Parameter fitting tool for the TLVP model – User guide

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Important note

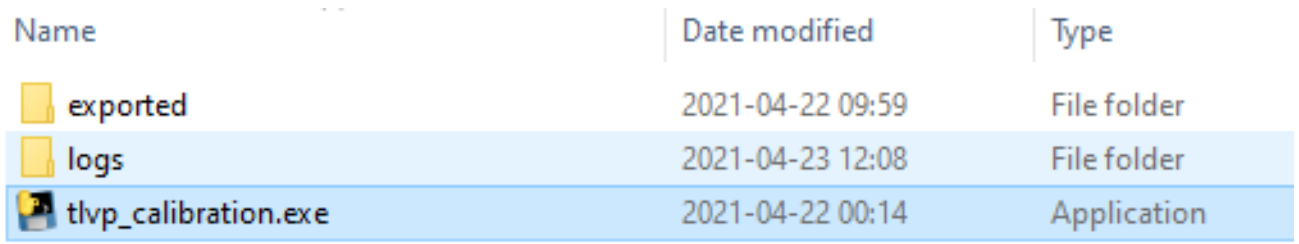
This program is distributed as an executable. Windows Defender (and other antivirus tools) may flag it as a dangerous application as the file has an “Unknown Publisher”.

I assure you it is not dangerous. This program will fit the TLVP parameters to measurement data and write some logs during the process. And nothing else.

This is simply a research tool, and I hope you find it useful in your work.

Installation

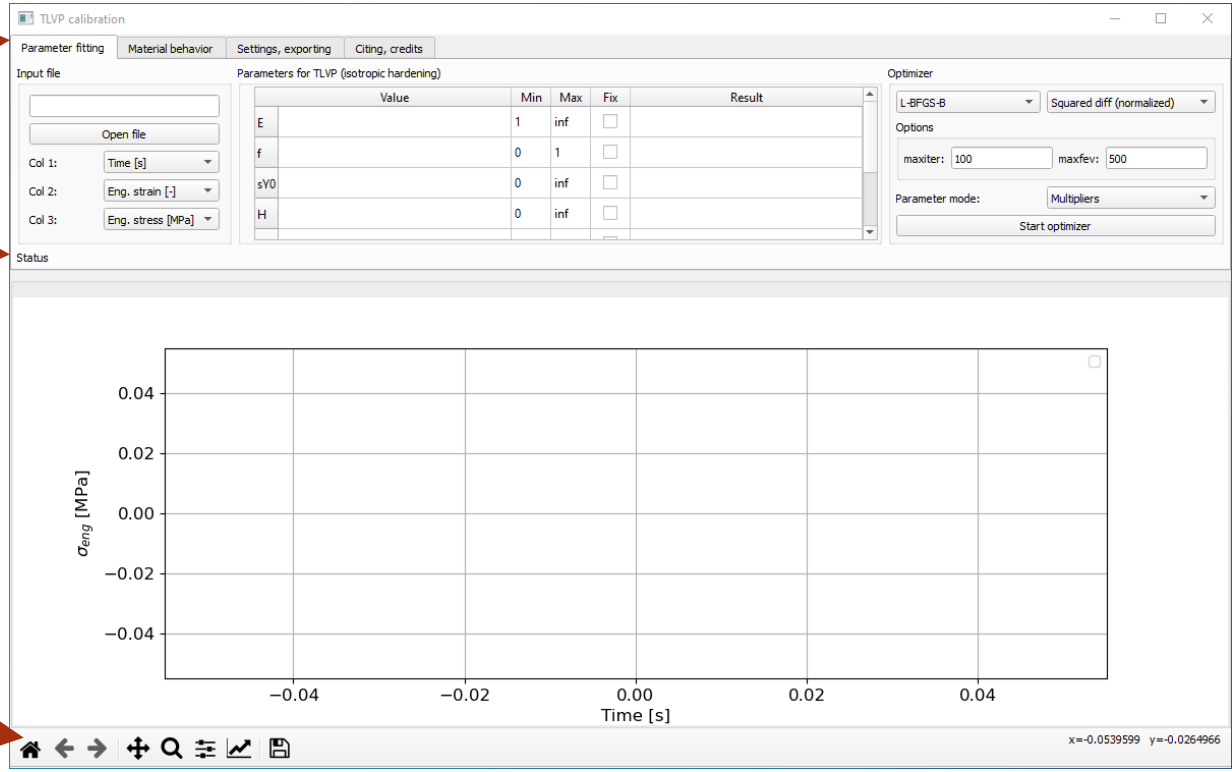
1. Download the executable from the website
   - This is the program itself, no real installation needed
2. Move it into some folder
3. Create folders named „logs” and „exported” in the same folder
   - This is not necessary if the program has permission to create the folders
4. You are done!



Recommended file structure

Using the program

- Features are organized in groups
- Status messages
- A command window opens with the GUI, don’t close it
- Plot controls



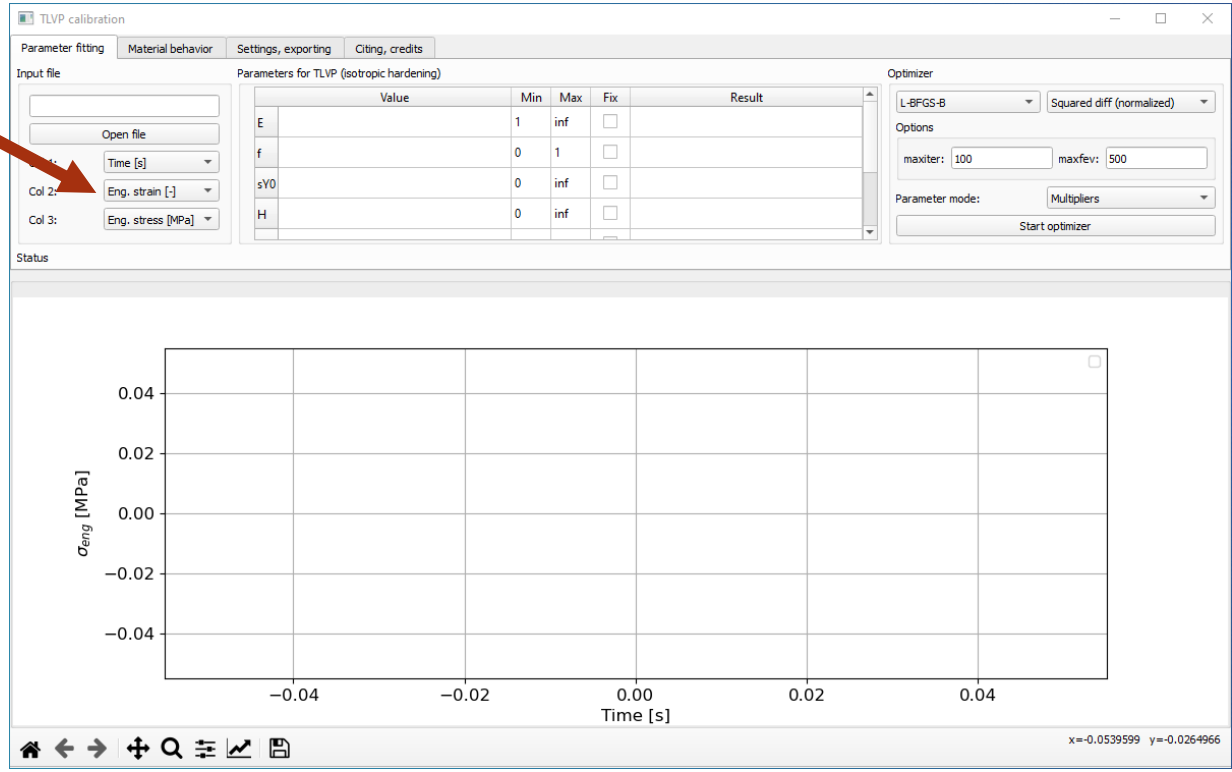
Parameter fitting (1): input file requirements

- .csv (or other text-based) format
- Separator: comma (,)
- Has 3 columns with time, strain, and stress data (additional columns are neglected)
- Time data in increasing order (equality not allowed)
- Lines with the same data as the line before are ignored
- Lines starting with # are ignored
  - You can use this to create headers

```
#header
#more header
0.,0.,0.
0.060603565066428104,0.0011993375389573004,0.4344397641987027
0.12120712912275561,0.002418403718207551,0.8707333925802879
0.18181069418918372,0.00363500383593981,1.2996113391077362
0.2423650409784661 6,0.004631300675787249,1.6475339383800032
0.2929686060448943,0.005855299031945852,2.0621983506565416
0.3535721701012217 7,0.007063678859320219 5,2.4663571071824077
0.4141757351676499,0.008273702750153402,2.851976471207087
0.4747792992239774,0.009496057056321283,3.2202924022306596
0.5353729996488042,0.010690751416688415,3.5722578198860937
0.5959765647152324,0.011918037886296 56,3.9121466824078466
0.6565801297816605,0.013120663525235303,4.2316422131782945
0.7171836938379881,0.014334797554513388,4.539087138822971
0.7777872589044161,0.015555507797222453,4.828610651716501
0.8383908229607436,0.016749913172739 49,5.097122853108685
0.8989943880271708,0.017978843692338358,5.353584449375099
0.9595979520834984,0.019179003256291016,5.5882622598481255
1.0202015171499264,0.020398891474004723,5.811198454279386
1.0808050822163544,0.021614669553273 53,6.015904246875494
1.141408646272682,0.022811541003776654,6.2046970605125775
1.20201221133911,0.024039649498380153,6.383602198149027
1.2625665581283925,0.025043344590122033,6.5180127937826295
1.3131701231948216,0.026252546442491757,6.671580761667458
1.3737736872511481,0.027476544798650363,6.813561608843537
1.4343772523175753,0.028669306124176674,6.9441098314349
1.4949808163739038,0.029898236630307454,7.062452953567473
1.555584381440331,0.031100040257718932,7.176624711991773
1.6161879465067 6,0.032314996311992 37,7.2870885927068505
1.6767915105630866,0.033534884529706 07,7.378781337525708
```

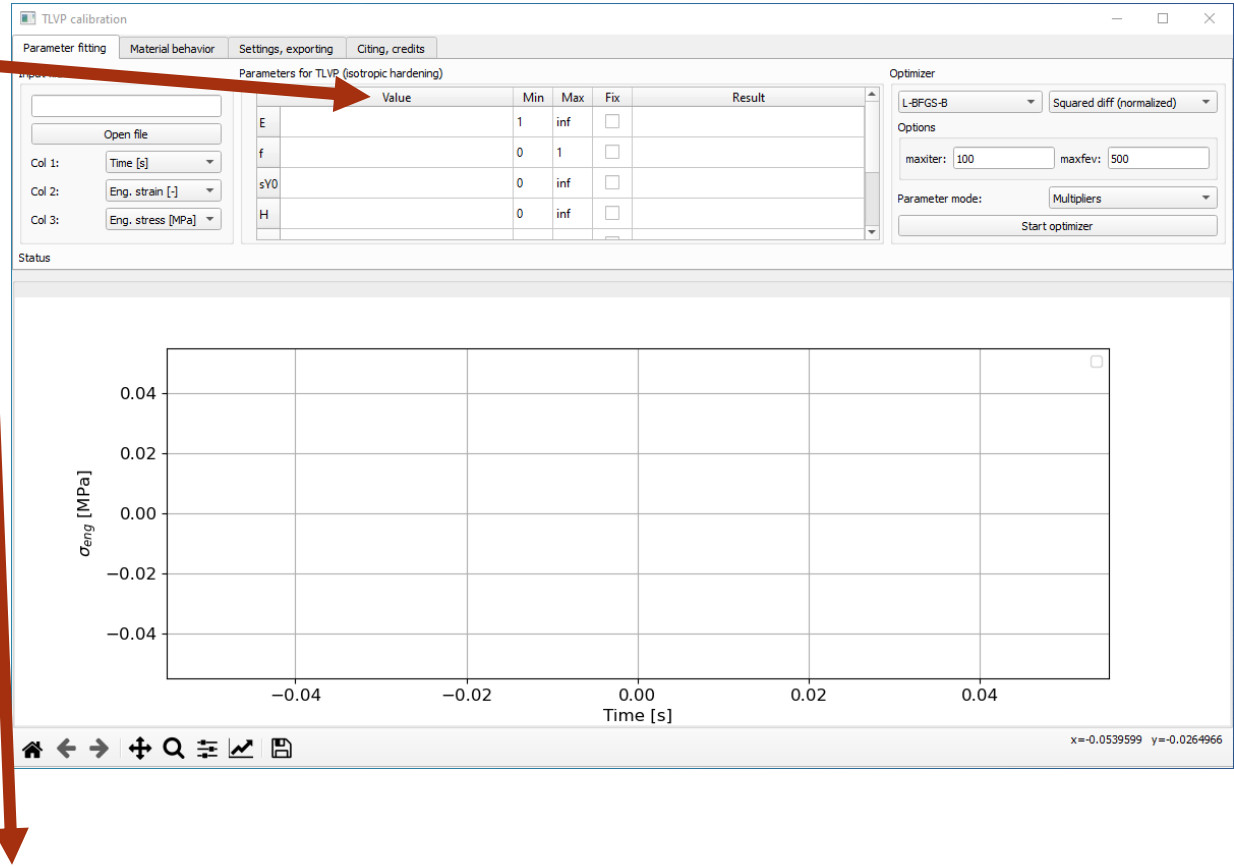
Parameter fitting (2): reading an input file

