

TIMPGUI: A graphical user interface for the package TIMP

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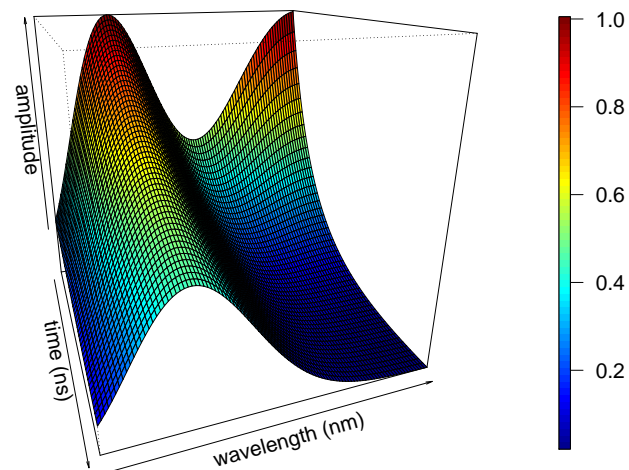


[Introduction: TIMP package]

TIMP is a package for fitting **superposition models** that has been applied to measurements arising in

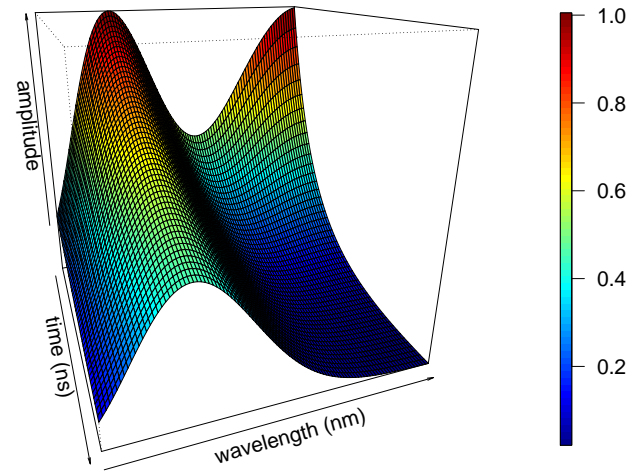
- time (and/or temperature, polarization, pH)-resolved spectroscopy
- fluorescence lifetime imaging microscopy (FLIM)
- time-resolved mass spectrometry data

this data can often be described as a (ragged) matrix representing possibly multiple experimental conditions

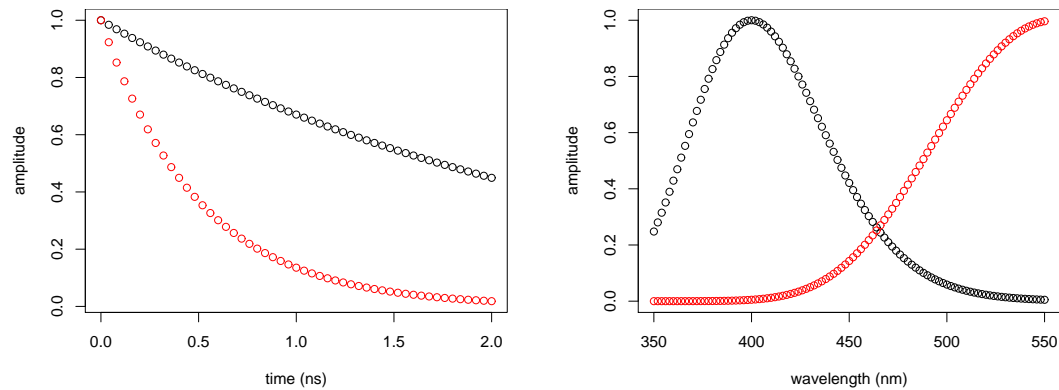


[Parameter estimation problem]

from the data



need to solve inverse problem to obtain a (parametric) description of components in time and in wavelength



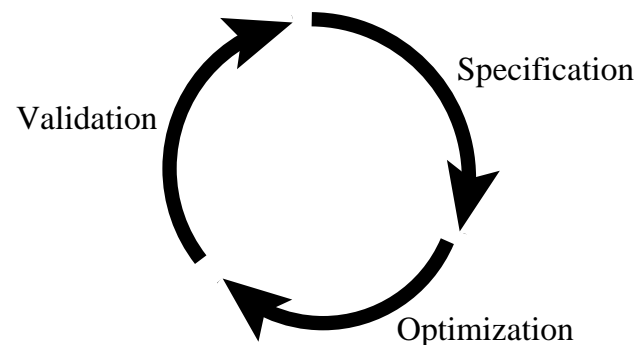
$$\Psi = C(\theta)E^T$$

[**Goals of data analysis and modeling**]

in modeling data arising time-resolved spectroscopy, microscopy and mass spectrometry experiments, often need to

