dimensionality of the optimisation vector, and may modify other settings used in the parameter estimation algorithm (Fig. 8).

(b) Choose one option from the top two panels. Typically, select "Approximated Hessian Method" and "Wolfe Conditions".

(c) After this, the user can choose to include an arbitrary number of variables in the optimisation vector by selecting or deselecting the corresponding checkbox in the bottom table. By scrolling this table to the bottom, other settings (resolutions) can be edited.

4.3 Change Result Format

Selecting this menu item allows the selection and ordering of results in the result table. The user can type any combination of allowed characters in text field, which will set up the output format. Hover over the headers in the result table for a tooltip definition. The results can be sorted by clicking the header similar to the task table. The columns

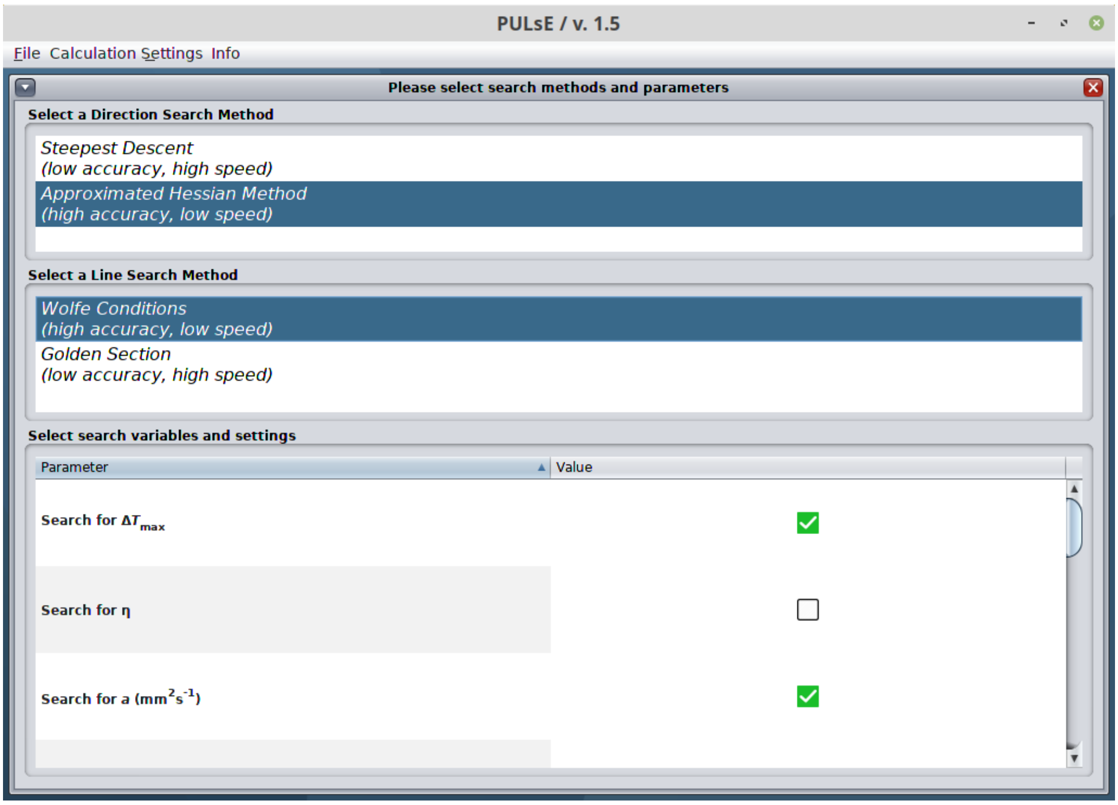


Figure 8: Search settings view

can also be rearranged by clicking and dragging the column headers into the desired order.

5 Execution

Clicking the "Execute" action will submit a batch of tasks to a dynamic queue for parallel processing using multiple threads, according to the settings previously selected. When execution is in progress, the running man green icon is replaced by a red stop sign. Pressing this button during execution will cause tasks to terminate prematurely, which changes their status to "terminated". The calculation can be resumed at any time.