- The order of the columns in the input has to be given *before* opening the file
- True strain and stress are converted to engineering strain and stress internally
  - Assumption: incompressible material
- Successful input status message:
  - „File read done, valid input”



Parameter fitting (3): initial values

- Initial guess is put in the first column
  - Missing value: filled up from table below
- sY0: better to use a „too low” value, than a „too high” one
  - If sY0 is too high, plastic deformation never starts, the optimizer cannot fit sY0 and H.
  - If sY0=0, plastic deformation is always present, this is also undesirable

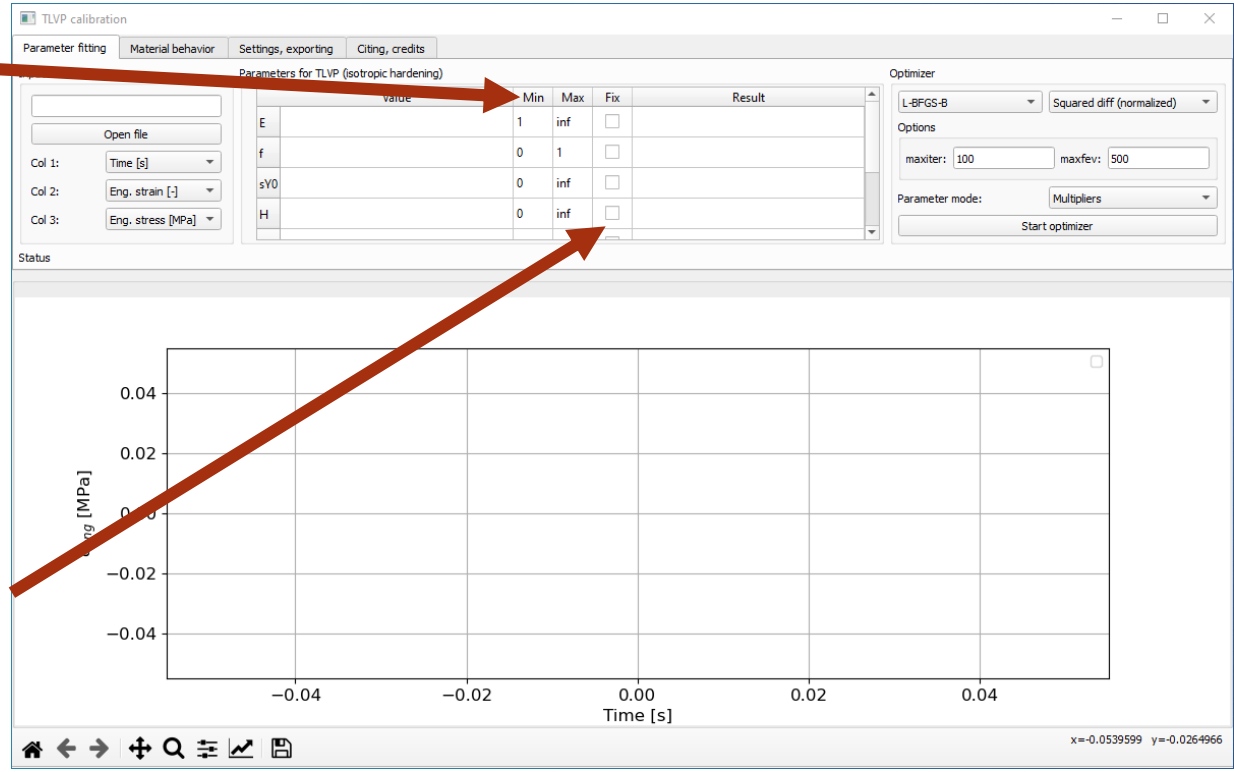


E [MPa]	f [-]	sY0 [MPa]	H [MPa]	A [$MPa^{-n}s^{-m-1}$]	n [-]	m [-]
1000	0.5	10	100	0.001	2	-0.5

Parameter fitting (4): boundaries, fixing

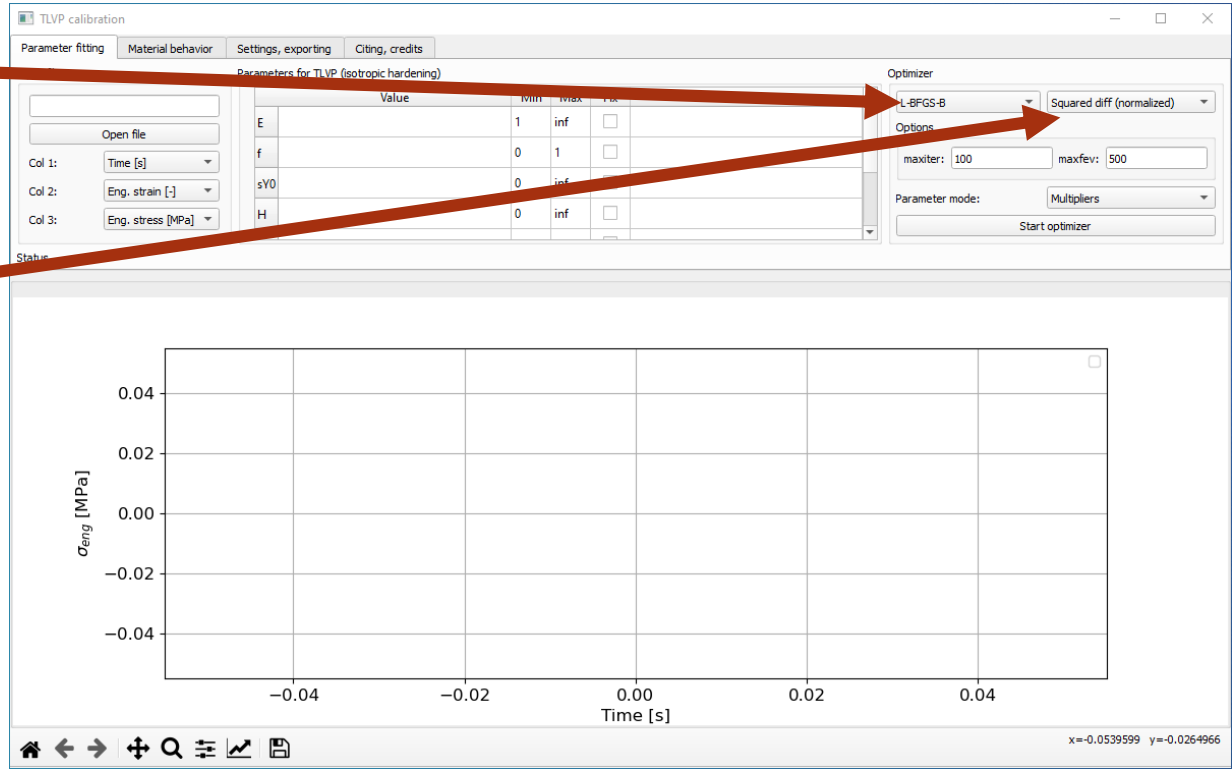
- Min and max for the optimizers
  - Not all algorithms keep them strictly
- „Focuses the search” in a narrower range
- Too small range:
  - Can lead to stability issues
  - The optimum might not be found, even if it’s in the range
- Fix parameter: the optimizer won’t change it
  - At least one value must remain changeable

- Note: Ctrl+C and Ctrl+V works in the entire table



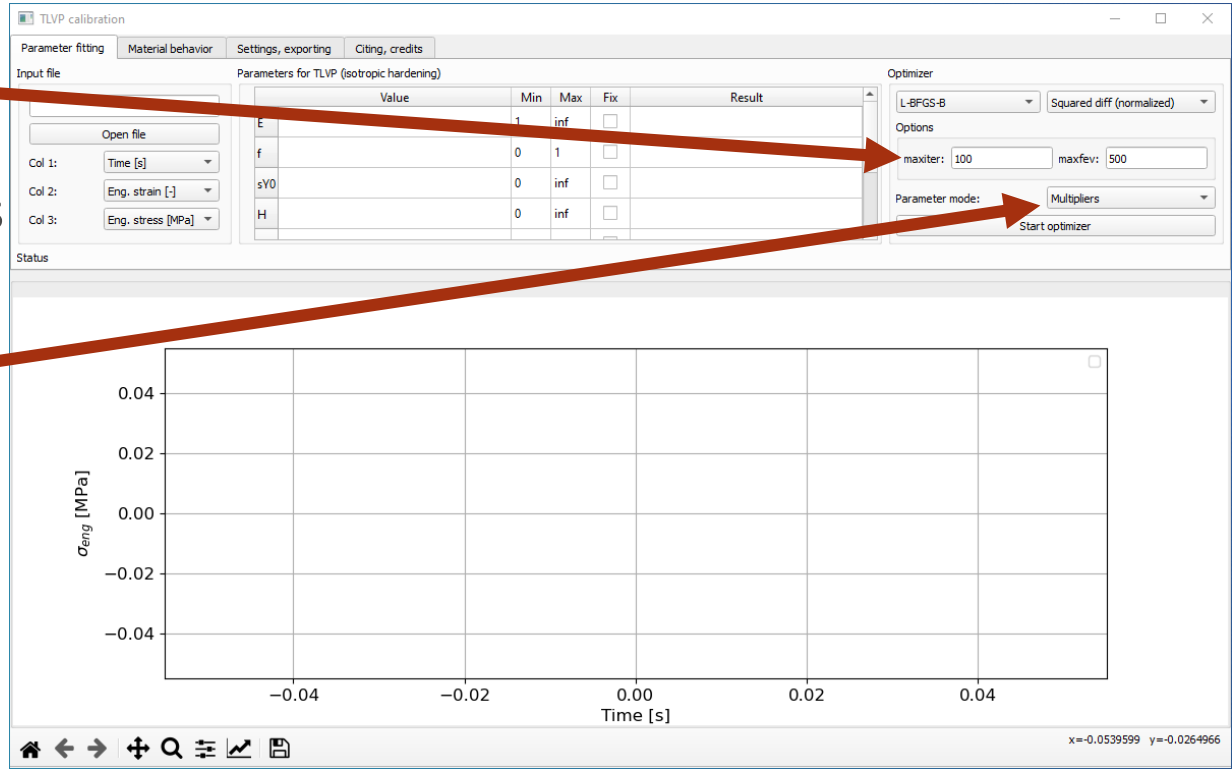
Parameter fitting (5): optimizer settings

