EURADOS 2023 COURSE

ANALYSIS OF LUMINESCENCE SIGNALS FOR DOSIMETRY APPLICATIONS

Vasilis Pagonis

Professor of Physics Emeritus
McDaniel College, Westminster, MD, USA

Many thanks to WG10 group and Dr Liz Ainsbury for the invitation!

OUTLINE OF THE TALK

- Luminescence signals for dosimetry

  How do we analyze them?

  Open access software

- Computerized analysis and models

  - Classification
  - Organization
  - Standardization

- The Jupyter notebooks

- Adapting the software codes to analyze your data

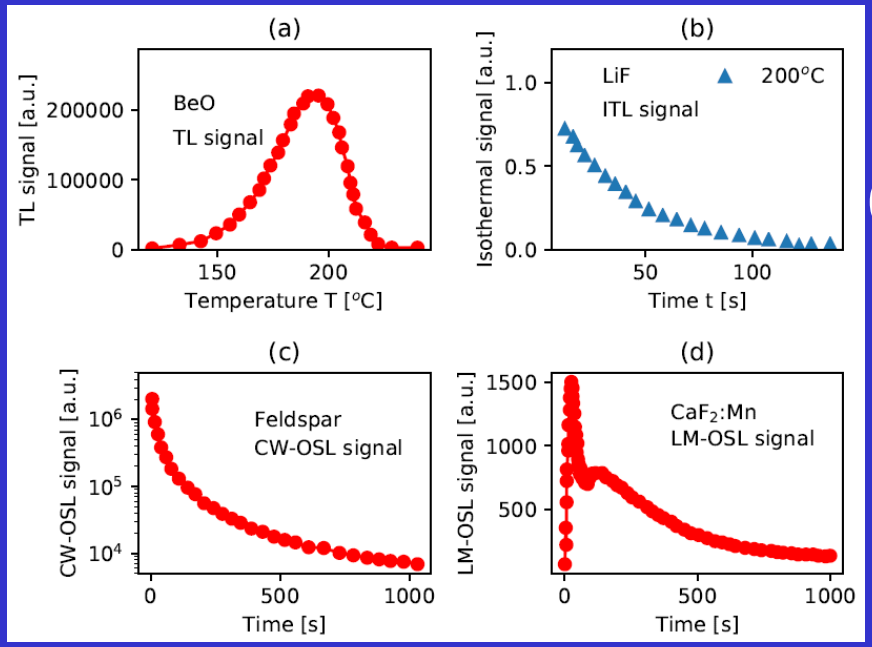
LUMINESCENCE SIGNALS

TL

Thermoluminescence (linear heating)

OSL

Optically stimulated luminescence (blue/infrared LEDs)



ITL

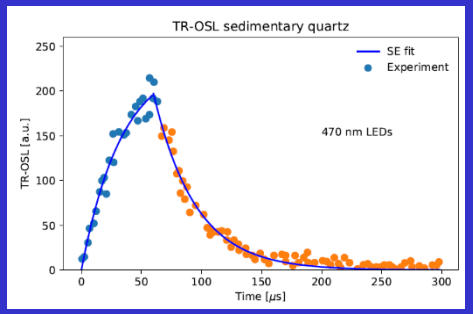
Isothermal signals (constant temperature)

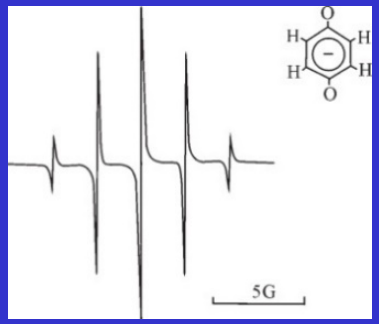
LM-OSL

Linearly modulated OSL

TR

Time resolved luminescence





ESR

Electron spin Resonance

Purpose of the new R and Python codes

Classification, organization and standardization of :

Computerized analysis of luminescence signals
Modelling of luminescence phenomena.

- Although a significant number of open access codes is already available in the literature, there is a ***lack of common standardization and homogeneity***.

- We developed ***new codes*** and ***included the latest modelling:***

New equations based on the Lambert W function for
TL, OSL, dose response

New equations for localized transitions in *feldspars* for
TL, CW-IRSL, LM-IRSL, Time-resolved signals

New codes for most available luminescence models

The new R and Python Open access codes

- Why we chose R and Python
- How the codes are organized

  By type of signal: TL, OSL, IRSL, dose response etc
  By type of transition: delocalized, localized, semilocalized

- All open-access codes are available in GitHub
  - 99 R codes
  - 87 Python codes
- Examples of currently available codes as Jupyter notebooks
- Running the codes in Google Colab

Why choose

R versus **Python**

Many excellent R packages already available (e.g. *Luminescence*)

Various R packages are already incorporated in Analyst

Steeper learning curve than Python

R is all about vectors, manipulation of large amounts of data can be very efficient

Structure of commands is not obvious to a new user.

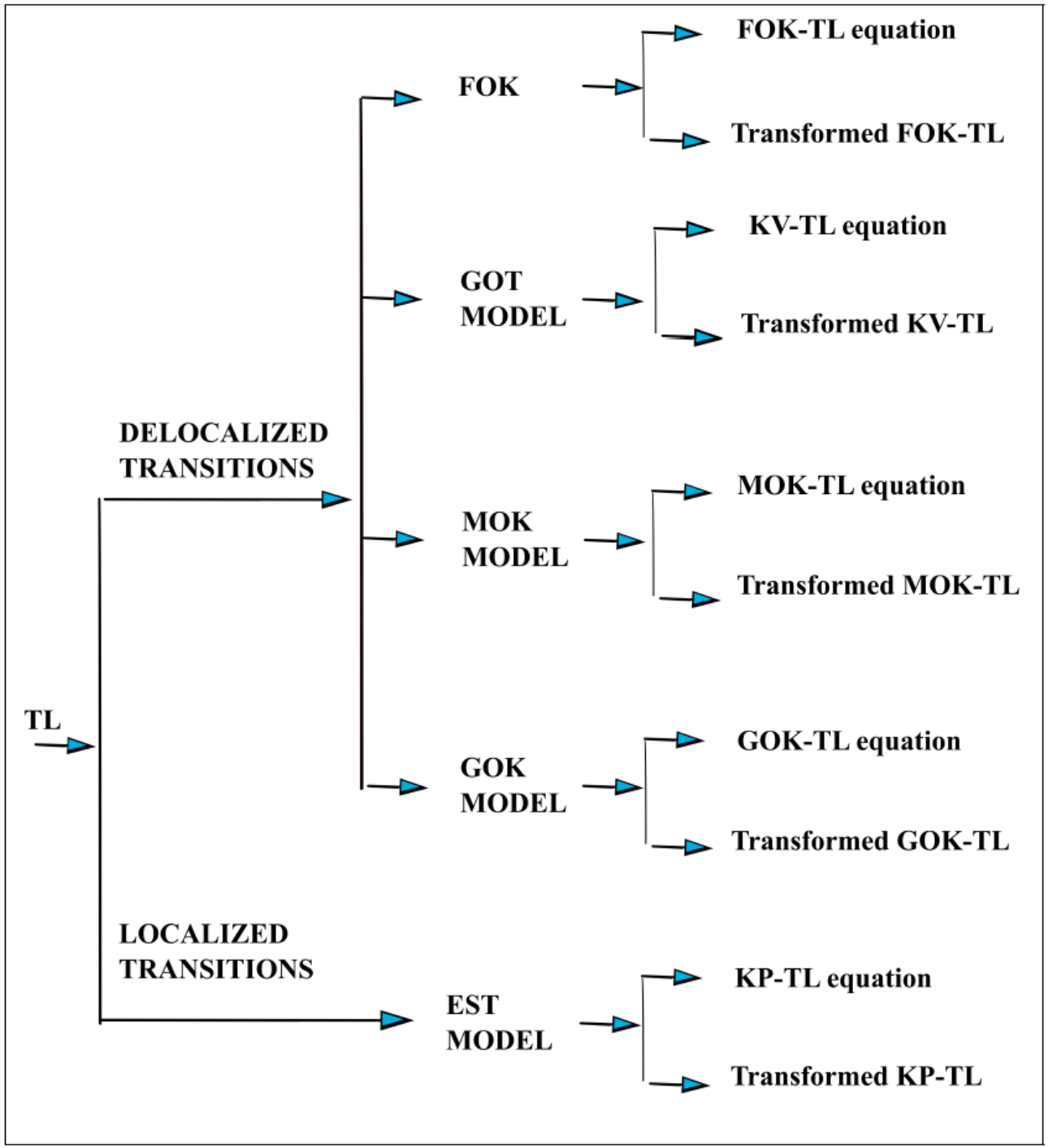
R is ideal for statistical analysis

Huge number of libraries for scientific analysis

Learning curve less steep, more researchers are familiar with it

Structure of codes easier to read

Very large online community and websites available, that can help us find a solution quickly



TL MODELS

First order kinetics (FOK)

