Documentation for calculating relaxation time from NIST Polymerization Stress Tensometer (SRI 6005)

If you are using this software please cite:

Sarkar, S., Baker, P. J., Chan, E., Lin-Gibson, S., & Chiang, M. (2017). Quantifying the sensitivity of network structure and properties from simultaneous measurements during photopolymerization. *Soft Matter*.

Directory Organization:

We recommend that the code directory **get_tau** and experimental data folder be organized in the following way.

get_tau	(contains python code for calculating relaxation time)
GlobalDataFolder	(contains all experimental data)
ExperimentFolder	(contains all trials of specific experiment)
<TrialName>.txt	(text file containing the information about the trial setup)
<TrialName>.csv	(Results of experiment in CSV format)

Example <TrialName>.txt file

Experimental Conditions

Measurements: Stress, Temperature, Degree of conversion

Beam type: Rigid steel

Sample Description: 70_30_50%
Diamater of sample (cm): 0.2500
Sample height (cm): 0.2000
C-Factor: 0.6250
Position of sample along the beam (cm): 20.0000
Compliance of the beam (cm/N): 1.2322E-3

Integration time (ms): 25.0000
Scans to average: 3.0000
Sample rate (s): 0.2000

Irradiation Mode: Standard
Start time of irradiation (s): 20.0000
Light Intensity (mW/cm2): 500.0000
Duration of irradiation (s): 40.0000

Duration of experiment: 10.00 minutes and 0.00 seconds

Additional comments on the experiment:

The NIST tensometer records the experimental condition in the above format. If the user's instrument records the information in a different way, it must be converted into the above one.

Example <TrialName>.csv

Time (s)	Voltage (V)	Disp. (cm)	Stress (MPa)	DC (%)	deltaT
0.142216	-0.00008416	-0.00000107	-0.00010018	2.926763	-0.12565
0.342656	-0.00009116	-0.00000107	-0.00010918	1.078467	0.016231
0.543096	-0.00026116	-0.00000207	-0.00031118	0.381026	0.300331
0.743536	-0.00071016	-0.00000707	-0.00084418	2.357989	0.959891
0.943976	-0.00145116	-0.00001407	-0.00172418	1.337635	2.112882

Lastly, we need a provide some additional information regarding for the material, which are provided using <inputfile>.txt.

# Inputs for folder location
Superfolder = GlobalDataFolder
Subfolder = ExperimentFolder
Testname = TrialName

Information about the composite
Initial viscosity (in Pa.s) = 1.0
High-frequency Youngs modulus (GPa) = 4.5
Maximum shrinkage strain = 0.10
Coefficient of thermal expansion (in 1/T) = 1E-4,0.5E-4
Molecular density (in moles/m^3) = 2500

Numerical calculation details
Calculation time (s) = 250.0
Regularization parameter = 1E-2
Denoising window = 5

# Analysis outname
Casename = TrialAnalysis

The coefficient of thermal expansion asked for are the limiting values for the resin and the cured polymer at a high DC.

Once, the input file and rest of the information has been organized. The code can be executed as,

python get_tau/get_tau.py -i <inputfile>.txt

The outputs of the calculation will be stored in a folder <Casename> under the directory ExperimentFolder.