- Optimization algorithm
  - Our tests: L-BFGS-B and SLSQP are the „best”, most efficient
  - Documentation: SciPy
- Quality function:
  - How the difference is measured
  - Absolute and squared difference
  - dX weighted: less weight to densely packed set of points
  - Normalized: normalized with the number of measurement points



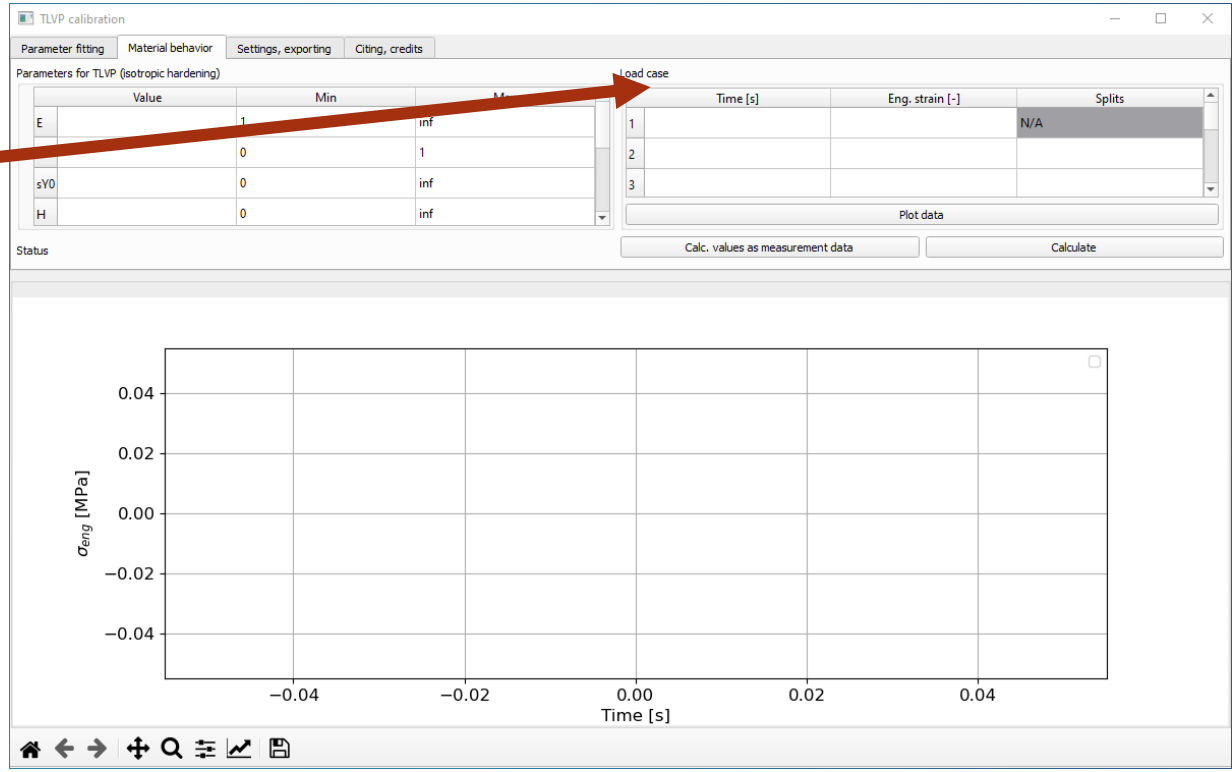
Parameter fitting (6): optimizer settings

- Stopping conditions:
  - Maxiter: max. allowed iterations
  - Maxfev: max. allowed function evaluations (some algorithms ignore it)
  - The optimizer stops if either is met
- Parameter mode:
  - Values: the parameters are optimized directly. Not recommended.
  - Multipliers: initial guesses are used as internal multipliers. The optimizer „sees” values in more similar magnitudes
  - Normalized: parameters are transformed to the [0,1] range based on their boundaries



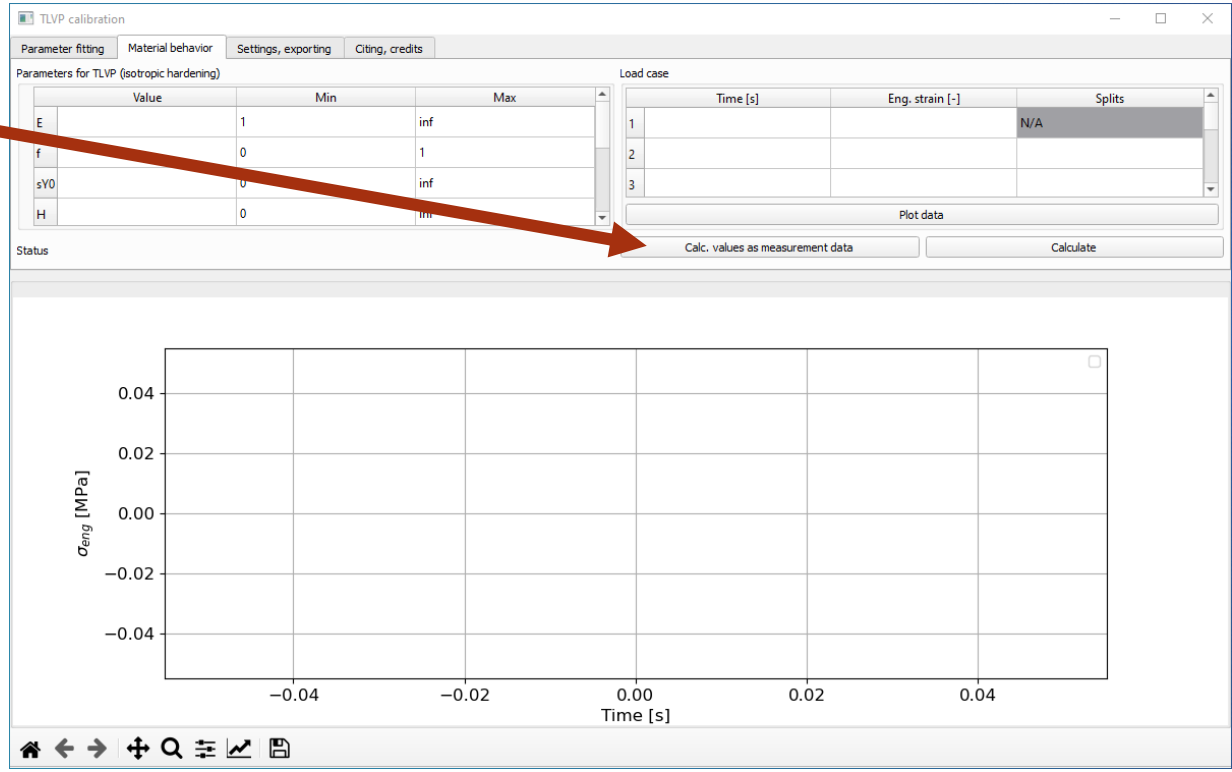
Material behavior (1): general

- Values are give directly
  - Boundaries only serve as reminders
- Uniaxial load:
  - Time-engineering strain history given by points (linear path assumed in between)
  - Number of division between points: 3rd column (must be >0 integer)
  - The „Plot data” only plots the load specified in the table
- If the table has no valid load data:
  - The measured strain history is used (if a measurement file was loaded)



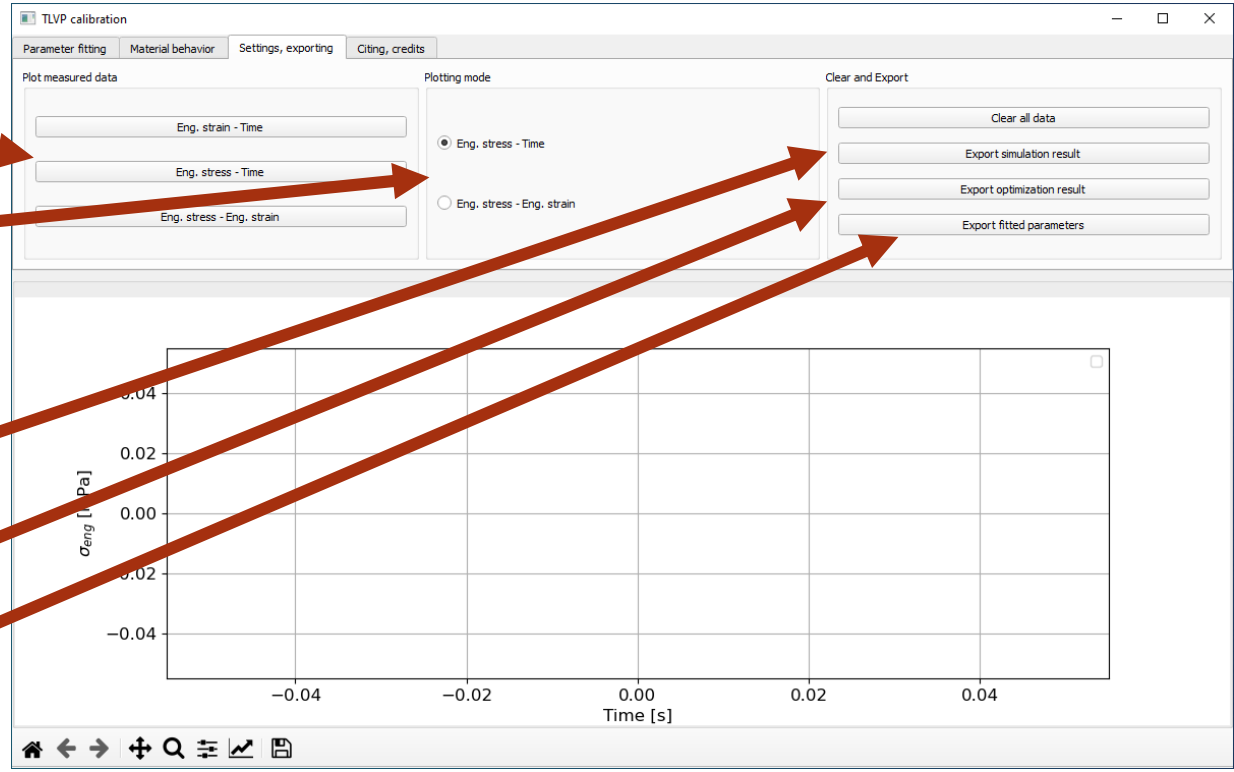
Material behavior (2): testing of optimizers

- Results can be interpreted as measurement data
- Test the optimizer settings in the first tab, while knowing the exact values it should converge to



Settings, exporting

- Plot the measured data
- X axis: time or strain data
  - Cannot be changed during optimization
- Clear all data:
  - Forget about the loaded values
- Export results from the material behavior tab
- Export the fitted and measured behavior
- Export fitted parameters