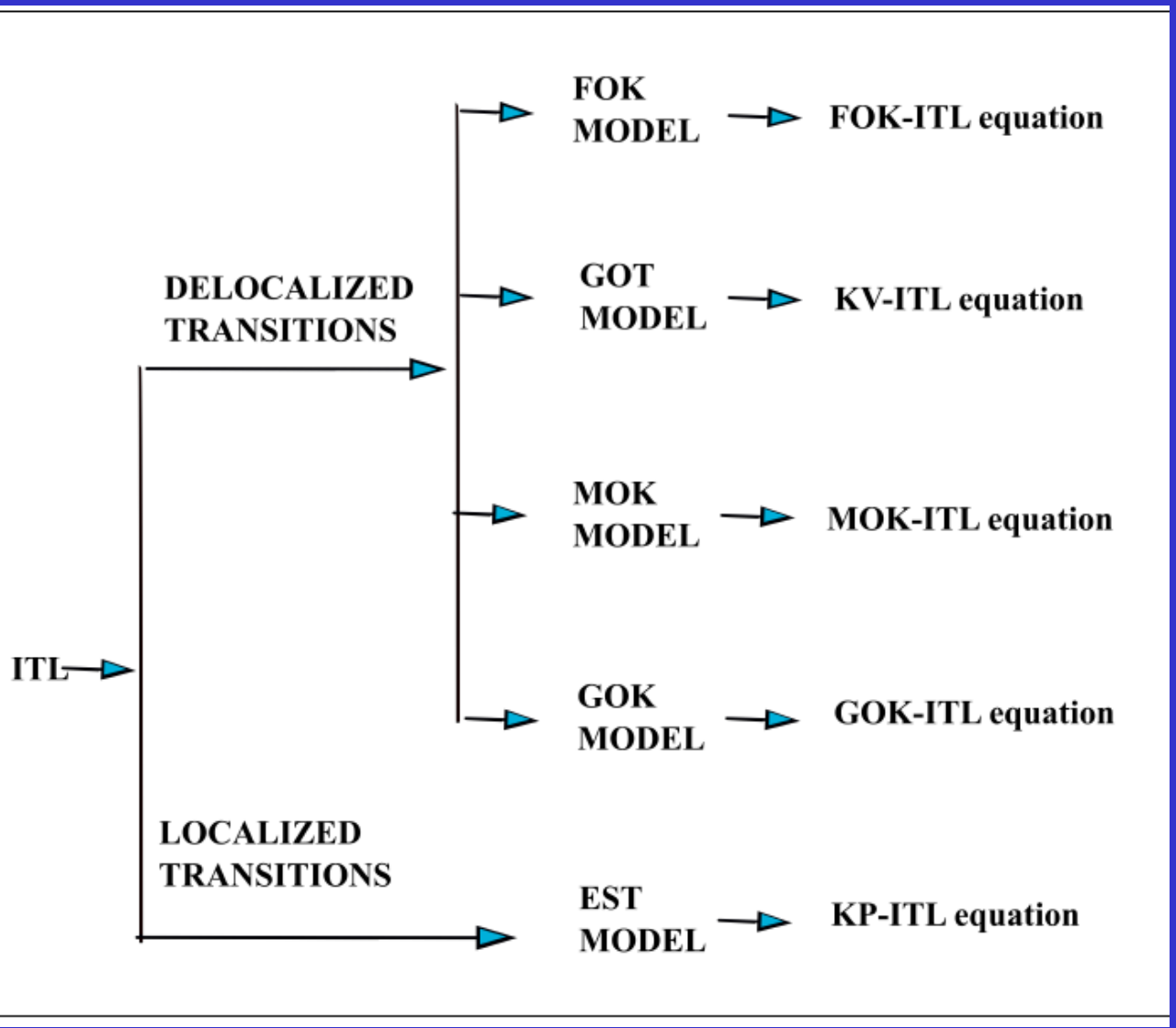
General one trap (GOT)

Mixed order kinetics (MOK

General order kinetics (GOK)

(EST) localized transitions model

ISOTHERMAL TL (ITL)



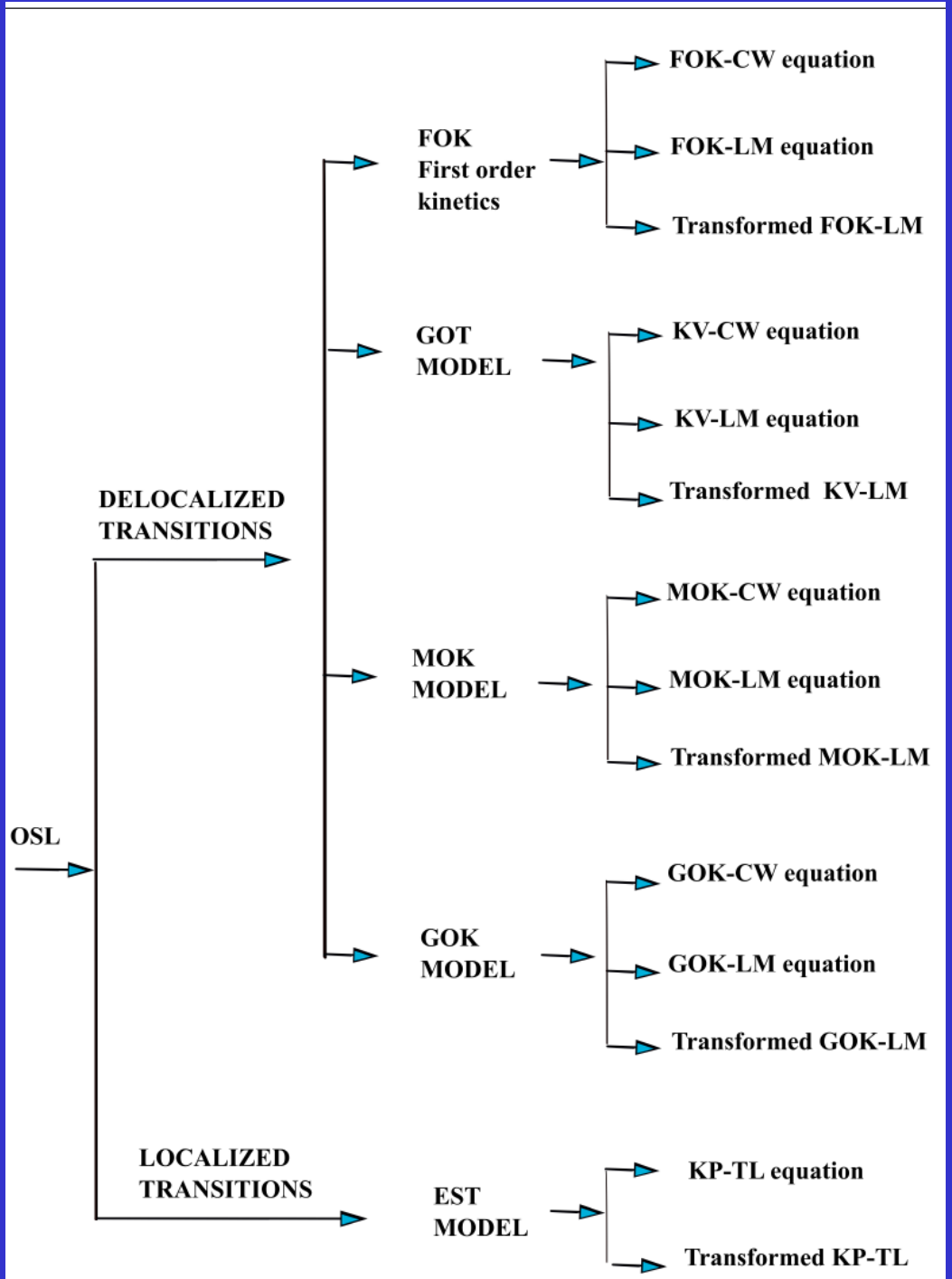
First order kinetics (FOK)

General one trap (GOT)

Mixed order kinetics (MOK)

General order kinetics (GOK)

(EST) localized transitions model



OSL

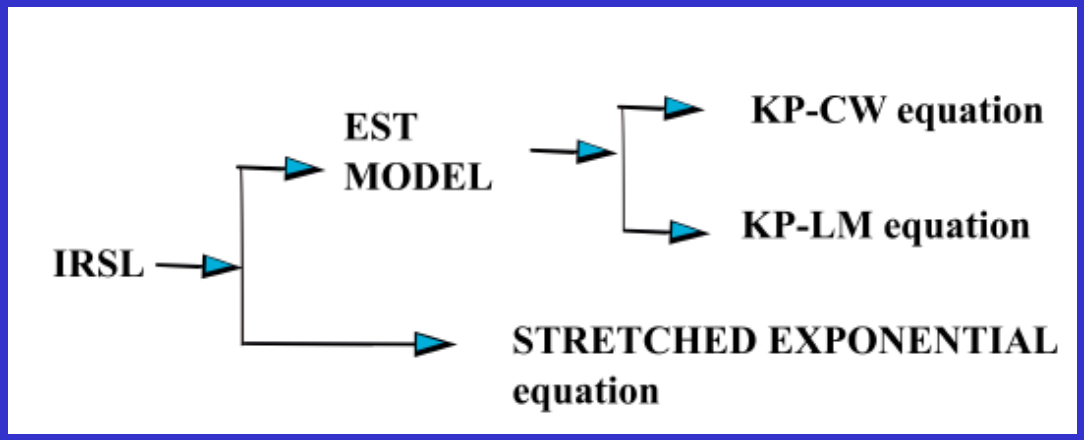
First order kinetics (FOK)