5.1 Statuses

The statuses of tasks will change as a result of this (Fig. 9).

(a) "ready" means that the settings have been chosen for the task, but calculation has not yet been executed;

8	473.0	∞	-∞	ready
9	473.0	∞	-∞	queued
10	572.0	306.95689	0.98184	done
11	573.0	509.31304	0.95583	timeout
12	573.0	∞	-∞	incomplete
13	573.0	455.79095	0.95646	terminated

Figure 9: Examples of tasks with statuses

(b) "queued" means that the task will execute once other tasks have finishing executing;

(c) "done" means that the calculation for the task has completed. You can find the results for this task in the results pane;

(d) "timeout" means that the calculation took too long to complete. This may be due to an error in calculation (if the R^2 looks particularly low) or due to the search algorithm being unable to find the optimal values fast enough. The results will not be shown in the results table. Right-clicking the task and clicking "Execute" for this task only will continue calculation, and may be able to complete the calculation. Right-clicking the task and choosing "Generate result now" will generate a result immediately based on the most recently output values;

(e) "incomplete" means that no execution has taken place yet as the settings (heat problem and least squares methods) have not yet been chosen. Additional status description may be shown on request;

(f) "terminated" means that the execution was manually stopped before completion. Similar to tasks with a "timeout" status, re-executing may allow completion of the calculation.

5.2 Charting

Switching between tasks in the task table or in the settings view, pressing the "Graph" button in the task toolbar, or selecting the corresponding option from the pop-up menu for individual tasks will result in the calculated solution to be shown in the top-right internal frame, along with the raw data (Fig. 10). Raw data is plotted as a scatter chart, while the solution is plotted as a line series. It may happen that the solution line is not visible because of dense raw data – in this case try moving the slider on the right down, this will decrease the opacity of raw data.

The graph toolbar combines the following elements:

(a) Search range selection tools. The text fields show the current search domain for the selected task. Both the lower and upper bounds may be changed by entering their respective values in the text fields and pressing the "Limit Range To" button.

This will show a confirmation dialog where the user will be prompted to confirm their choice. Note that the bounds will not be changed if the button is not pressed. Selecting and confirming a new search range will result in the vertical dashed lines in the graph to shift according to the selection. Only the raw data contained between these vertical lines will be used to calculate the sum of squared residuals;

(b) A "Sanity Check" toggle button. When activated, this will show how the calculated solution deviates from the analytical solution of the adiabatic problem given by Parker *et al.* Note that the model and the Parker's solution will be different in most of the cases [1];

(c) "Plot Residuals" toggle button. When activated, this will show a graph of residuals. The residuals are calculated by comparing the raw data values to the interpolated values from the solution curve. If the parameters are chosen appropriately and if no systematic error is present in the calculations or in the experimental data, the graph of residuals will show white noise. For more details, please see [1].