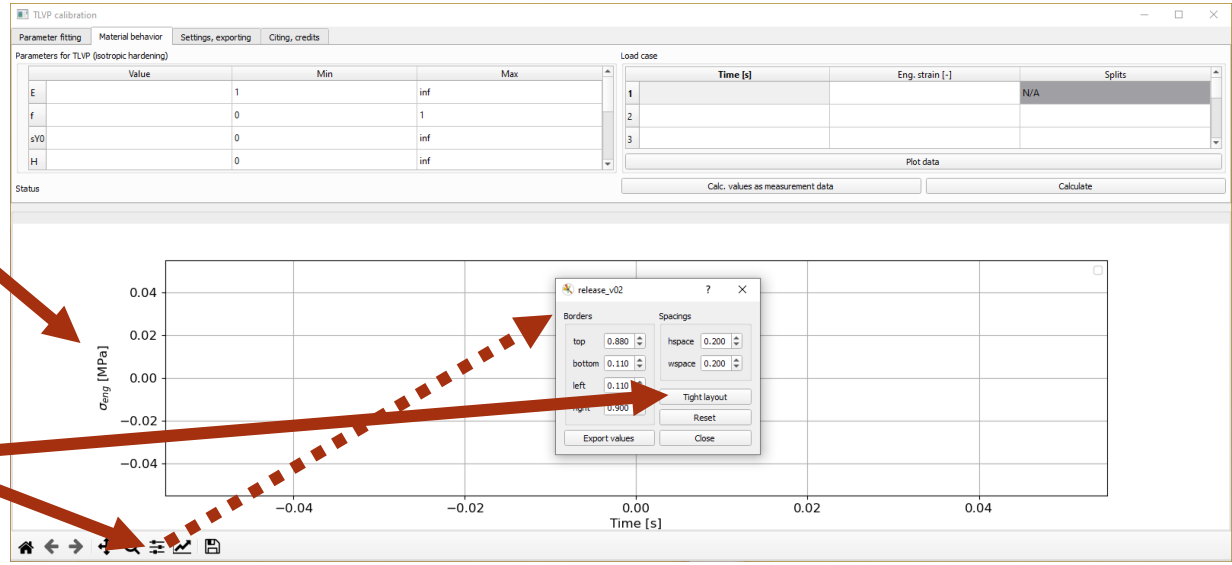


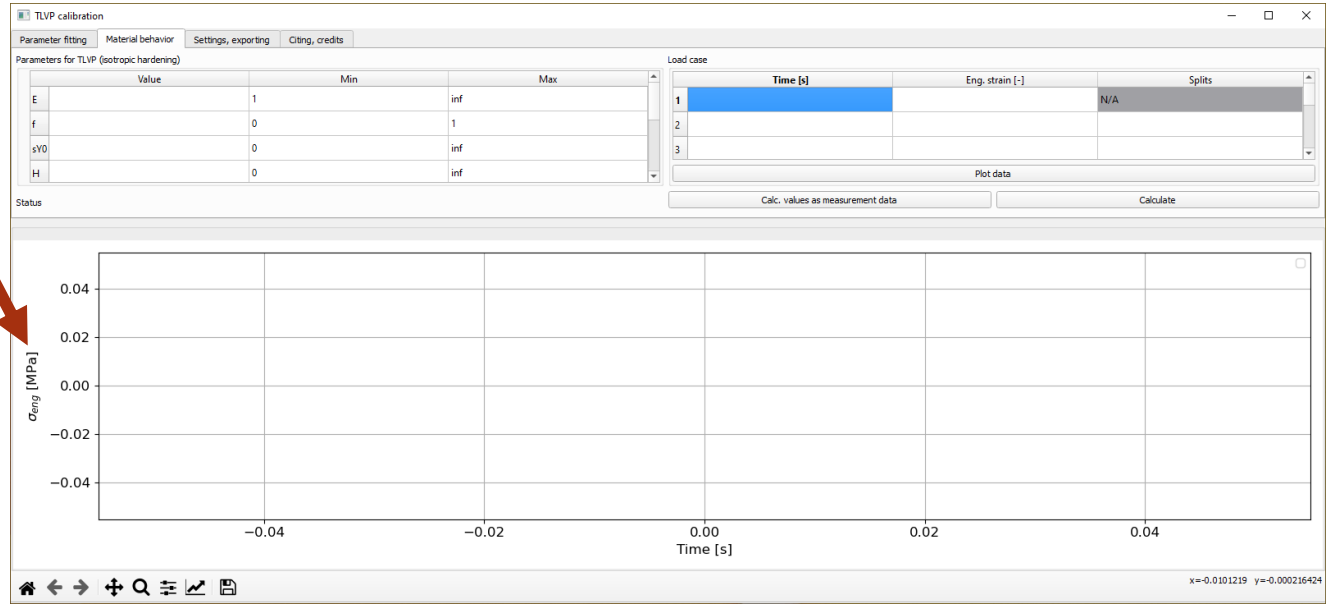
- Files are put in the „exported” folder

Tips (1): fixing axis labels

- Sometimes labels are placed incorrectly
  - Should be at the edge of the window

1. Bottom menu, configure subplots
2. „Tight layout” button
3. Labels moved to correct positions



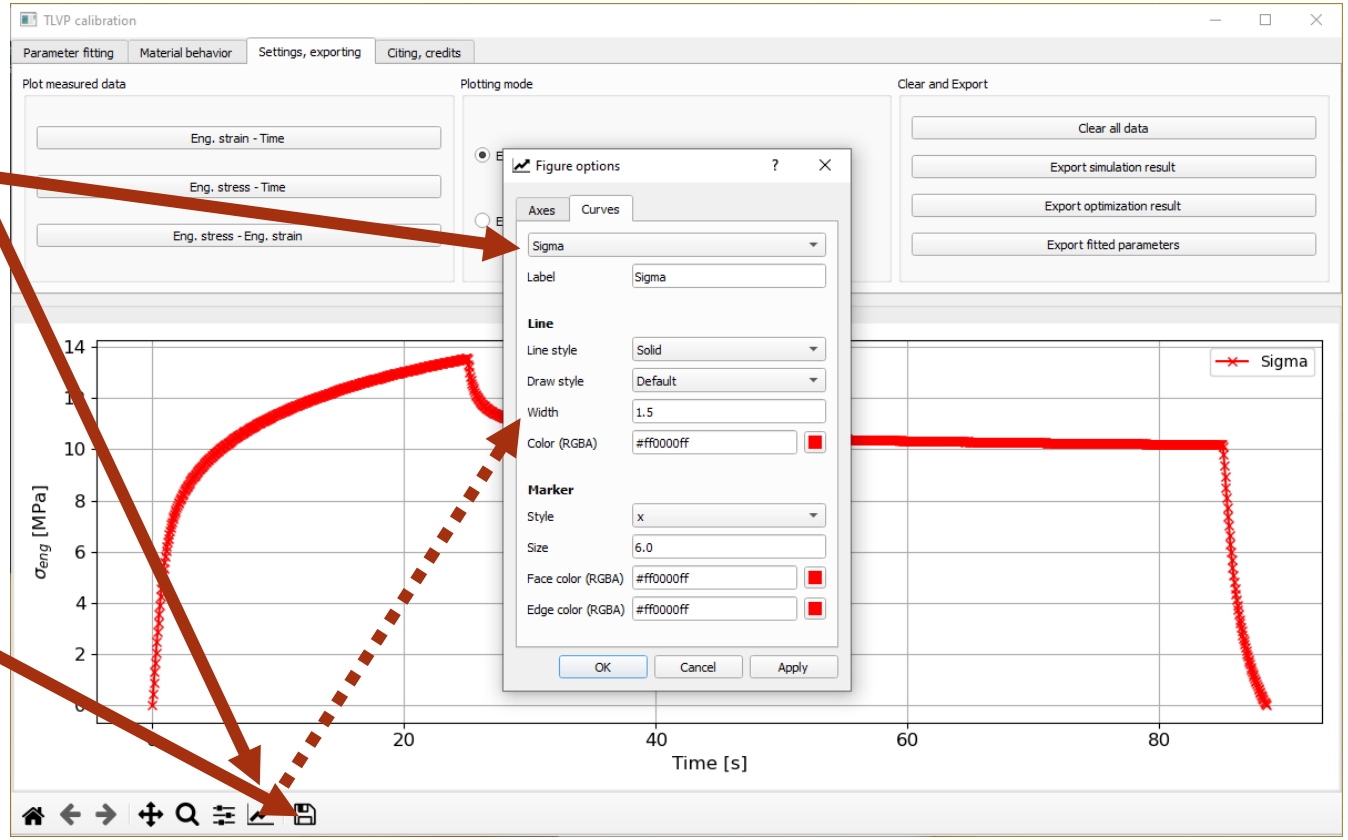


Tips (2): Changing curve properties

1. Bottom menu, edit axes, curve…
2. Select the curve
3. Edit properties (line width, markers, etc)

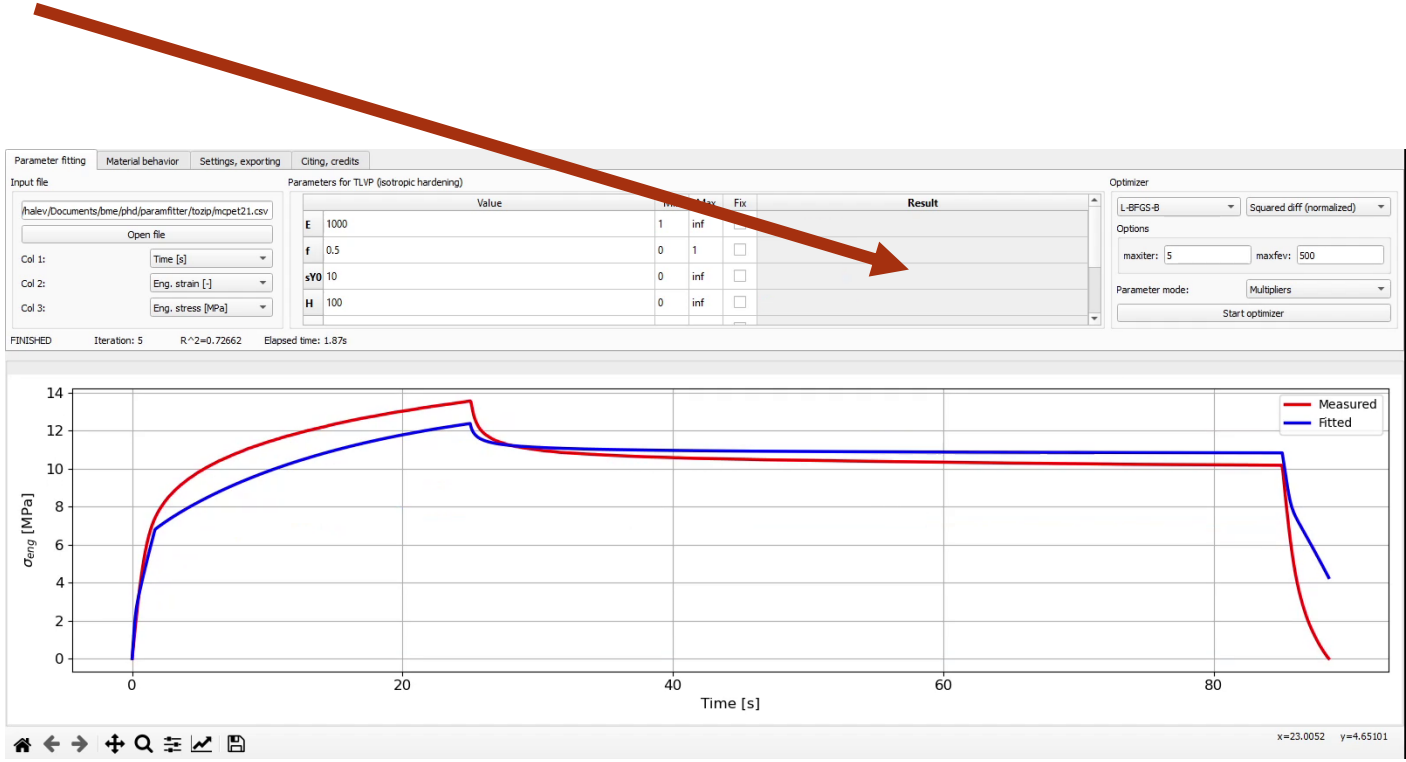
- Note: these setting are reset when replotting

- Save the figure (several formats)



Tips (3): result column not rendering/updating

- Sometimes the values in the result column don’t show up or update
  - Only when using Windows
- Solution:
  - Click into the cells
  - Select the column header
  - Use the scrollbar