General one trap (GOT)

Mixed order kinetics (MOK)

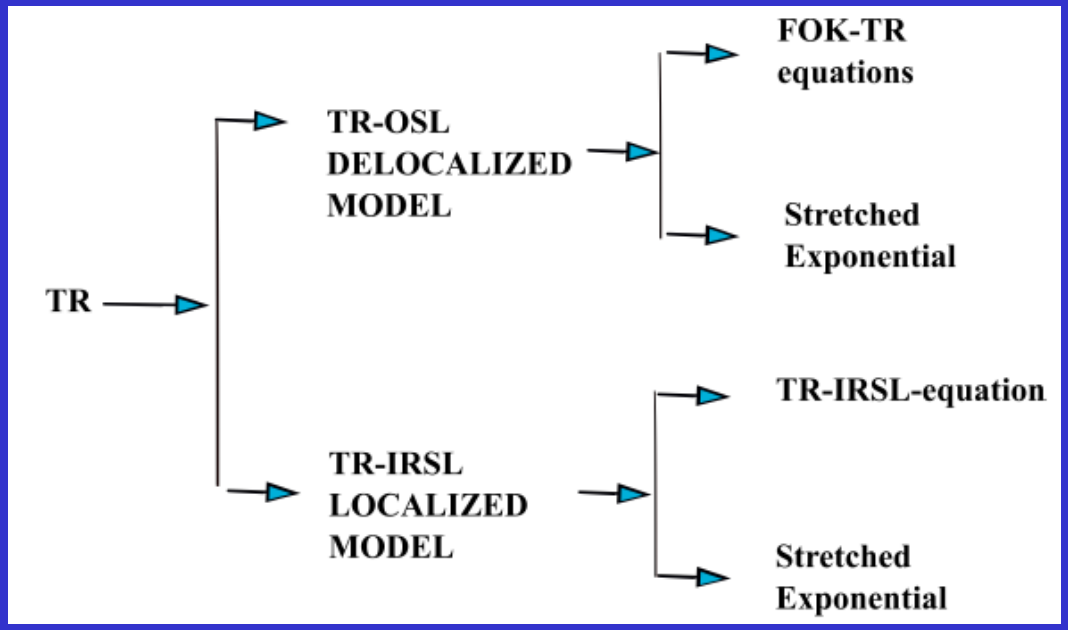
General order kinetics (GOK)

(EST) localized transitions model

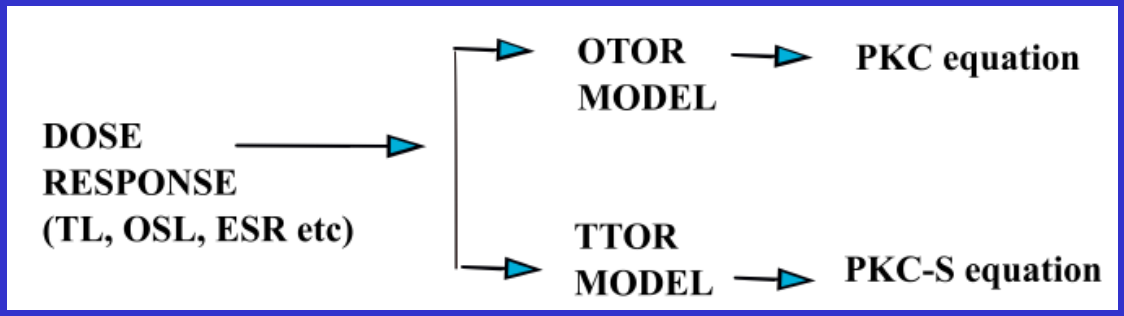


INFRARED SL (IRSL)

Based on localized transitions model



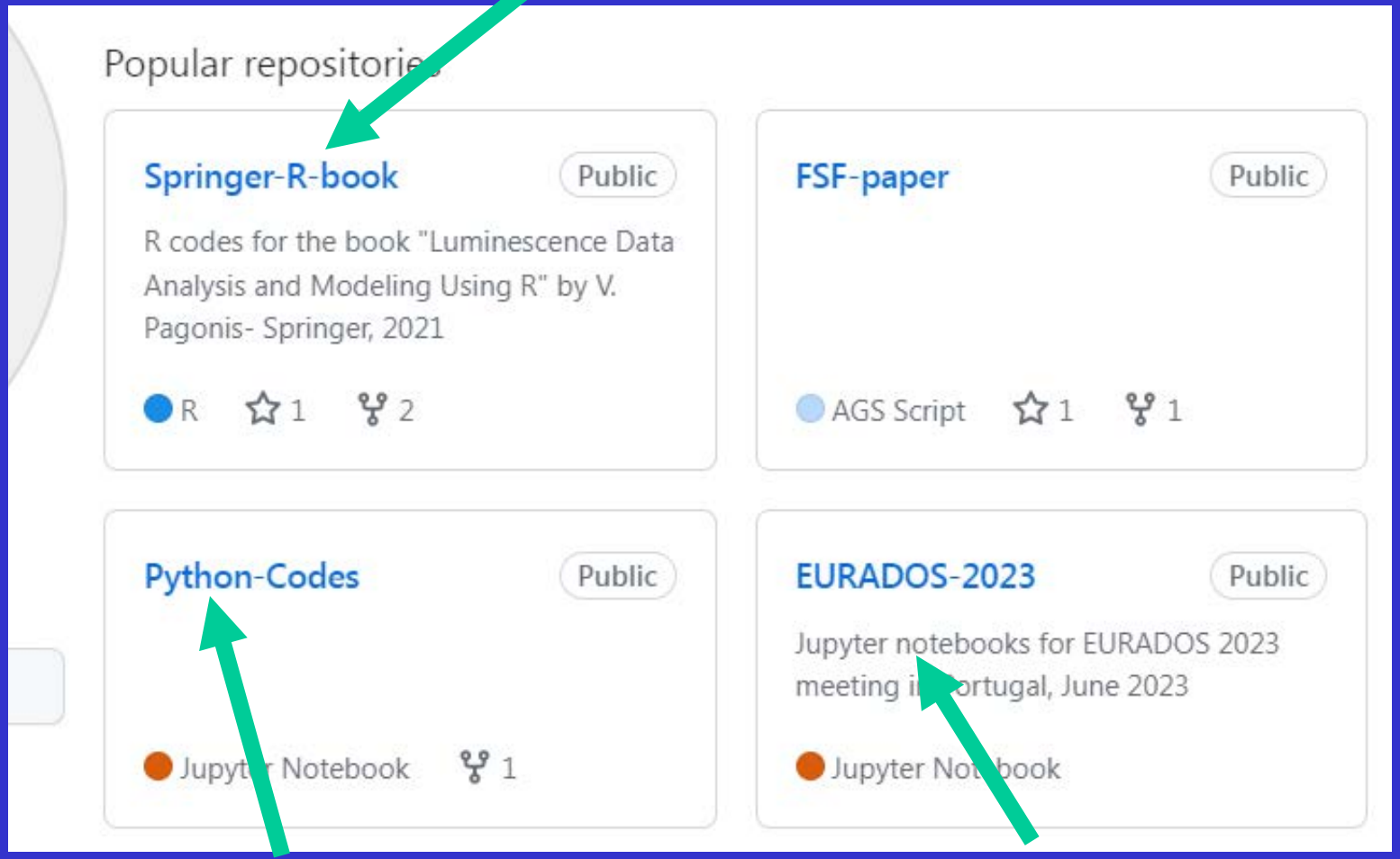
TIME-RESOLVED (TR)