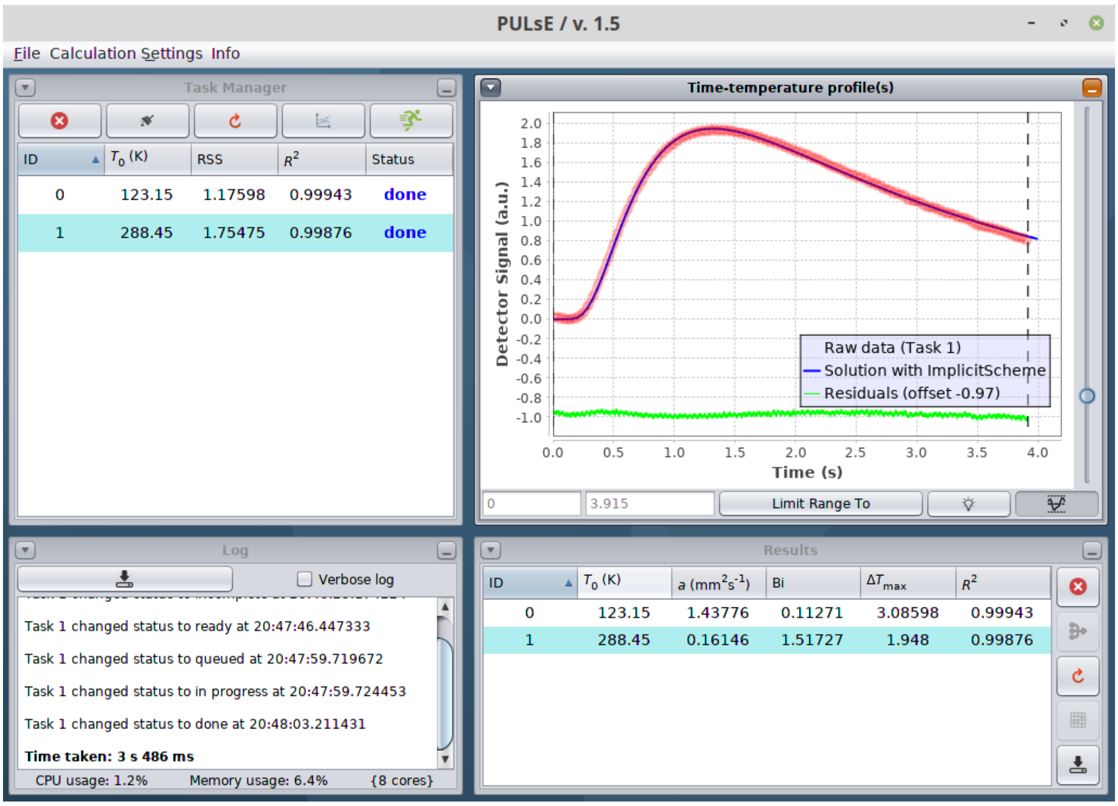


Figure 10: All tasks completed successfully.

6 Results

Once execution has completed, the result table at the bottom right will look similar to Fig. 10.

Actions that can be performed on these results are as follows:

(a) “Delete Entry” removes the selected result from the table.

(b) “Merge (auto)” allows calculating averages (and averaging errors) for tasks that are within a small interval of ambient temperatures. Clicking this will bring up a context window. The results will be grouped according to the selection;

(c) Clicking “Undo” returns the results to their individual values, ungrouping them;

(d) “Preview” allows you to plot the results on a chart. Clicking it brings up the preview mode, which includes a large chart panel on top with the results plotted against user-selected axes and the results table in the bottom. Chart axes are selected by clicking the combo boxes. Any column of the results table can be selected as an axis. Clicking the ”Preview” button will update the chart, e.g. after merging or removing specific results (Fig. 11). The graph can be saved as a .png image, but the users are recommended to use the results table to produce cleaner graphs. Along with the axis selection, the preview panel has a toggle button enabling spline fitting of data. This can be turned off or on (on by default);