Parameter fitting:
An example

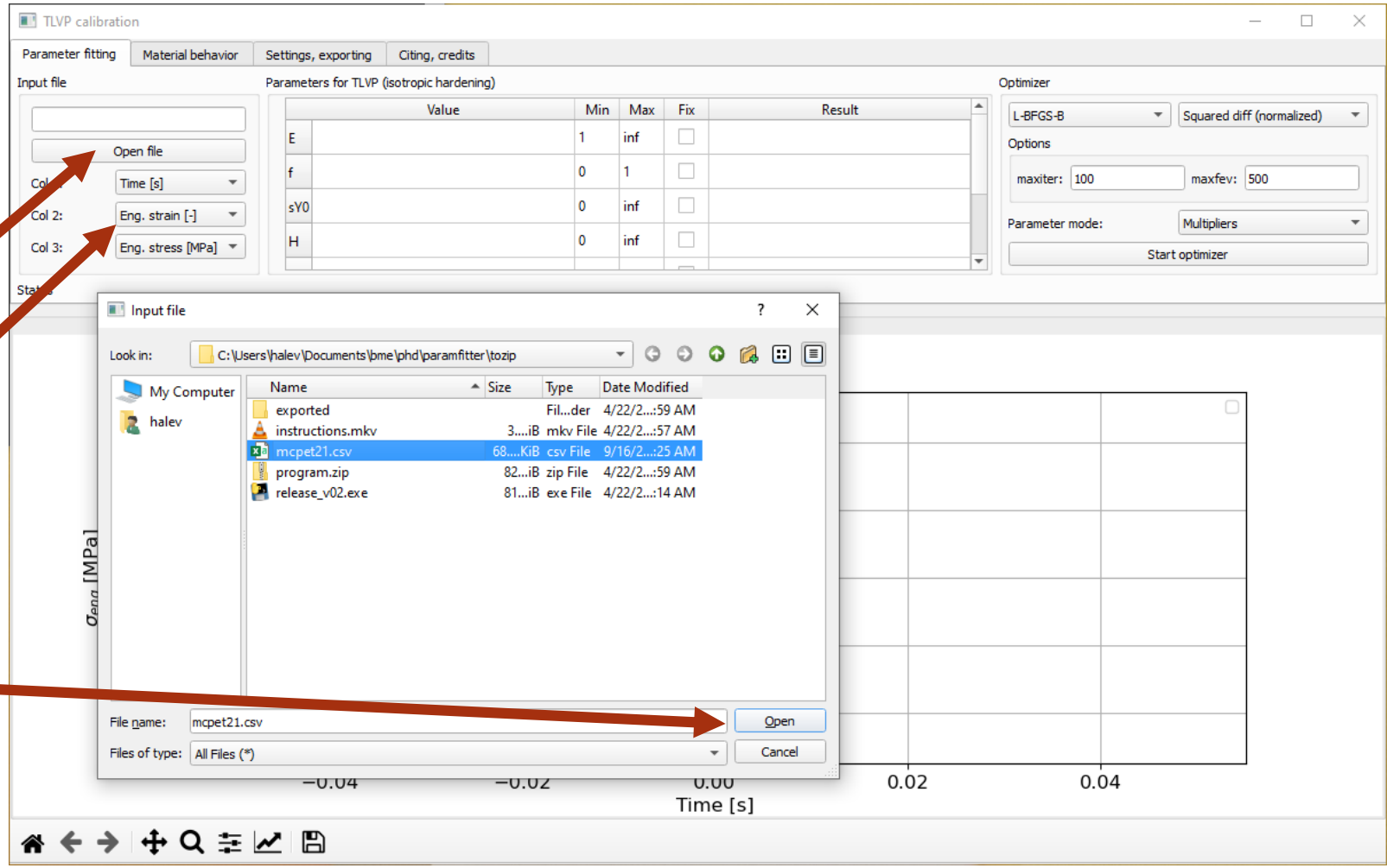
Goal

- Show a fitting example using real measurement data
  - Measured material: MC-PET at room temperature
- Show how to judge the obtained results

Start the program, load the measurement file

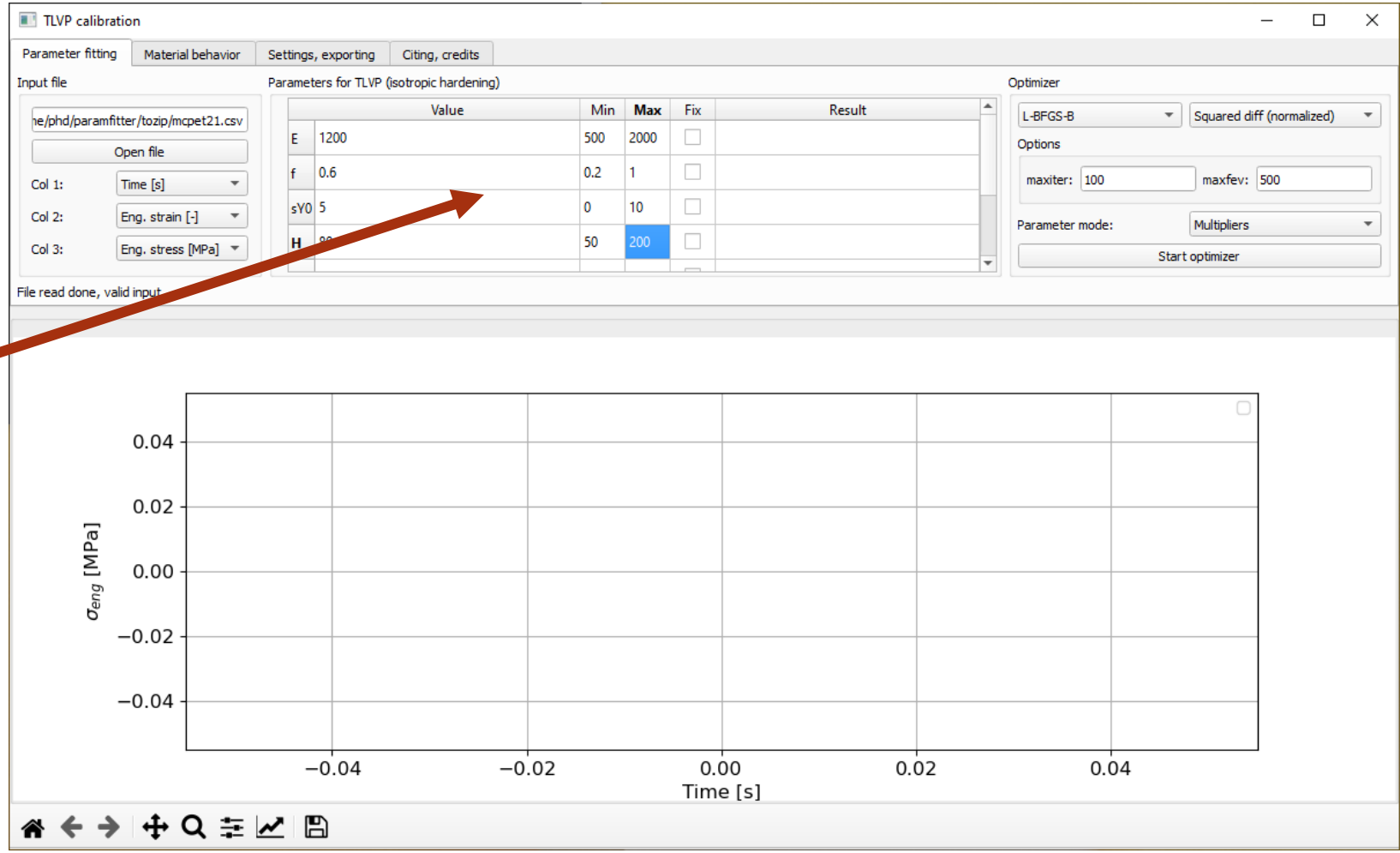
- Measured material: MC-PET @ room temperature
- Known: column order

1. Setup column order
2. Open file
3. Open



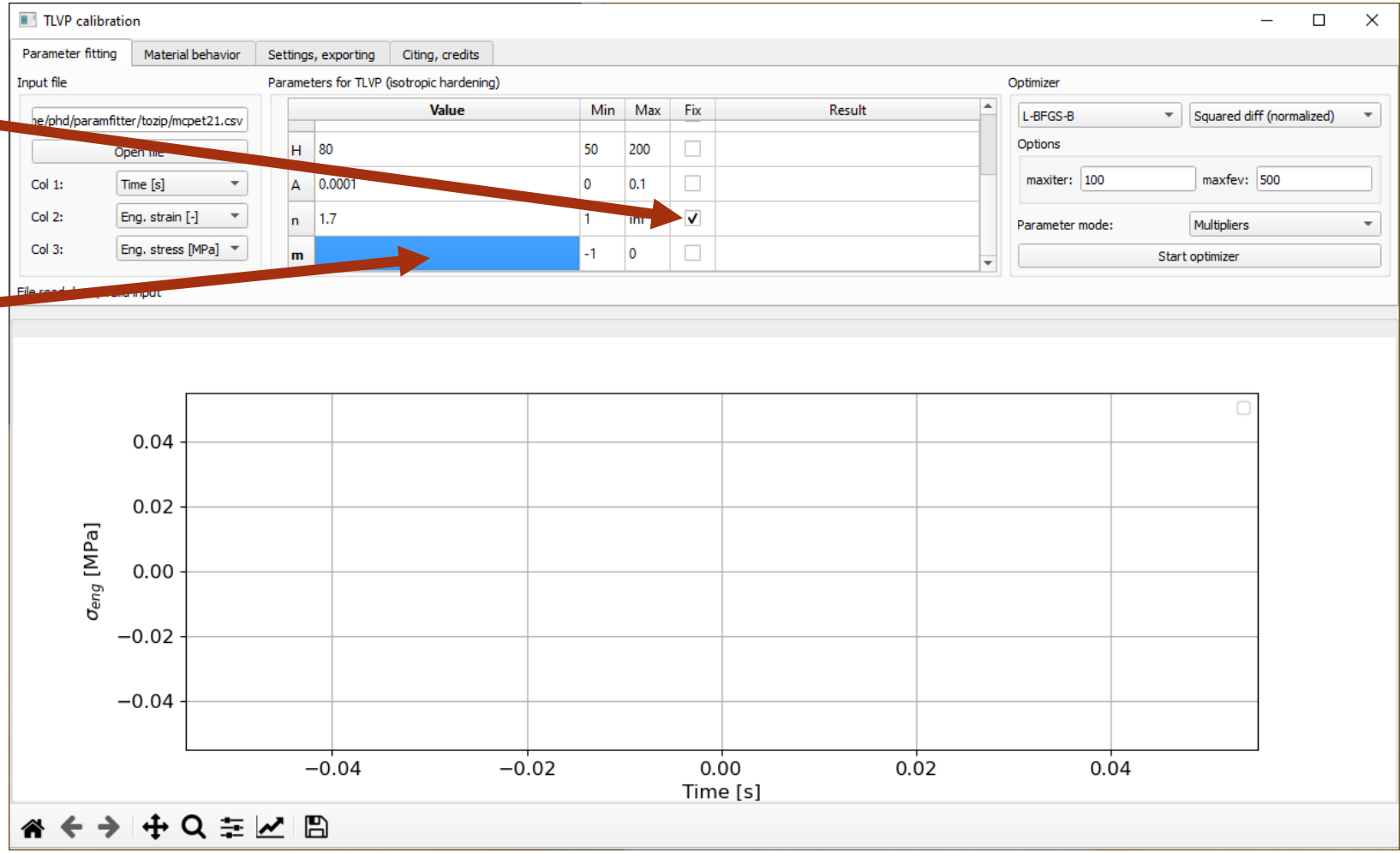
Initial guess (1)

- We have following ideas for some parameters before starting (values; ranges):
  - E≈1200; 500<E<2000
  - f≈0.6; 0.2<f<1
  - sY0≈5; 0<sY0<10
  - H≈80; 50<H<200
  - A≈0.0001; 0<A<0.1