DOSE RESPONSE
Exponentials
Double exponentials
Linear+exponential
PKC equations

CODES CURRENTLY AVAILABLE AT GITHUB:
https://github.com/vpagonis

R CODES



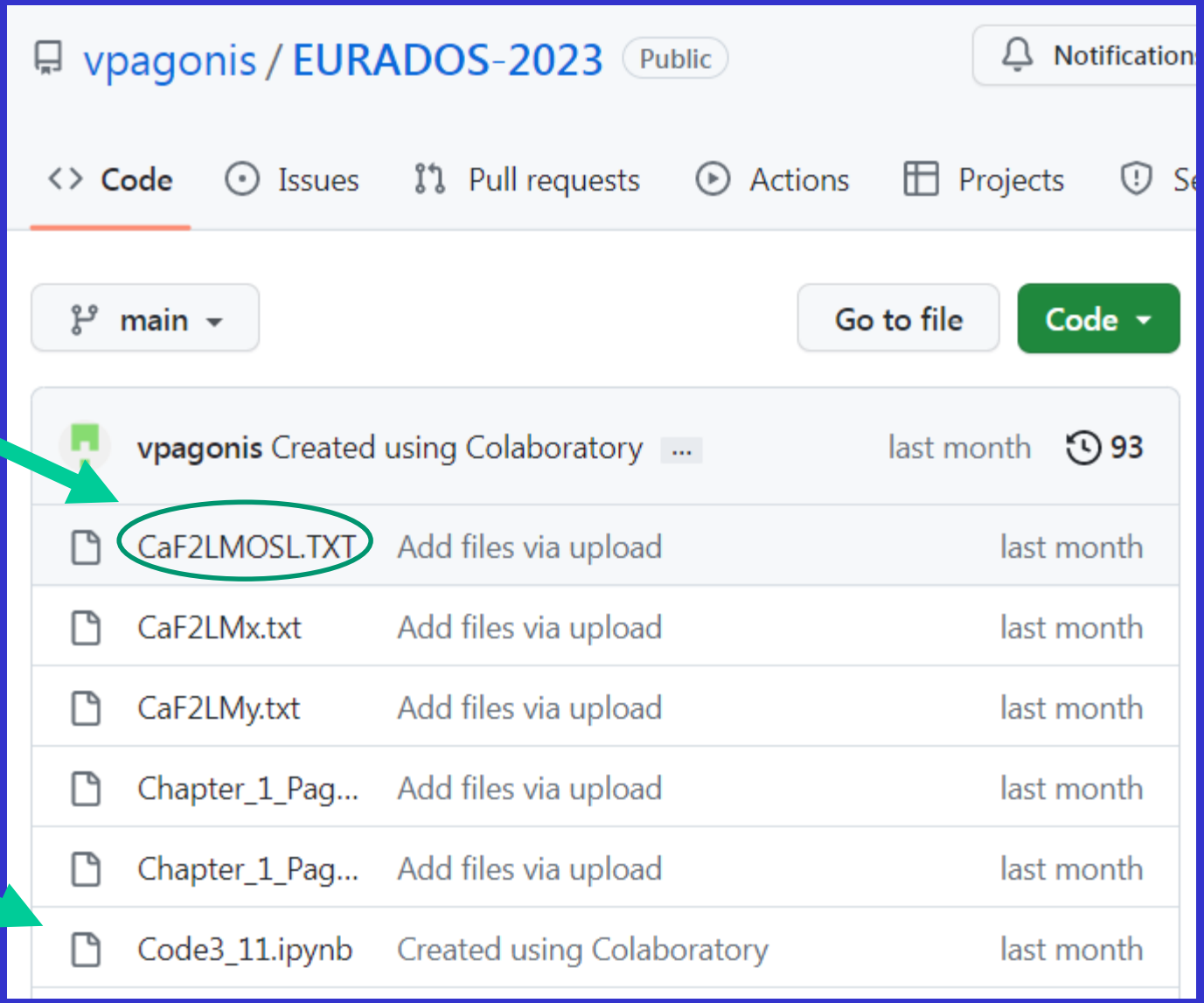
PYTHON CODES

JUPYTER NOTEBOOKS

https://github.com/vpagonis/EURADOS-2023

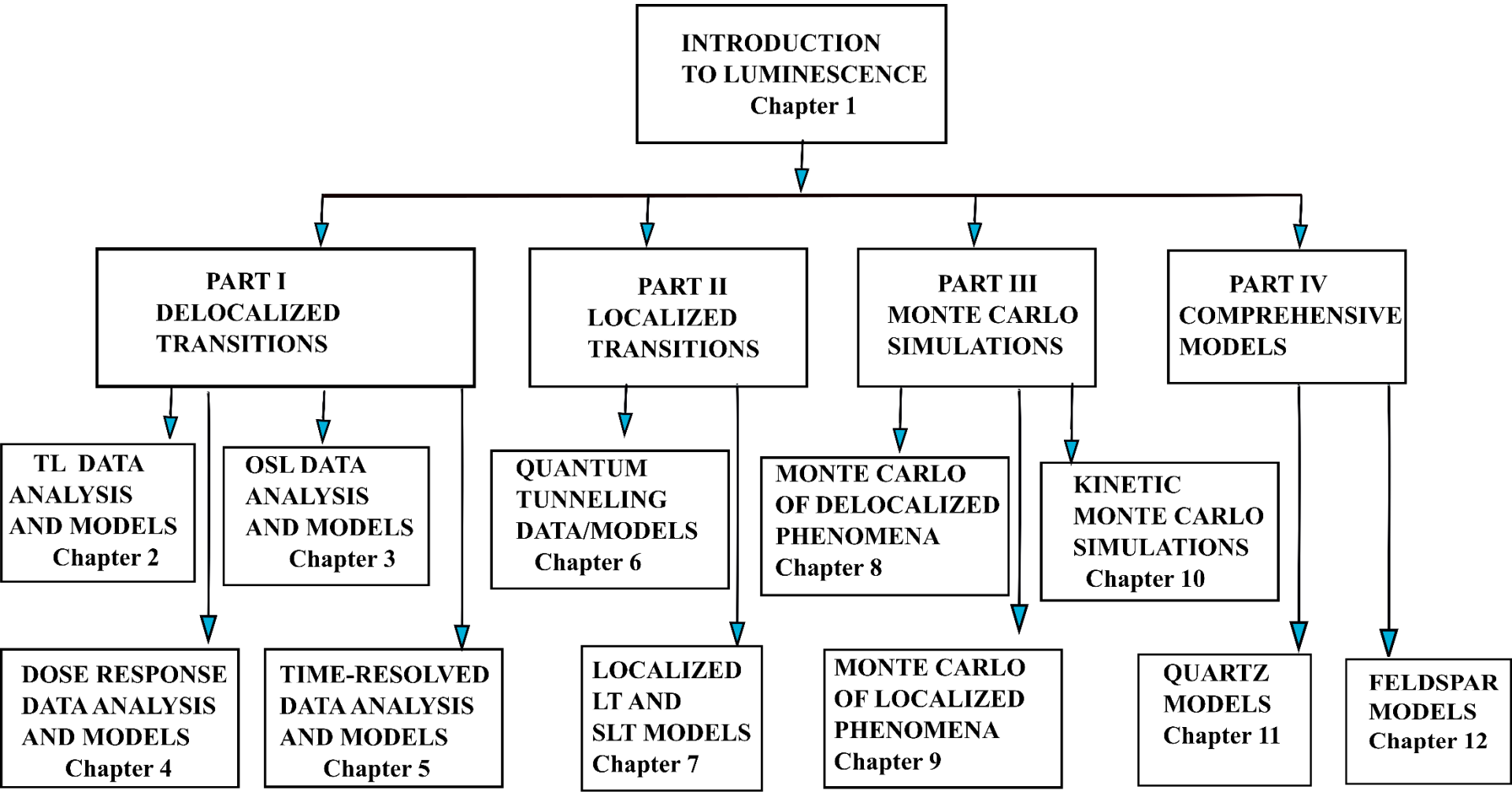
Data file
(.txt)

Jupyter notebook
(.ipynb)



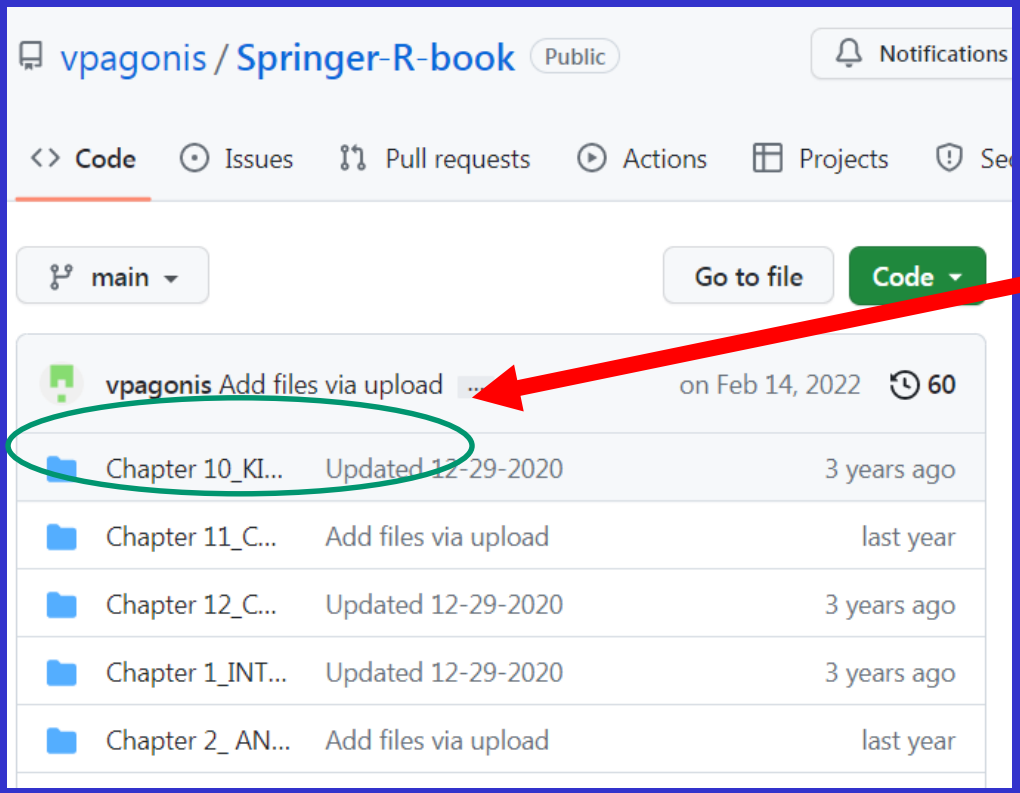
99 R CODES CURRENTLY AVAILABLE AT GITHUB