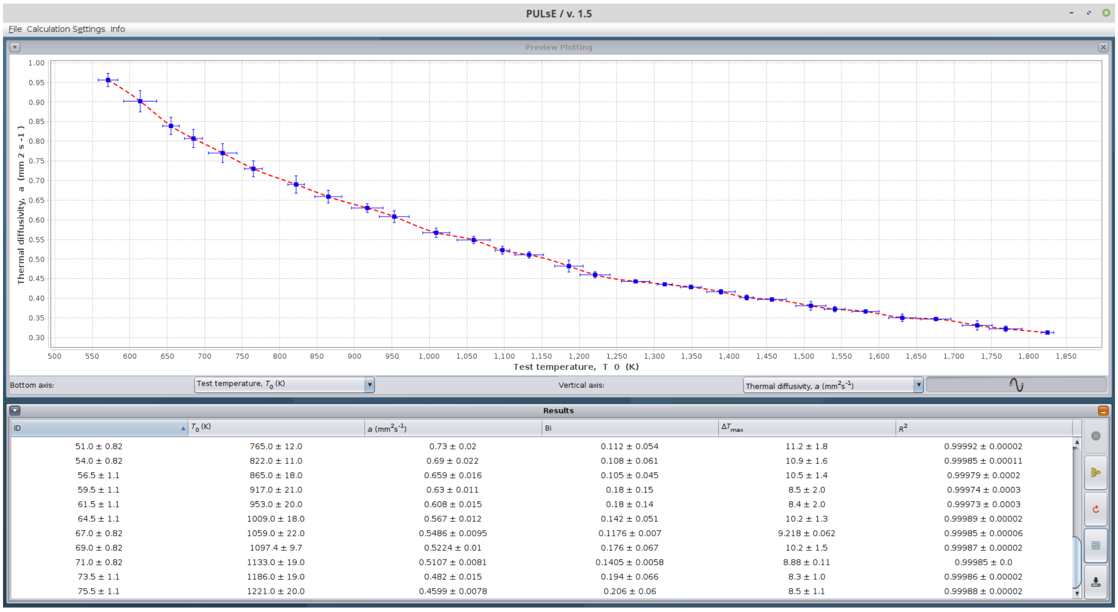


Figure 11: Preview mode.

(e) “Save” button allows to export the results in an .html or .csv format. Saving while the results are merged will save both the merged results and the individual results.

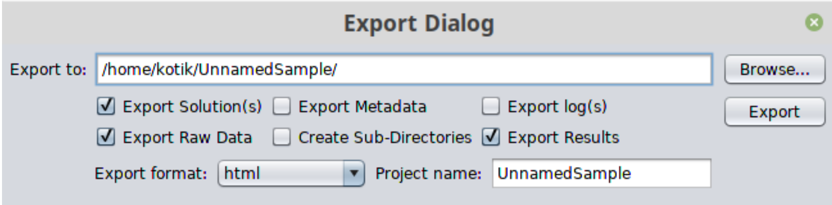


Figure 12: Export dialog.

6.1 Export

Clicking "File - Export..." in the main menu brings up the export dialog (Fig. 12). The destination directory is shown in the non-editable text field at the top, which is updated by clicking the "Browse..." button. A file chooser dialog is then initiated, which allows to choosing a parent directory for the exported data. By default, files are saved in a sub-directory in the user's home. Editing the project name (bottom right) or selecting a new parent directory will be reflected in the text field on the top. The exported format is selected with the combo box in the bottom left. If the selected format is unsupported for this specific data type, the export will revert to the default format (html), but only for this specific category of property holders. Names of all exported files are formed of the prefix, which indicated the type of the exported data, and the ID of the task, to which this property holder belongs to, and which matches the ID in the task table and the results table. Finally, after configuring the desired output, the "Export" button may be pressed creating a new directory (if necessary) and populating it accordingly.

7 Log

The log pane is found in the bottom right of the main window, and displays the status of currently executing tasks. Ticking the "Verbose log" checkbox forces more information to be written in the log pane to show the changes in various search parameters while trying to reach the minimum of the sum of squares. By default, this option is not selected, and only time events, such as change of statuses and task completion, will be recorded in the log. In addition, any errors that come up during execution will also be shown in this frame as red text. Clicking "Save Log" saves the current contents of the log to a location of choice.

8 Advice to maximise accuracy

8.1 Identifying systematic errors

The Preview graph is useful for identifying which data points may arise from erroneous heating curves or searches, if any points are far outside the expected range. Once the corresponding task is identified in the results table, it is mandatory to review the heating curve graph for that task to see if the calculation has been done correctly. Incorrect calculations are usually easy to identify, since they reveal an ordered arrangement of the residuals, e.g. slopped data sample. If this is the case, the user needs to:

(a) manually change the search range, as explained in Sect. 5.2;

(b) change the individual heat problem parameters (Sect. 4.1);

(c) or revise the optimisation vector by including additional or excluding redundant variables (Sect. 4.2)

. The result of the task needs to be removed from the table of results, and the task needs to be re-executed by right clicking on it the task table and pressing the Execute menu item again. This is the art of fine tuning in the laser flash analysis, explained in more detail in [1].