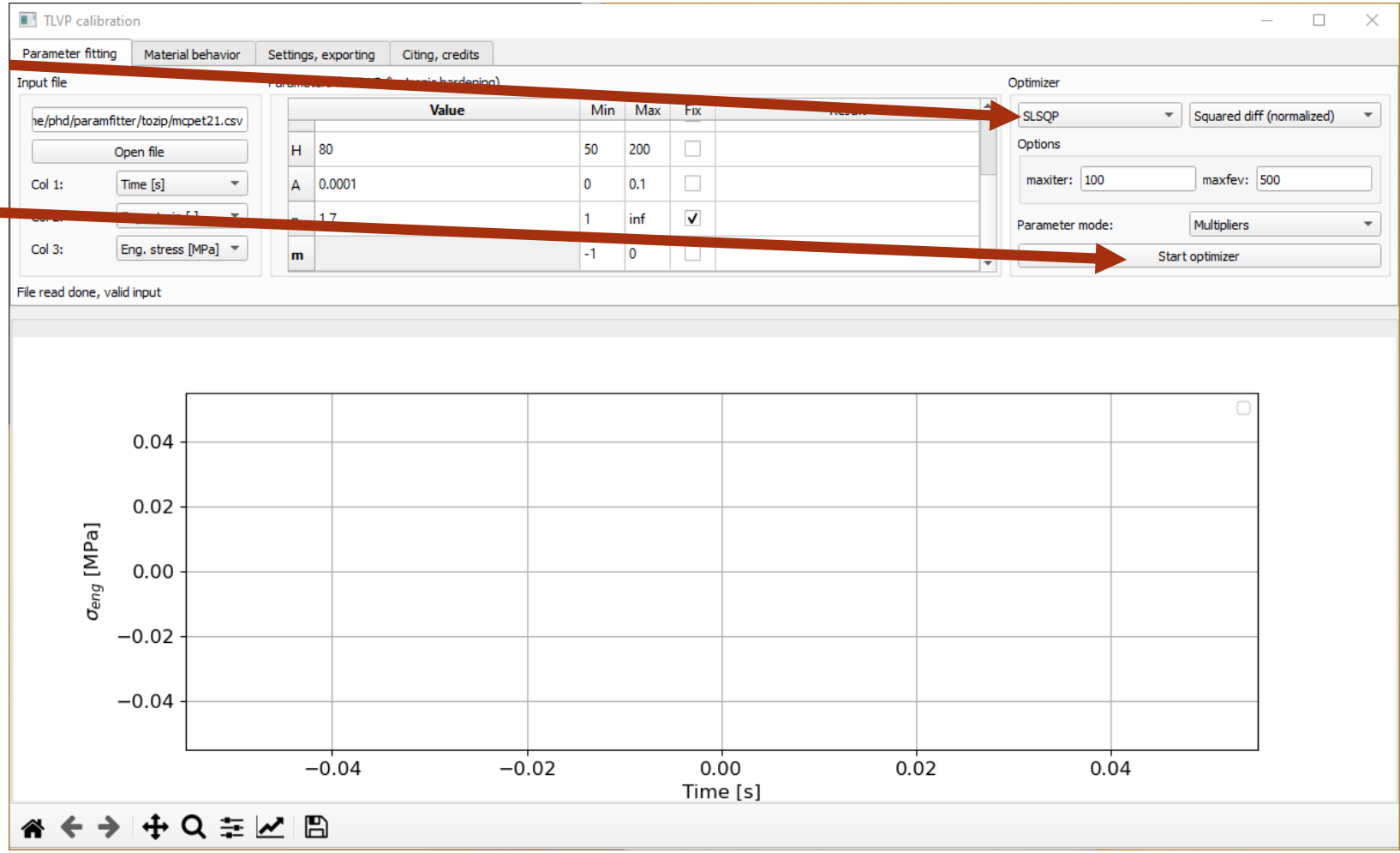
Initial guess (2)

- For some reason we are certain that n=1.7 -> fix
- We have no idea about m -> leave the field empty
  - The program will fill in the default value of m≈-0.5



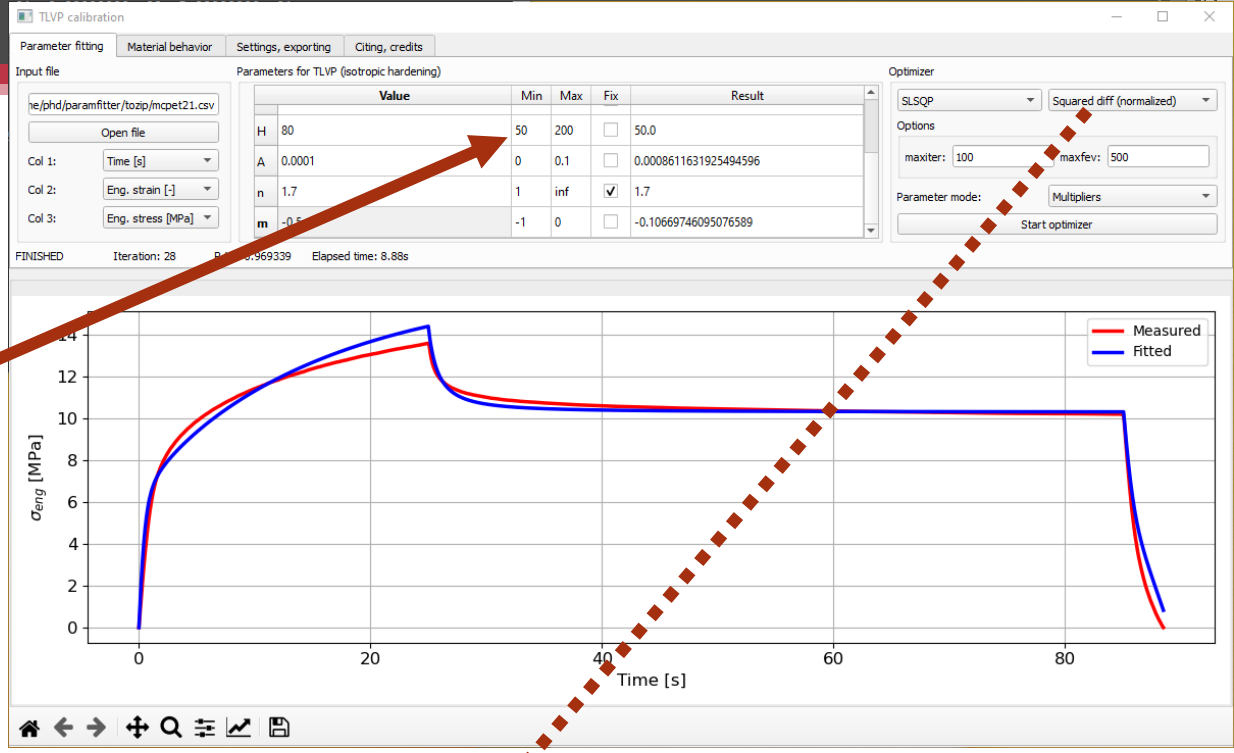
Optimizer settings

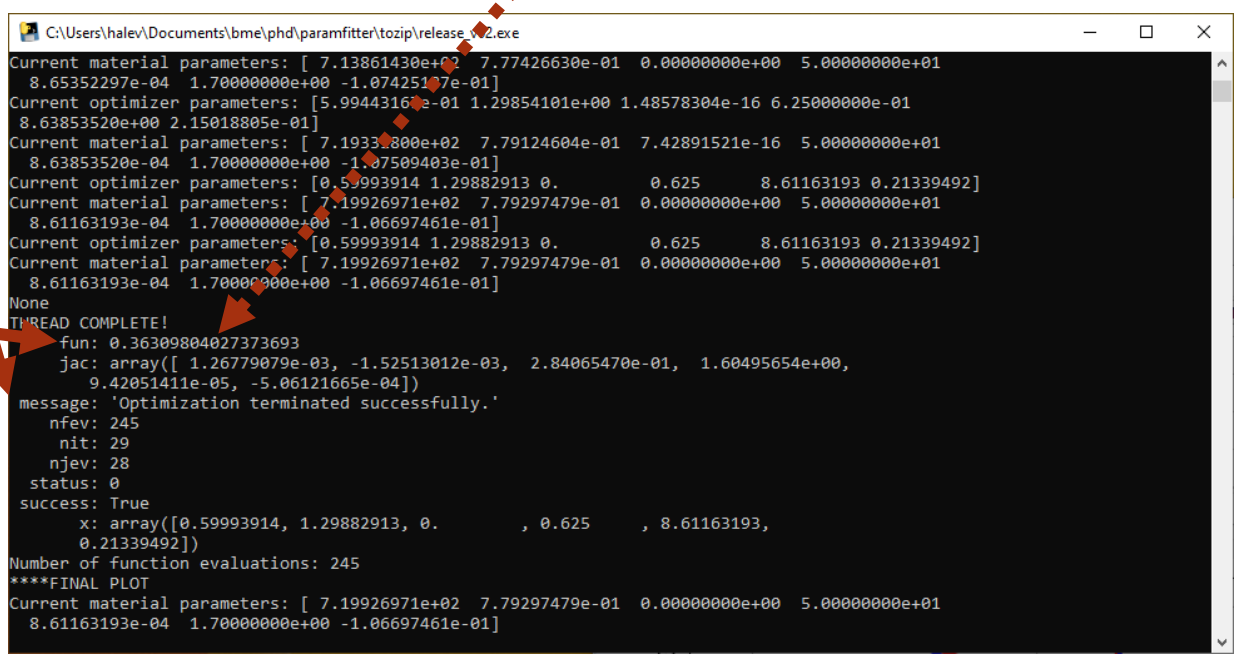
- Let’s use the SLSQP algorithm
- Start the optimizer



Check results

- Did we „hit” any boundaries?
  - Yes, H=50 in the results, our initial guessed range was probably wrong
- The console also has useful information:
  - The optimizer „terminated successfully”, it didn’t reach the maxiter or maxfev limit
  - The final value of the normalized squared differences was 0.363
- Conclusion: let’s try again with different boundaries for H