ORGANIZATION OF 99 R-CODES IN THE R BOOK

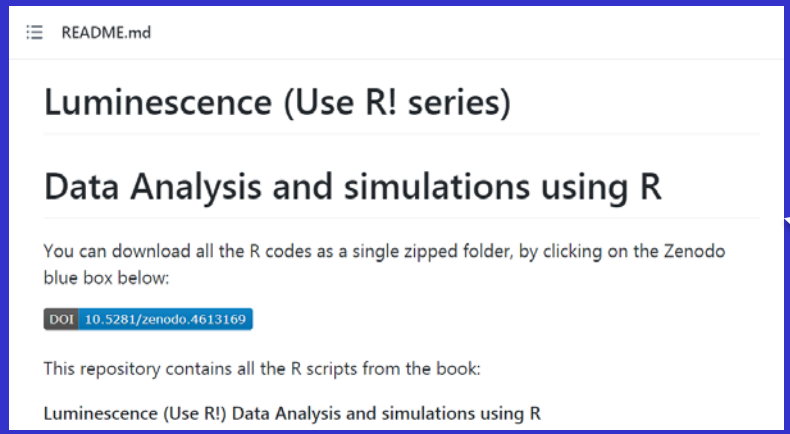


The 99 R codes from the Springer Luminescence book are at GitHub

https://github.com/vpagonis/Springer-R-book



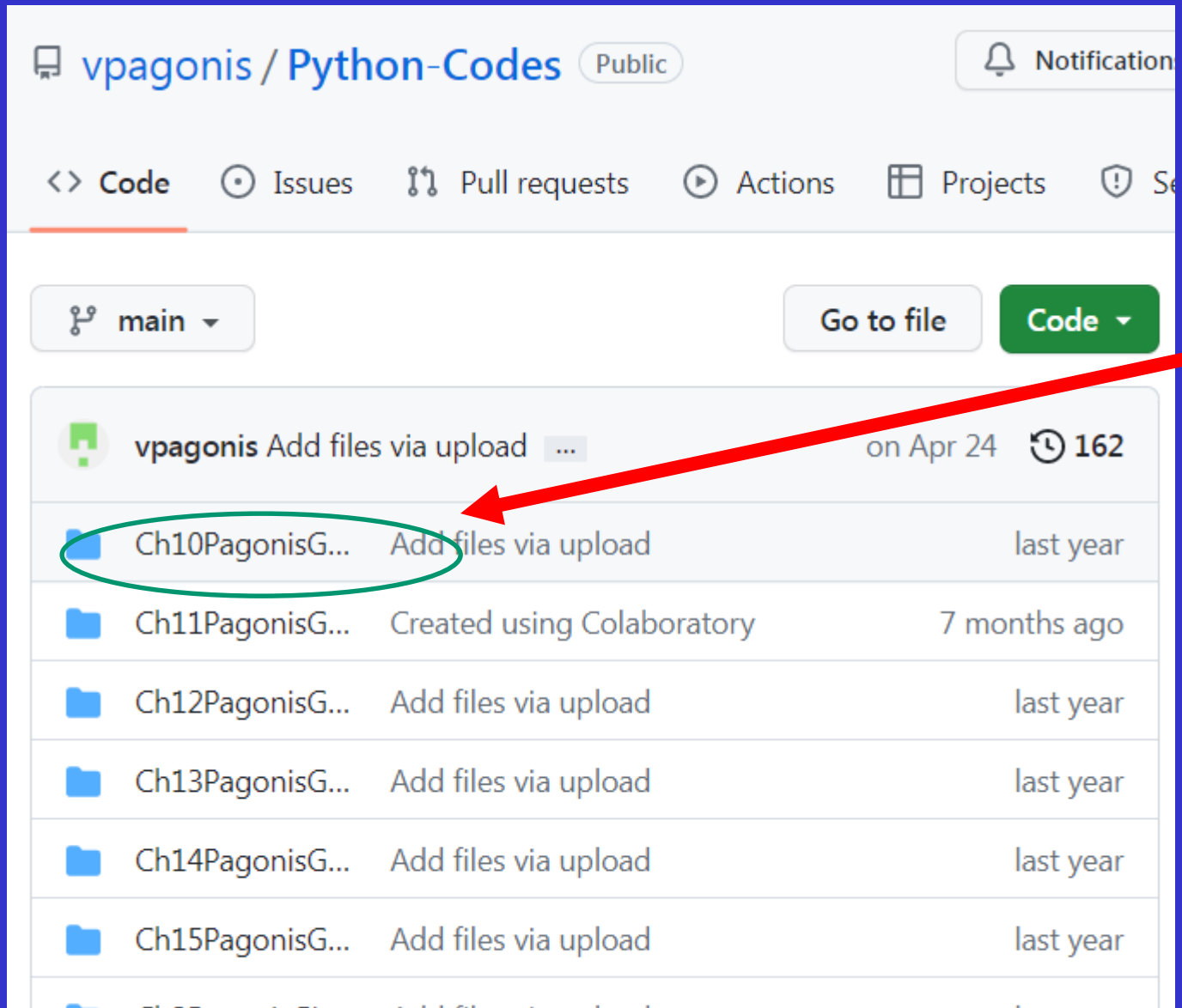
CODES are organized by chapter



All R codes can be downloaded as a single ZIP file from ZENODO

The 87 Python codes from the Springer Luminescence book are at GitHub

https://github.com/vpagonis/Python-Codes



CODES are organized by chapter

FAQ: Luminescence meets Google Colaboratory (CoLab)

Are the Python and R codes open access? **Y**

Can I run the codes without installing Python or R in my computer? **Y**

I am new to Python and R, can I use the codes without too much suffering? **Y**

What is the easiest way to use the codes in the web?

Use the website link emailed to you:

https://blog.mcdaniel.edu/vasilispagonis/python-codes-for-eurados-2023/

What is the easiest way to download the codes in the web?

https://github.com/vpagonis

Code3_12.ipynb

File Edit View Insert Runtime Tools Help

+ Code + Text Copy to Drive

Code 3.12 FITTING TL DATA WITH GENERAL ORDER KINETICS (TRANSFORMED GOK-TL equation)

The transformed GOK-TL equation for analysis of TL signals is:

$$I(T) = I_m b^{\frac{b}{b-1}} e^u \left[Z_m + (b-1)\left(1 - \frac{2kT}{E}\right)\left(\frac{T^2}{T_m^2} e^u\right)\right]^{-\frac{b}{b-1}}$$

$$u = \frac{E}{kT}\frac{T - T_m}{T_m}$$

$$Z_m = 1 + (b-1)\frac{2kT_m}{E}$$

The fitting parameters in this expression are b and E, while the parameters T_m, I_m can be estimated fro

```
##Deconvolution of 9-peak data with transformed GOK-TL eqt
from scipy import optimize
import numpy as np
import matplotlib.pyplot as plt
from prettytable import PrettyTable
import warnings
warnings.filterwarnings("ignore")
import requests

# read data file from GitHub
url='https://github.com/vpagonis/EURADOS-2023/raw/main/Refglow009.txt'
response=requests.get(url)
a=response.text
```

