

zlambda v. 0.73 - User manual (not yet completed - we are working on it)

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1 The software overview

The **zlambda** is a numerical simulation software for modeling *Z*-scan experiment and analysis of the heat transfer caused by laser radiation.

In order to speed up the calculations, the program supports multithreading of modern processors with support from 1 to 32 threads. The number of threads used during the calculations is defined by the user. Therefore, in order to parallelize the calculations, for example, on a 32-thread unit, it will be possible to run 4 simulations running 8-thread simultaneously or 2 simulations running 32, etc.

2 Software operating and files structure

2.1 Start the program

The **zlambda** is a console application that can be run in the terminals of operating systems such as Linux, macOS or Windows. To start a program, open a terminal and go to the directory where the program is located. Then simply write the command:

```
1 ./zlambda
```

After pressing the enter button, the program will start calculations. Depends on the mode selected in **ConfigExperiment.txt** the application will perform the full or single shot calculation.

2.2 File structure

The structure of the program files and directories is as follows:

```
zlambda <Parent Folder>
  |-Results <Folder>
  |   |-Surfaces <Folder>
```

```
|    |-HeatMaps <Folder>
|-zlambda <main application>
|-ConfigExperiment.txt <ascii txt file>
|-ConfigSample.txt <ascii txt file>
```

The `zlambda` is the main application, that can be run in the system console. The main application uses the `ConfigExperiment.txt` and `ConfigSample.txt` files for calculation. First config file contains the physical parameters of the *Z*-scan experiment. The second file configures the thermal, physical and numerical parameters of the calculation. The wider description of the `ConfigExperiment.txt` and `ConfigSample.txt` files are presented in the section 2.3 and 2.4 respectively.

2.3 Setting up the ConfigExperiment.txt file

The `ConfigExperiment.txt` file contains the set of variables which control the *Z*-scan experiment, simulated by the `zlambda` software.

The hash symbol comments the line. If the line starts with a #, anything after that symbol will not be interpreted by the program.

Syntax

```
# This is a comment, and this line is not interpreted
# by the program.
```

SingleShot The value of this variable indicates the calculation mode of the `zlambda` software. There is a two available mode implemented in the software. If the value of **SingleShot** variable is equal to **1** the calculation will start with single mode and only 1000 iteration will be perform according to other variables set in both `ConfigExperiment.txt` and `ConfigSample.txt` files. In this mode the sample is irradiated by one pulse of the laser at the sample is located at the z_0 .

Syntax:

```
SingleShot = <index>
```

Where the `<index>` is equal 0 or 1.

ZScanRange indicates the distance between $-z$ and $+z$. This is a distance which the sample moves in the *Z*-scan experiment with the constant velocity.

Syntax:

```
ZScanRange = <real_value>
```

Where the <real_value> is a real number representing the distance. Example:

```
# Z-scan range. Distance between -z and +z [mm]
# Below the range is set for 100mm.
ZScanRange = 100
```

SampleVelocity This variable sets the sample's velocity at the range from $-z$ to $+z$.

Syntax:

```
SampleVelocity = <real_value>
```

Where the <real_value> is a real number of the sample's speed. The unit of the variable **SampleVelocity** is (mm/s). Below example sets the sample speed at 5.5 (mm/s):

```
#Sample velocity [mm/s].
SampleVelocity = 5.5
```

SimulationTime This variable controls the time that is simulated during numerical calculations. This value should be selected appropriately to the modeled experiment, taking into account the time needed to simulate the *Z*-scan experiment. For example, if the sample speed is set to 1mm/s and the variable **ZScanRange** is set to 30mm, the time needed to simulate the full *Z*-scan experiment (and Simultaneously the heat transfer) will take 30s. If this variable is set to less than 30 seconds, the program will finish the calculations earlier, before the *Z*-scan experiment is modeled. Therefore, it is good to set simulation time for longer than the modeled *Z*-scan experiment takes. Then it will be possible to observe the cooling processes of the material after the end of the laser irradiation resulting from the simulated *Z*-scan experiment.

Syntax:

```
SimulationTime = <integer_value>
```

Where the <integer_value> is a integer number. The unit of this variable is one second - (s). Example:

```
#Simulation time set for 100 seconds
SimulationTime = 100
```

NumericalTimeStep This variable specifies the time step that is used in the numerical calculations. If we divide the values of **SimulationTime** and **NumericalTimeStep** by ourselves, we get the number of iterations that the program must perform to complete the calculations. If the **SimulationTime** is set on 100s and the **NumericalTimeStep** is set on 0.2ms the number of iteration will be 500000.

Syntax:

```
NumericalTimeStep = <real_value>
```

Where the **<real_value>** is a real number of the numerical differential time step. The unit of this variable is one second (s). Below example sets the time step of numerical calculation to 0.2ms:

```
#Duration of the numerical time step. Real value in [s]
NumericalTimeStep = 0.2e-3
```

LambdaOfLaser This variable specifies the wavelength of the laser used in simulation. The type of variable is real number and the unit is nanometers (nm). Syntax:

```
LambdaOfLaser = <real_value>
```

Below example sets the laser wavelength to 532nm:

```
#Laser wavelength [nm]
LambdaOfLaser = 532.0
```

omegaZero is the beam waist ω_0 at $z = z_0 = 0$. Syntax:

```
omegaZero = <real_value>
```

Where the **<real_value>** is a real number of the beam waist expressed in meters (m). The following example sets ω_0 to $25\mu\text{m}$

```
#Beam radius at z0 [m] sets to 25 micrometers.
omegaZero = 25e-6
```

LaserPulseDuration is a real variable which specifies the pulse duration of the laser used in simulation. Syntax:

```
LaserPulseDuration = <real_value>
```

The **<real_value>** is the pulse duration expressed in seconds (s). The example sets pulse duration to 100ps:

```
#Laser pulse duration [s] (i.e. 5ns -> 5e-9, 100ps -> 100e-12)
LaserPulseDuration = 100e-12
```

```

#Laser Pulse Energy (if the LaserPulseDuration > 0) [J]
LaserPulseEnergy = 9.81748e-4

#LaserPower (if the LaserPulseDuration = 0) [W]
LaserCWPower = 10e-3

#Pulse Repetition frequency [Hz] for pulsed laser. Please notice that the value must be
LaserPulseRepetition = 10

#Save Zero Planes interval [s] If the value is 0, then data will be saved after each
SaveZPRInterval = 0.01

#Save Zero Planes (1 = Yes, 0 = No) - indicate that the program will be saved Zero Planes
DoesSaveZPRInterval = 1

#Save all sample Interval [s] - If the value is 0, then data will be saved after each
SaveASInterval = 25.0

#Save all sample (1 = Yes, 0 = No) - indicate that the program will be saved All sample
DoesSaveASInterval = 1

Threads = 4

```

If you want to comment some phrase in the ConfigExperiment.txt file, please use # at the beginning of the line # Below you can set the simulation condition. # Please notice that you have to use the units pointed in [] brackets.

2.4 Setting up the ConfigSample.txt file

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