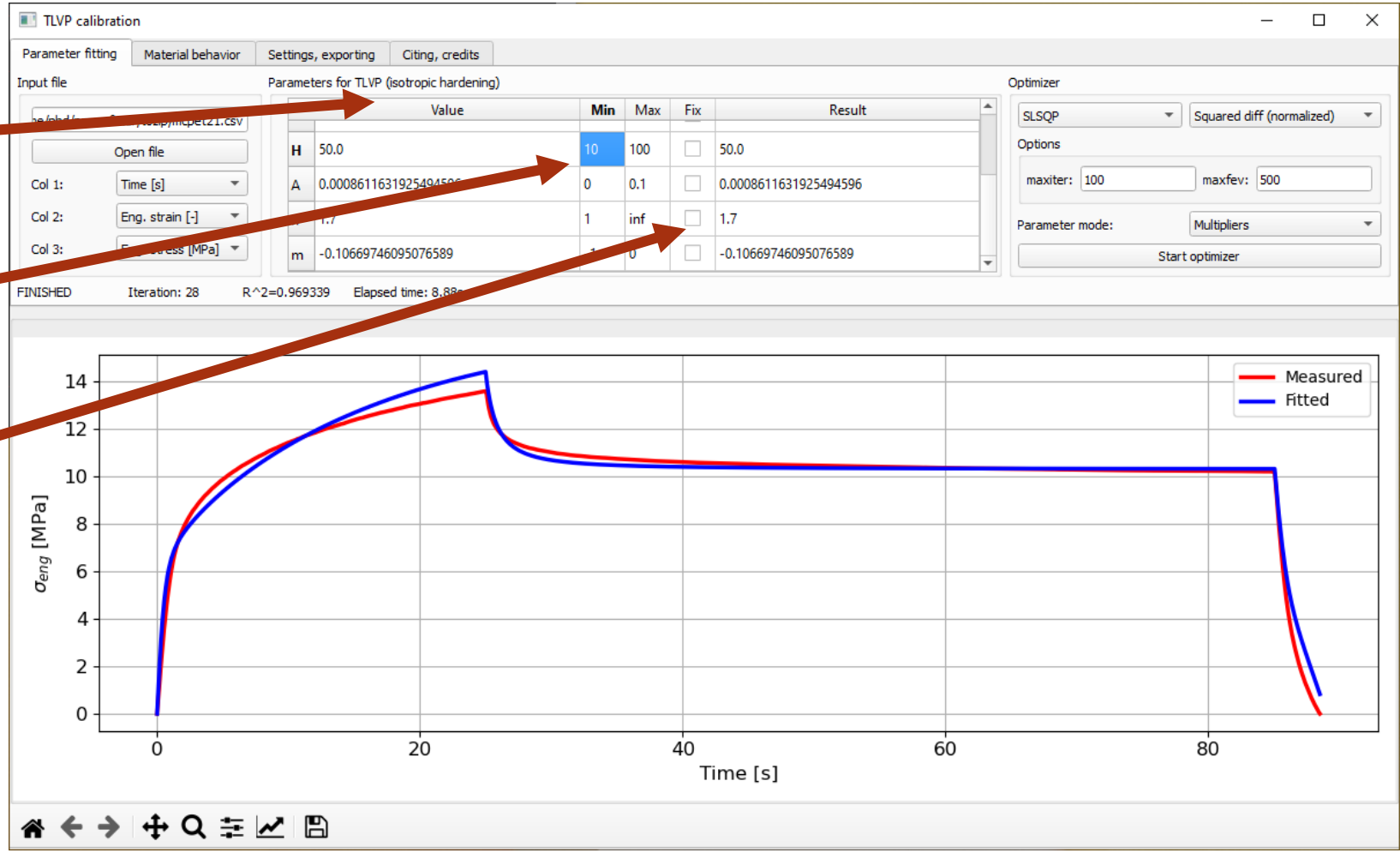




Retry

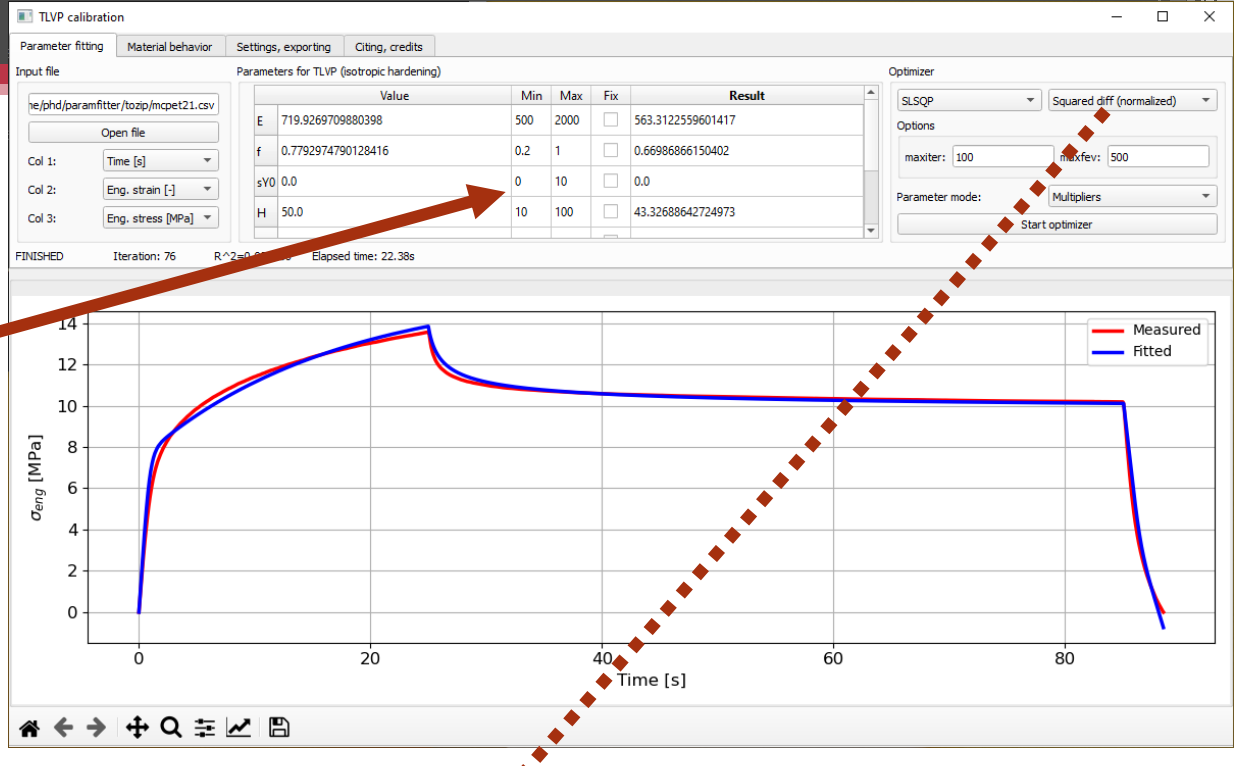
- Let’s use the old results as the initial guess:
  - Ctrl+C, Ctrl+V the values
- Change the limits of H to 10<H<100
- Let’s try with removing the „fix” from n

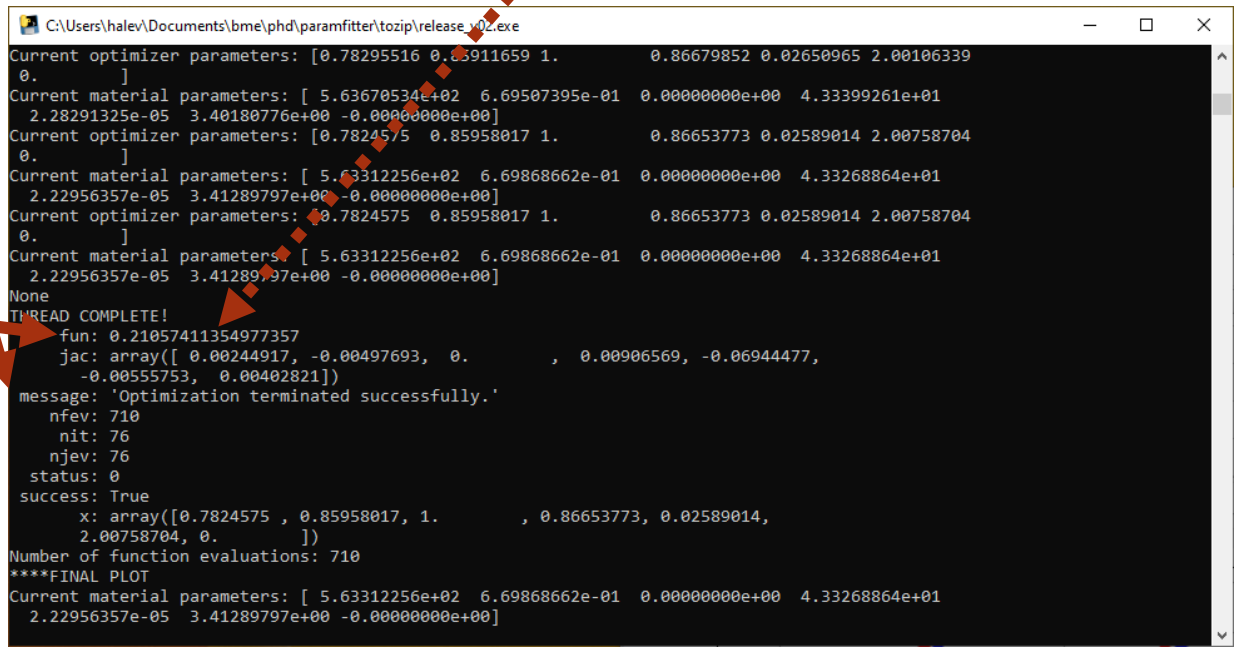
- Restart!



Check results again

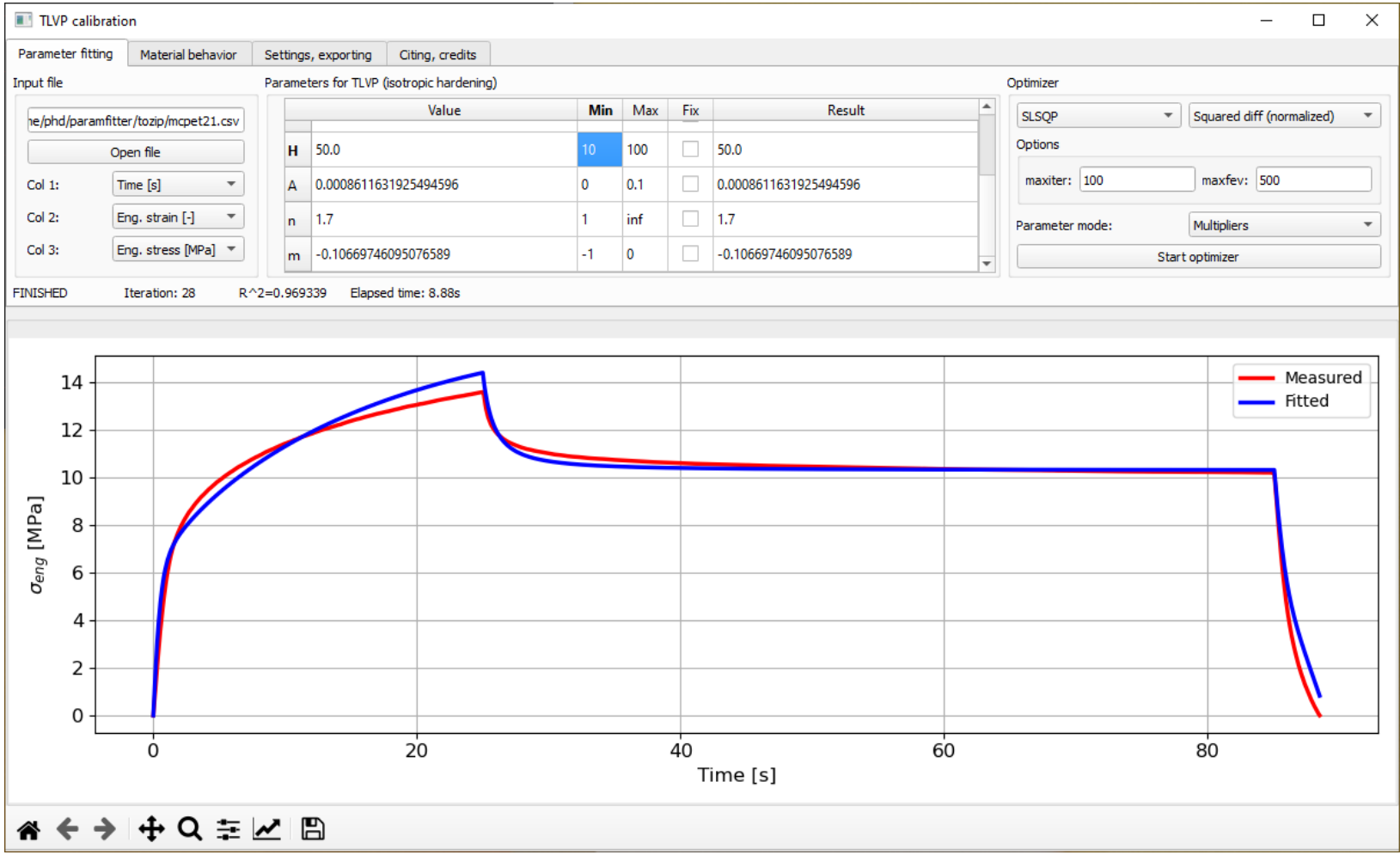
- Did we „hit” any boundaries?
  - Yes, sY0=0 in the results
- The console also has useful information:
  - The optimizer „terminated successfully”, it didn’t reach the maxiter or maxfev limit (well, actually SLSQP ignores maxfev…)
  - The final value of the normalized squared differences was 0.21
- Conclusion: let’s try again with changing sY0’s initial guess