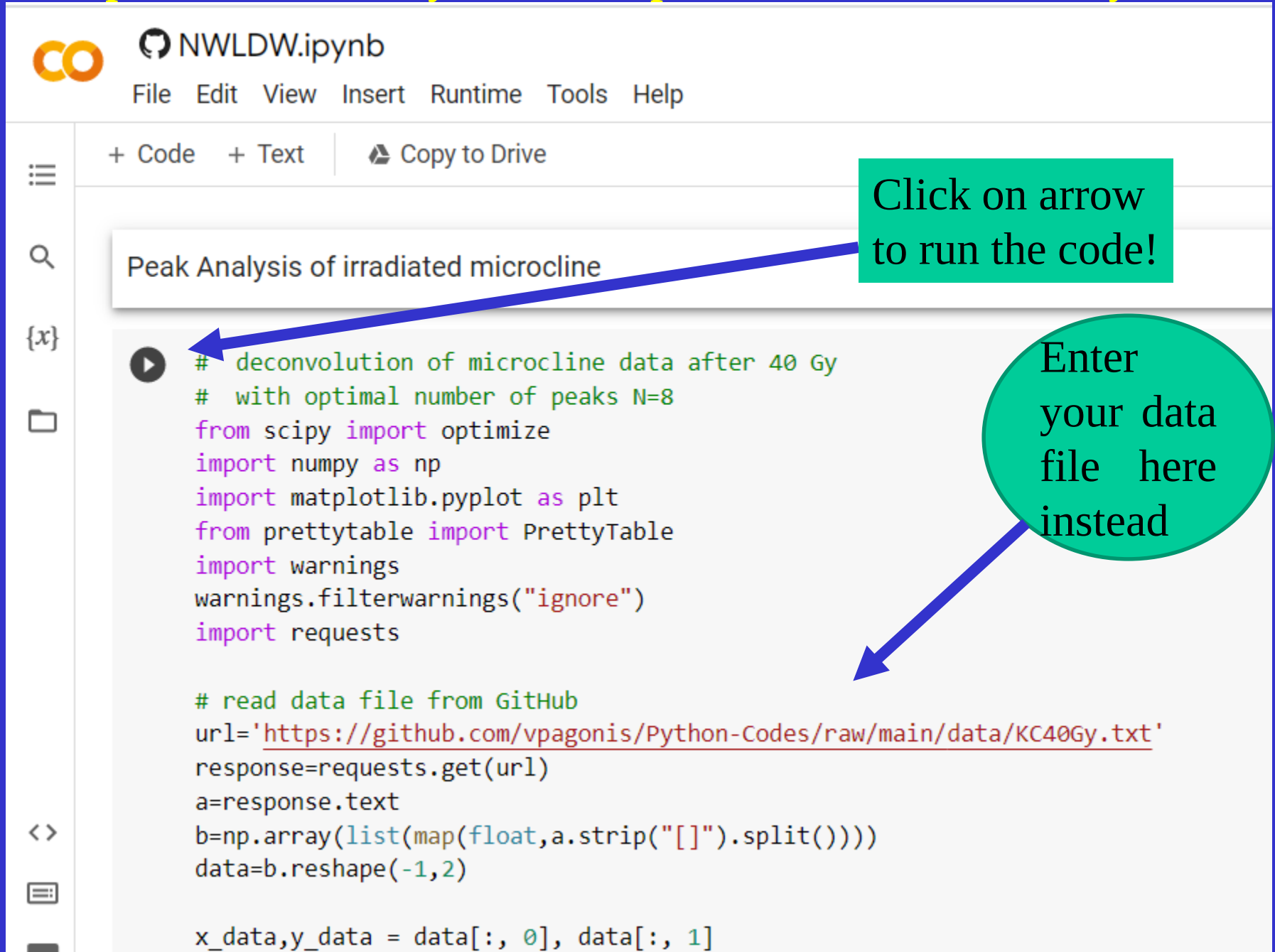
JUPYTER NOTEBO
contains several parts

This is the text and equations (you can edit easily)

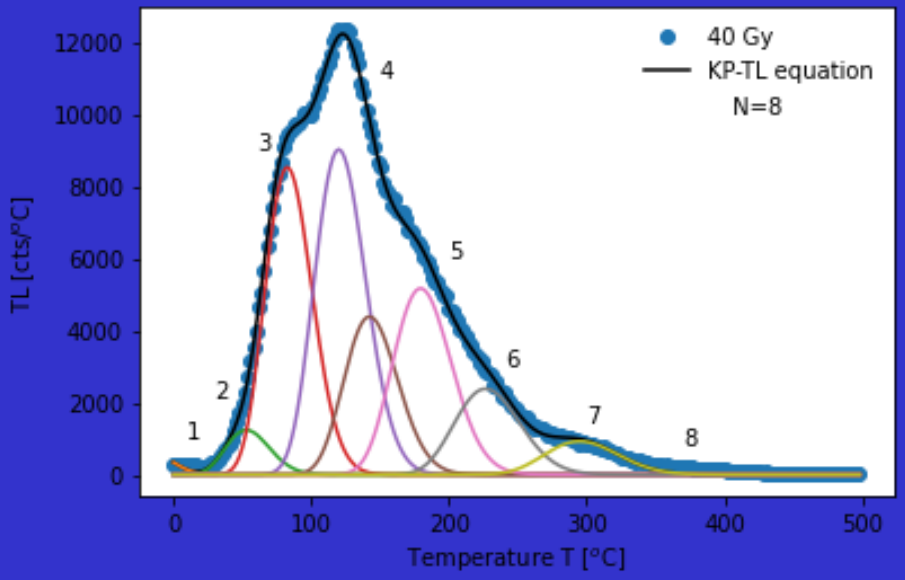
This is the Python code

(edit easily)

Example Code 1: Analysis of feldspar TL from dose=40 Gy



Jupyter notebook also contains the CODE OUTPUT



You can run, edit, modify, save the code and/or the notebook in your Google Drive, or in your computer

(The code plus the output are a Jupyter notebook)

Table of Best fit parameters
FOM= 2.82 %

Amplitude B (a.u.)	Energy E (eV)	frequency s (s^-1)
8.78E+16	7.01E-01	9.22E+13
7.00E+16	8.40E-01	2.28E+13
9.91E+17	9.39E-01	4.41E+13
1.82E+18	1.06E+00	7.07E+13
1.30E+18	1.13E+00	9.96E+13
1.67E+18	1.24E+00	1.00E+14
5.91E+17	1.35E+00	6.91E+13
3.55E+17	1.56E+00	9.54E+13

ρ'= 1.16E-02

PYTHON CODES- PART I

TL

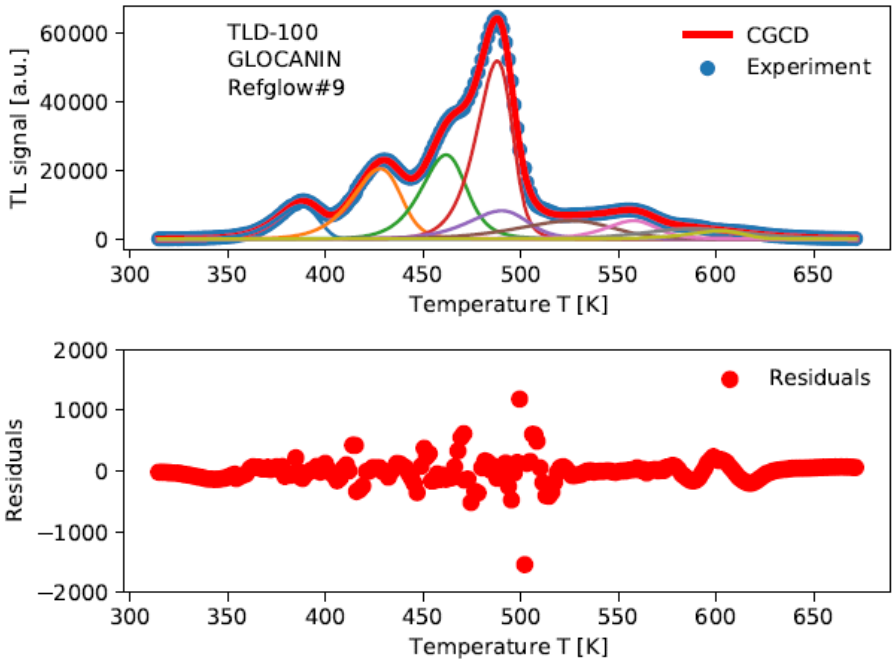
DELOCALIZED TRANSITIONS

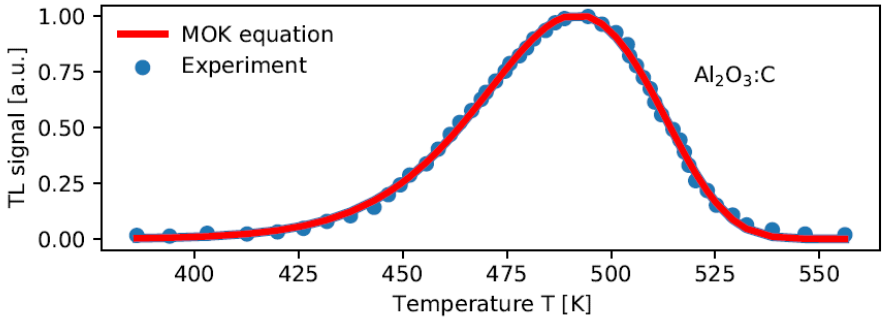
Kitis-Vlachos Equation with Lambert (KV-TL)

Mixed order Kinetics (MOK)

First order Kinetics (FOK)

General order Kinetics (GOK)