8.2 Changing individual settings

Open the problem view from the main menu, use the combo box on the top-left to select the task that needs to be adjusted. Ensure that "Apply to all tasks" and "Keep it simple" are unticked. Changing settings such as the initial thermal diffusivity a, baseline slope and baseline intercept to expected values and re-executing only that task (through the right-click menu) may also improve results. Comparing the fitted baseline to the $\mathrm{T}(t < 0)$ data seen in the "show $\mathrm{T}(t)$ profile" in the right-click menu may be of use when choosing values for the baseline.

9 Troubleshooting

9.1 Errors

If you encounter any errors, red text should appear in the log. If you are able to, copy this text into an email or save it to a file, and send it to the lead developer with the subject "PULSE Bug". If the error disappears before you can copy it, try running PULSE from the Terminal by opening a terminal in the same folder as PULsE.jar and typing:

```
java -jar PULSE.jar
```

and repeating what caused the error.

If any issues or errors cannot be resolved, please contact Dr. Artem Lunev (email `artem.lunev@ukaea.uk`) with the subject "PULsE Bug" and detail what you were doing before the error or issue occurred.

9.2 Ensure proper metadata formatting

Make sure the variable names in the metadata file is correct (see Sect. 2.3), especially if the metadata for a given task is not as you expected or if an error is encountered immediately after loading the metadata.

9.3 Ensure there are no unexpected zero values in the .lfr file

If the heating curve recorded by Linseis is erroneous, it may record a zero in the .lfr file for a crucial parameter. This can cause "divide by zero" errors in the program, often resulting in an infinity handling error. Remove this heating curve from the file and try again.

9.4 Check CPU and RAM usage

During execution, CPU or memory usage can be very high; this can cause the program to be slow to respond if run on a low-end computer. Usually, this will return to normal after execution is complete. If not, try removing half of the tasks from the queue before executing next time, which may improve performance. Opening graphs multiple times sequentially may increase RAM usage. If this gets too high, then it may cause performance issues on low-end computers.

10 For the lazy

Install PULsE and create the .lfr and .met files as detailed at the start of this manual. To quickly analyse a dataset:

(a) Open PULsE;

(b) "File" → "Load Heating Curve(s)..." and load the .lfr file containing your curve details;

(c) "File" → "Load Metadata..." and load your .met metadata file;

(d) "Calculation Settings" → "Heat Problem: Statement and Solution" to open the problem view. Select "Classical 1D Problem" and "Fully Implicit", ensure the sample thickness is correct, and close the view (cross at the top-right corner – be careful not to confuse this with quitting the program!);

(e) "Calculation Settings" → "Parameter Estimation: Method and Settings" to load the search view. Select "Approximated Hessian Method" and "Wolfe Conditions", and tick the checkboxes for rear-side heating, thermal diffusivity, baseline intercept (and baseline slope if you suspect the baseline is sloped). Close the view (again. ensure you are not quitting the program).;

(f) Click "Execute" and wait until all tasks have the "done" status. Right-click → "Execute" any tasks with the "timeout" status;

(g) "Merge (auto)" → "10" → "Apply";

(h) "Preview" → choose "T_0" as horizontal axis, "a (mm^{2}s^{-1})" as the vertical axis → "plot" → Save or Export graph. Close the preview mode;

(i) “Save results” and choose the directory, file name, and extension (you may want to select .csv);

(j) “File” → “Export...”, choose the location to export and the project name.

References

[1] Artem Lunev and Robert Heymer. Increasing the accuracy of laser flash analysis using noise-robust numerical algorithms in pulse. *arXiv preprint arXiv:1910.07499*, 2019.