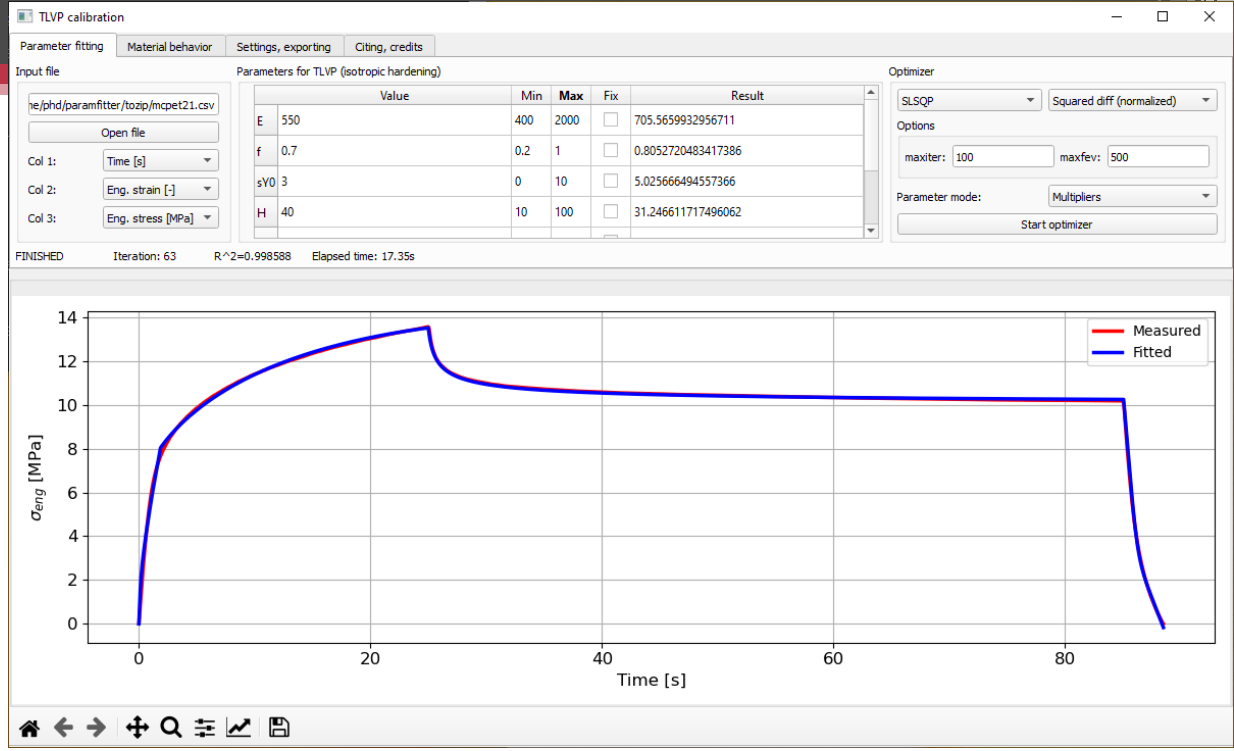
Retry 2

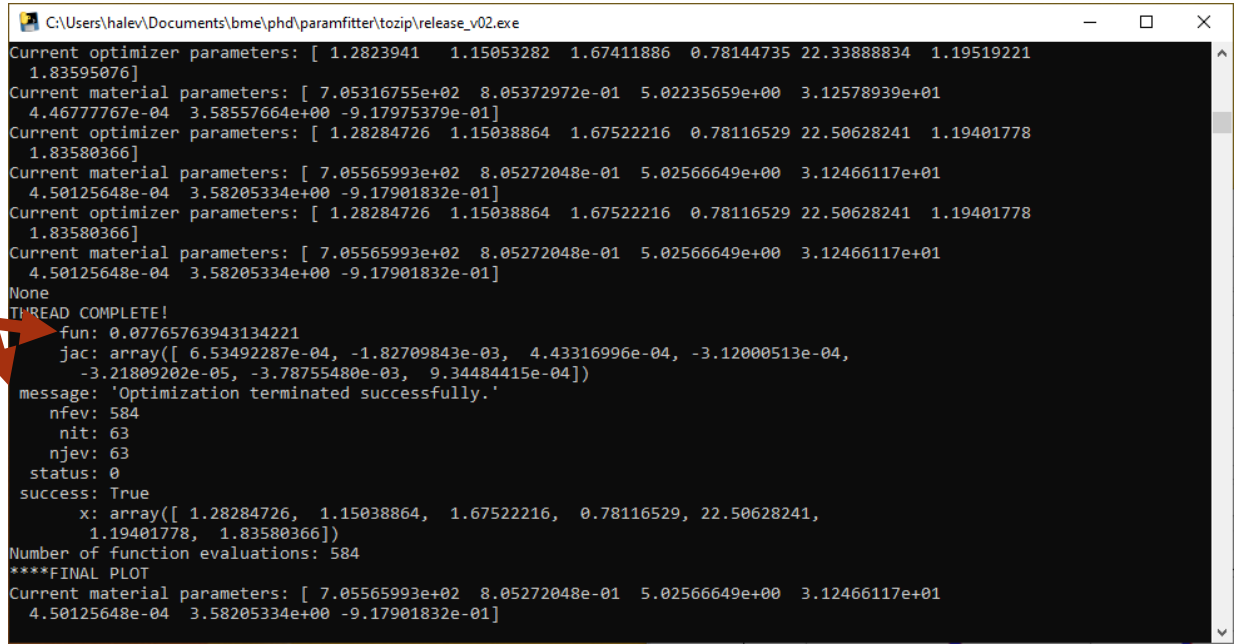
- Let’s base the new initial guess on the results
- Perturb the initial guess:
  - Change the copied values slightly (about +/- 10%) to help avoiding local minima
  - E≈550; 400<E<2000
  - f≈0.7; 0.2<f<1
  - sY0≈3; 0<sY0<10
  - H≈40; 10<H<200
  - A≈2e-5; 0<A<0.1
  - n≈3; 1<n<10
  - m≈-0.5; -1<m<0



Check results again

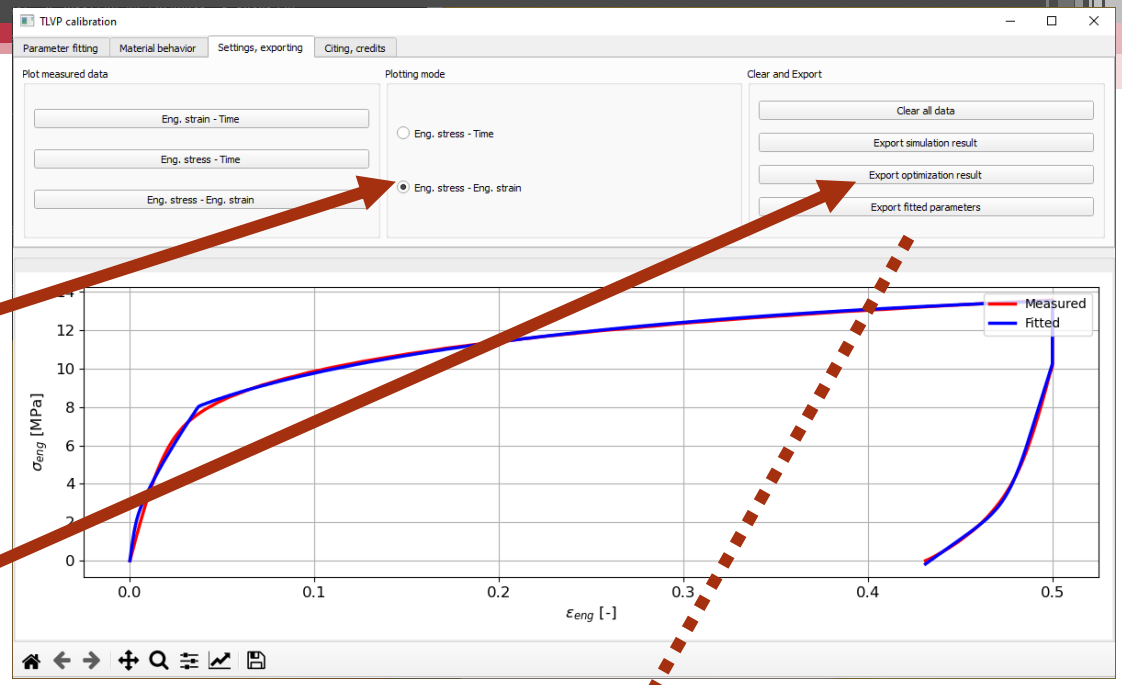
- Did we „hit” any boundaries?
  - No!
  - The plots are quite close too
- The console also has useful information:
  - The optimizer „terminated successfully”, it didn’t reach the maxiter or maxfev limit
  - The final value of the normalized squared differences was 0.077
- Conclusion: we are done

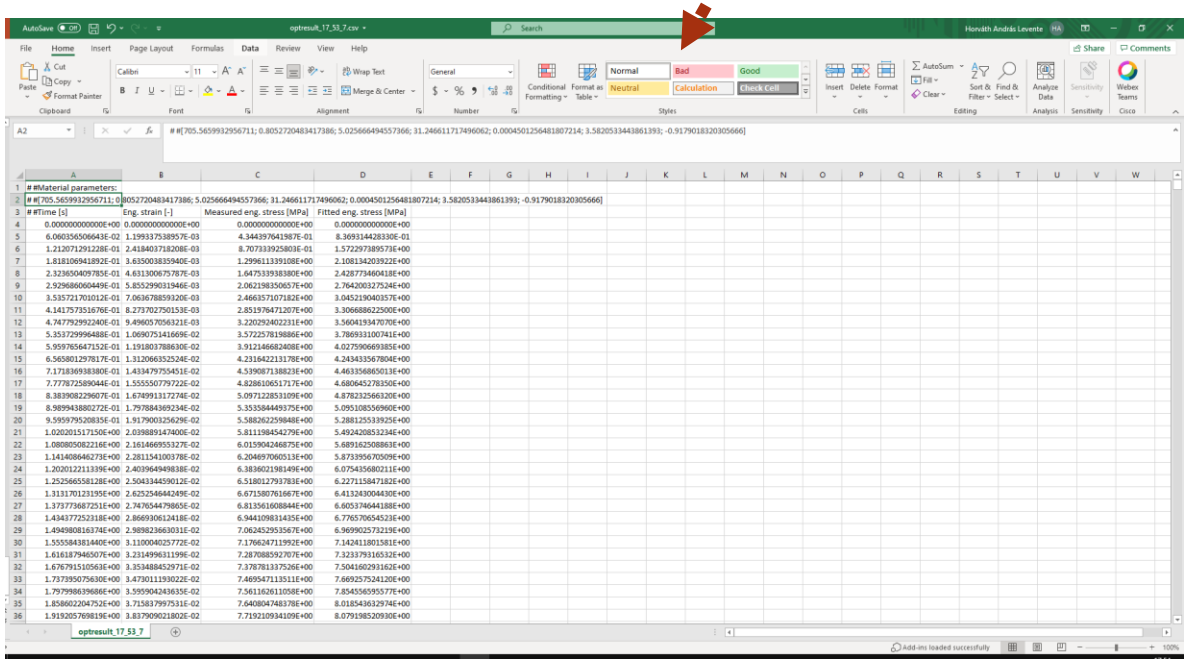




Plot the srtess-strain curve

- Sometimes the stress-strain graph can give additional insights
- Let’s export the results so they can be opened in an other program





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