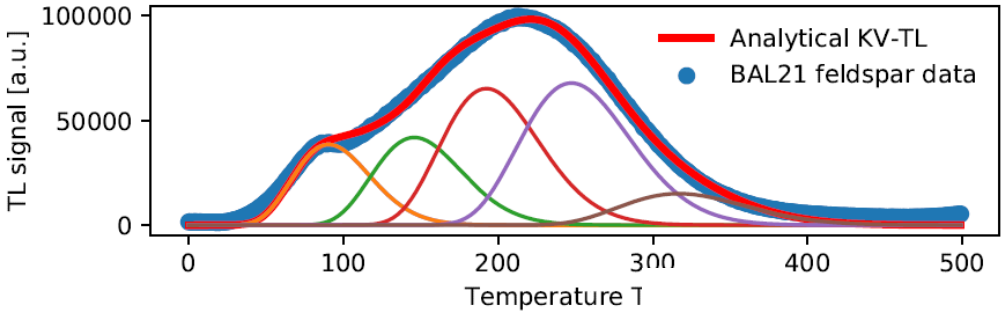
TL

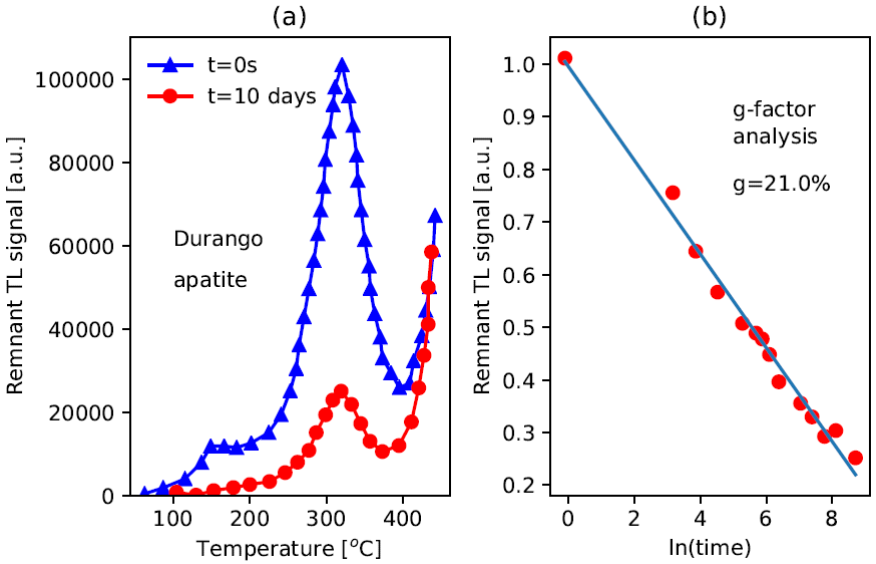
LOCALIZED QUANTUM TUNNELING TRANSITIONS

Kitis-Pagonis Equation for prompt TL signals (KP-TL)

Anomalous fading analysis (g-factor)

Transformed KP-TL equation for preconditioned samples





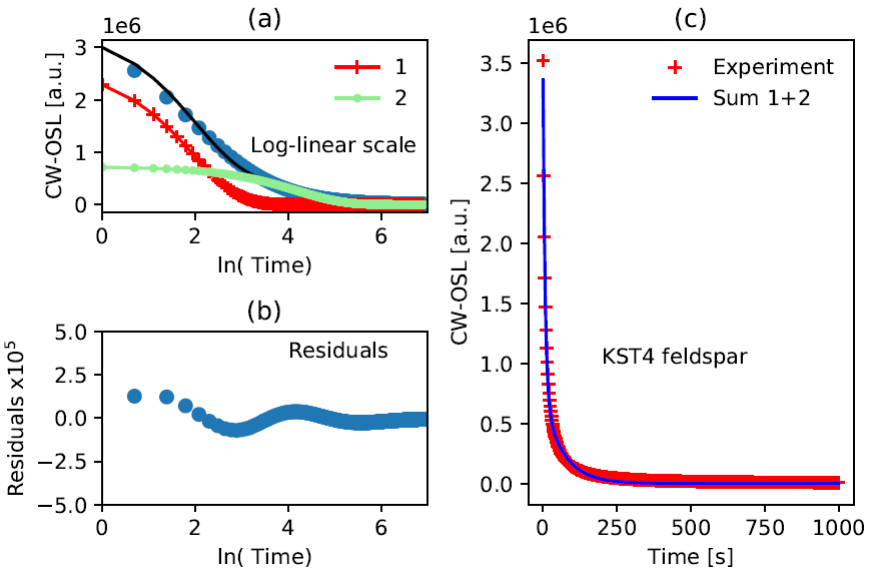
CW-OSL/LM-OSL

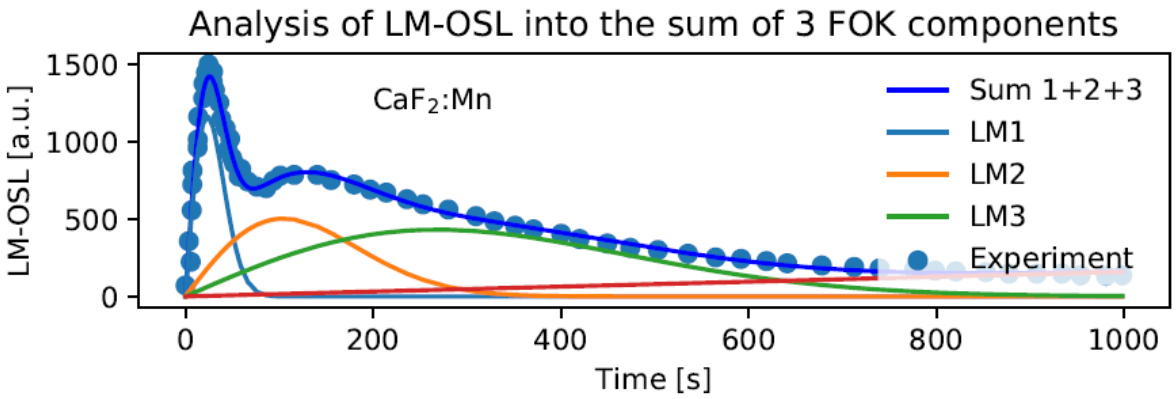
DELOCALIZED TRANSITIONS

Kitis-Vlachos Equation with Lambert (KV-CW And KV-LM)

First order Kinetics (exponential functions)

General order Kinetics (GOK)





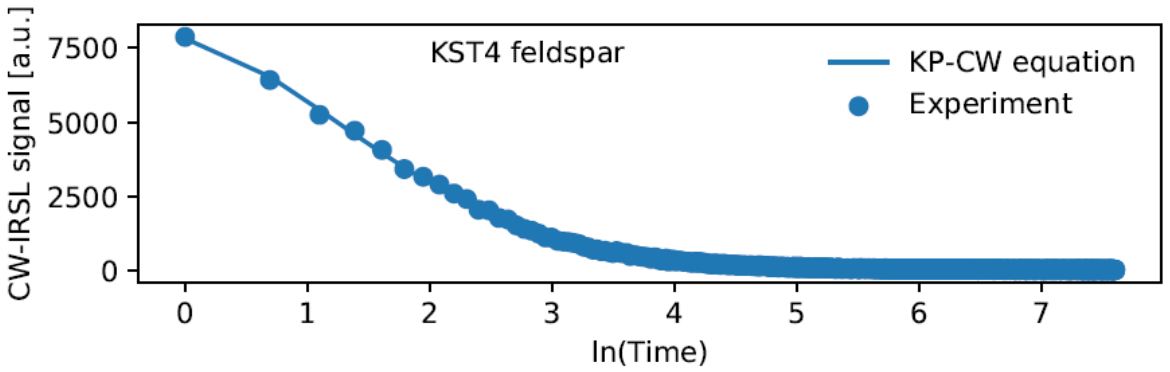
CW-IRSL/LM-IRSL

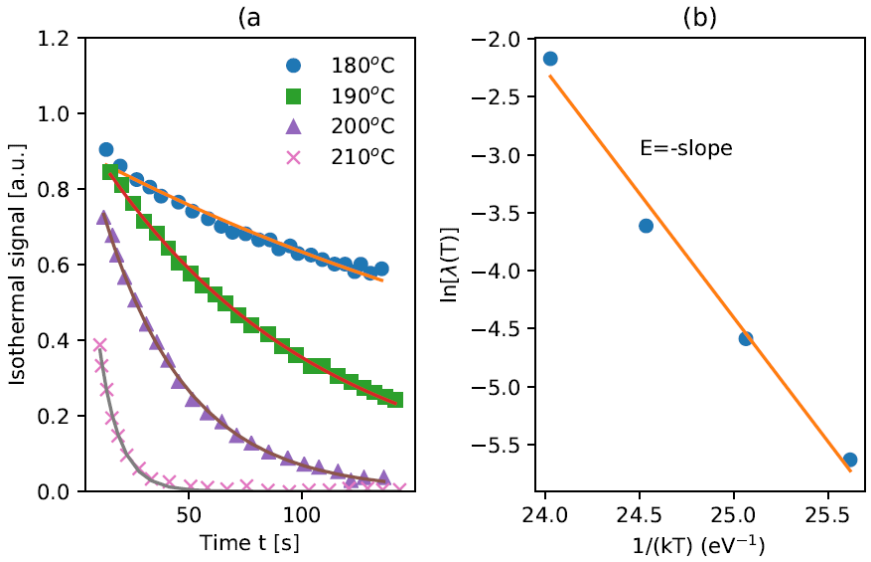
LOCALIZED QUANTUM TUNNELING TRANSITIONS

Kitis-Pagonis Equations for IRSL (KP-CWIRSL and KP-LMIRSL)

ITL (isothermal)

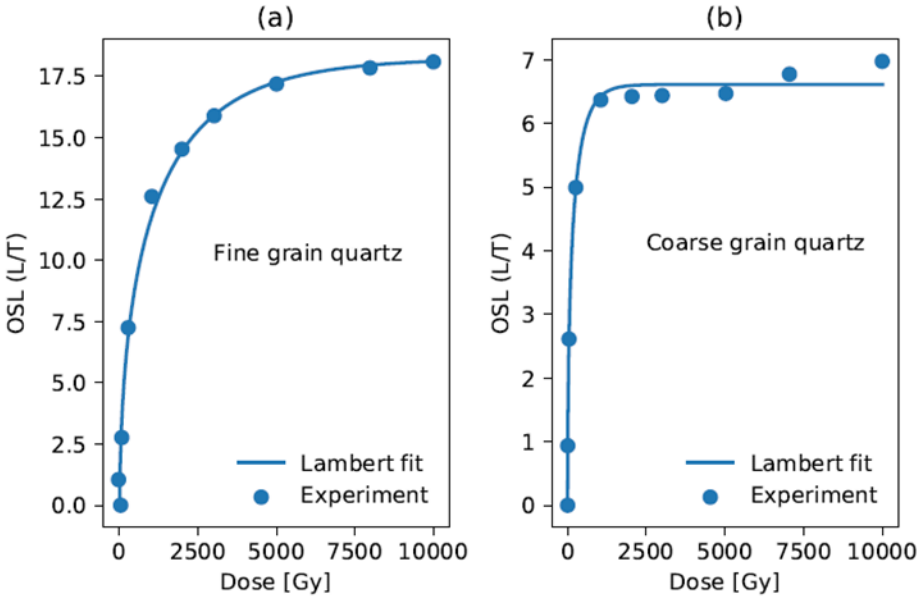
DELOCALIZED TRANSITIONS





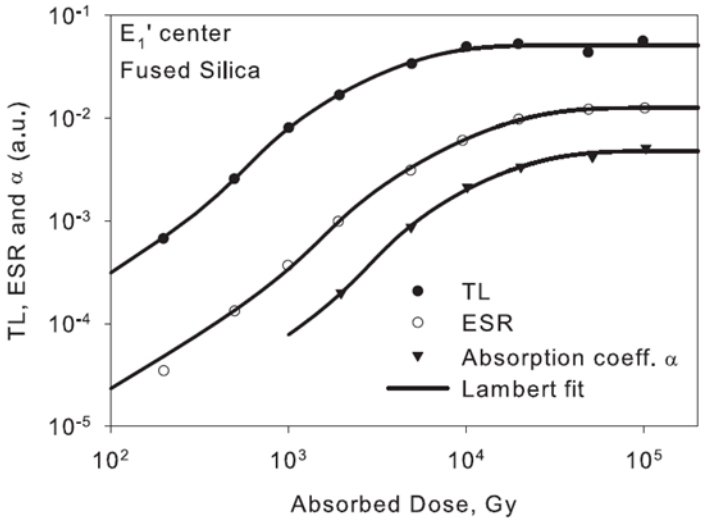
DOSE RESPONSE

Pagonis-Kitis-Chen Equation with Lambert Function (PKC)



Fit of experimental SAR-OSL experimental dose response data, for (a) fine grain and (b) coarse grain quartz samples, using the PKC equation..

Pagonis-Kitis-Chen Superlinear response equation with Lambert (PKC-S)

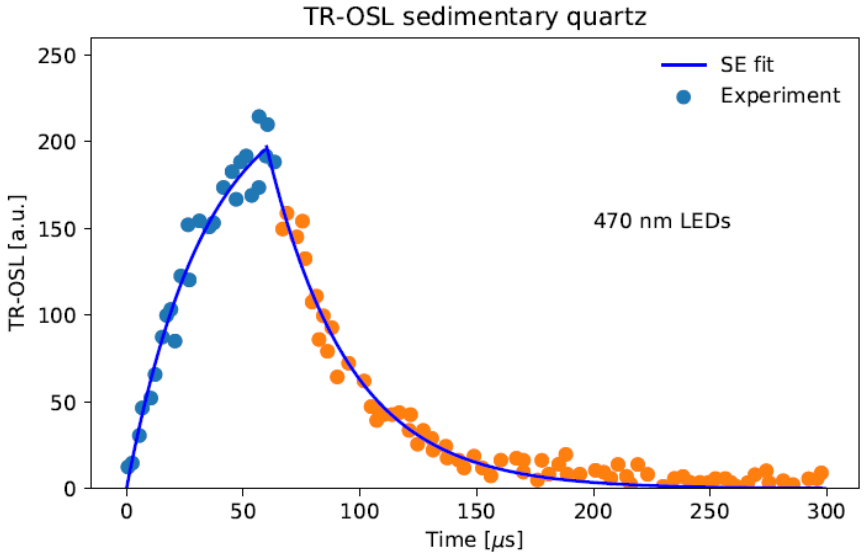


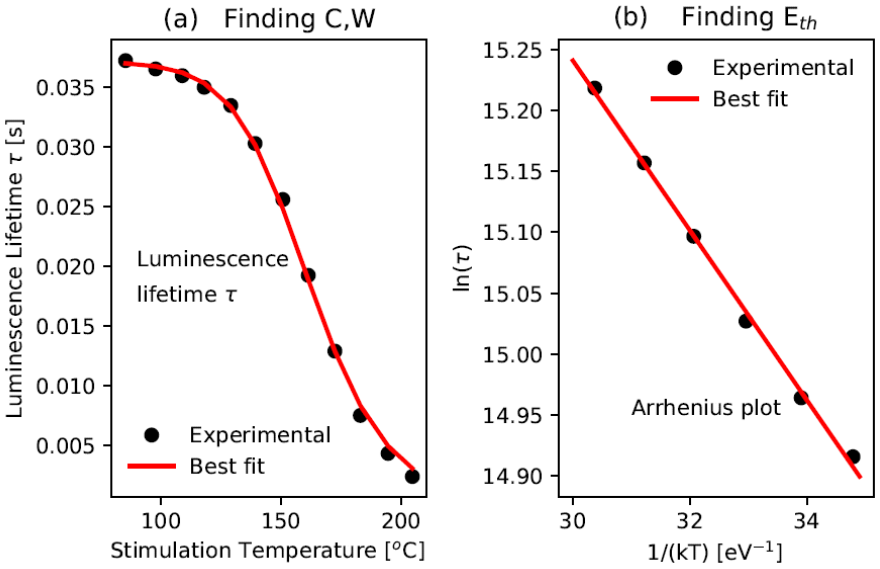
Superlinear dose dependence of the E_1' center concentration (ESR), TL and OA signals, from a single sample of fused silica.

TIME-RESOLVED

DELOCALIZED TRANSITIONS

First order Kinetics (FOK-TR exponentials)





WHERE TO FIND THE CODES, EQUATIONS, MODELS

R codes

The complete 99 R codes from the Springer Luminescence book are found at this GitHub website:

https://github.com/vpagonis/Springer-R-book

Recently published R book

V. Pagonis. Luminescence: Data Analysis and Modeling Using R. Use R!
Springer International Publishing, 2021.
(Contains all equations and models)

PYTHON

The complete 87 Python codes described here are found at this GitHub website:

https://github.com/vpagonis/Python-Codes

Recently published Python book

V. Pagonis. Luminescence Signal Analysis Using Python
Springer International Publishing, 2022.
(Contains all equations and models)

Things to watch for:

Peak shaped signals: How many peaks? First order or not?

Decay curve signals: How many components? First order or not?

Dose response: use two saturating exponentials, or linear plus saturating exponential or single component?

Thermal quenching

Discrete or continuous energy?

Fading

Reproducibility (accuracy and precision of dosimeter)

Local minimum in least squares always a possibility

Codes are blind to physics! It is best to place restrictions on the parameters

Where does this R and PYTHON software project go from here?

How can we make these codes most useful for researchers?

Ideally, we should have one website, sponsored e.g. by EURADOS ☺

Website can contain links to all Python and R codes, in form of Jupyter notebooks

99+87 codes= a LOT of Jupyter notebooks! help!

Users can download notebooks, software can be run immediately

The theory and results are available in the same notebook

CONCLUSIONS

Our goals are:

Make open access codes available to luminescence community

Classify, organize, standardize R and Python codes for computerized analysis and luminescence models

Currently 99 complete R-codes and 87 Python codes are available for downloading at GitHub

The codes have been tested and cross-checked with Mathematica

The Python codes are easier to use and understand (my personal opinion)

Further questions about the codes?

please send me an email: vpagonis@mcdaniel.edu

Thank you very much for your attention!