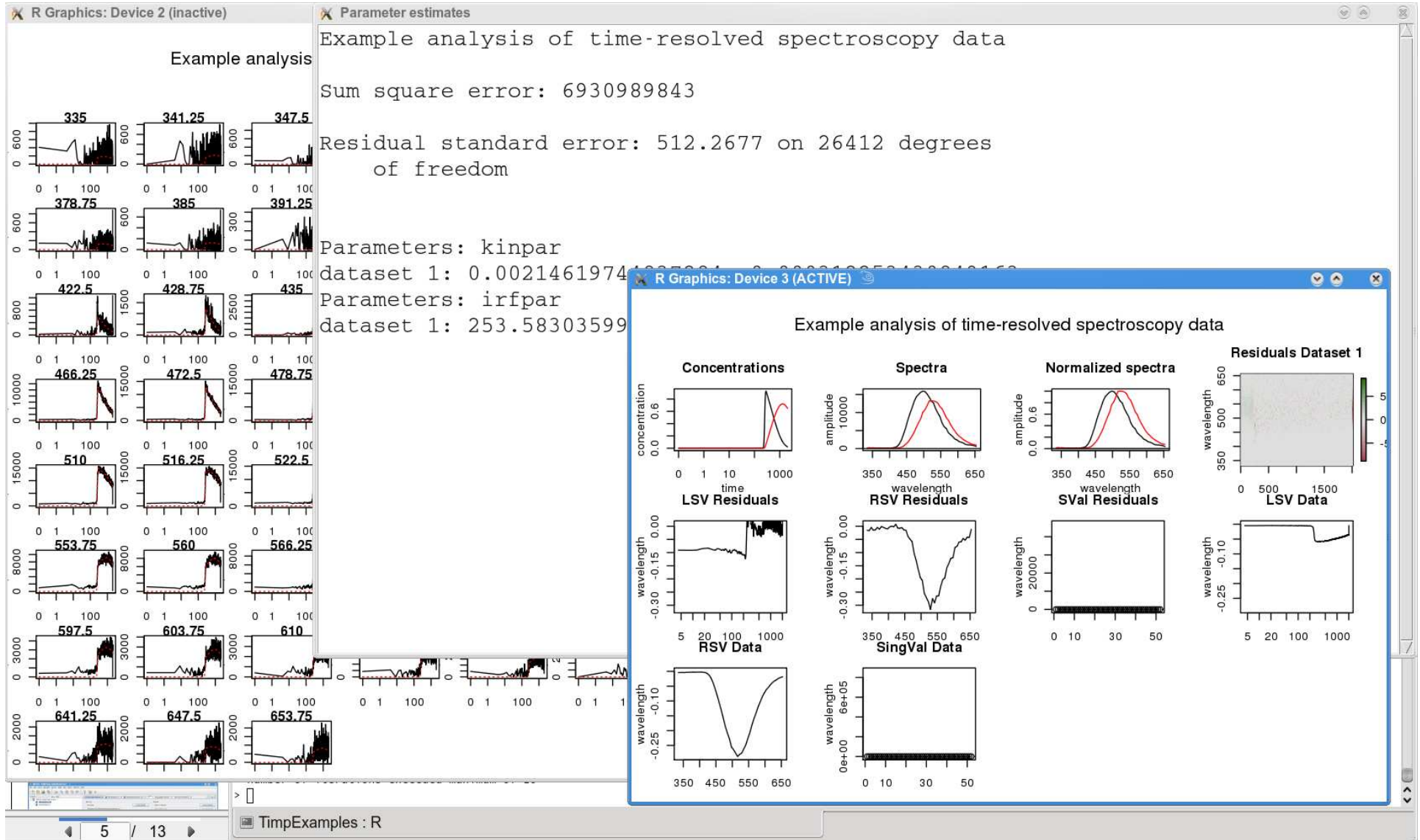
- test many different models
- evaluate the estimated parameters for physical interpretability
- explore the data and fit interactivity

TIMP is designed for easy model postulation, optimization and validation ...



but ... the interface has some disadvantages that are best explained by example

[LIVE DEMO SCREENSHOT: of model fitting via TIMP script]



[Motivation for a Graphical User Interface to TIMP]

In order to provide:

- possibilities for model specification via a graphical user interface (GUI)
- cross-platform software, to allow collaboration between Linux/Unix, MS Windows, and Mac OS users
- possibilities for interactive exploration of data and fit

we developed the java-based graphical user interface **TIMPGUI**

- built on top of the Netbeans platform
- calls **TIMP** via **JRI** from RoSuDa
- persistent storage of models and fitting options via XML files

The results are also best explained by example ...

[LIVE DEMO SCREENSHOT: loading data]

The screenshot displays the TIMPGUI software interface. The title bar reads "MPUR: TIMPGUI 200805300101". The menu bar includes File, Edit, View, Navigate, Source, Build, Run, Tools, Window, and Help. The toolbar contains icons for file operations and execution. The left sidebar shows a project tree with "TIMPGUI Streak Demo Project" containing "FittingOptions.xml" and "StreakModel.xml". The main window is titled "Streak Loader Window" and contains a "Data File" section with a "File Name" field set to "/home/jsg210/2008UseR/TimpExamples/jex.ivo" and a "Load Sample" button. To the right is a "Dataset" section with a "Name of Dataset" field set to "NameOfDataset1" and buttons for "Create Dataset" and "Save to Ivo File". Below these sections are three plots: "Selected trace" (Number of counts vs Time (ns)), "Selected Spectrum" (Number of counts vs Wavelength (nm)), and a 2D heatmap. The "Selected trace" plot shows a signal that rises sharply at approximately 250 ns and then gradually decays. The "Selected Spectrum" plot shows a broad peak centered around 500 nm. The heatmap shows a vertical band of high intensity (yellow/red) centered around 500 nm, with a color scale on the right ranging from 0 to 17,000 counts.

MPUR: TIMPGUI 200805300101

File Edit View Navigate Source Build Run Tools Window Help

Projects Files

TIMPGUI Streak Demo Project

- FittingOptions.xml
- StreakModel.xml

Streak Loader Window x StreakModel.xml x StreakModelOptions.xml x TimpguiMain Window x FlimTimpJFF Window x

Data File

File Name Load Sample

Dataset

Name of Dataset Create Dataset

Save to Ivo File

Selected trace

Number of counts

Time (ns)

Selected Spectrum

Number of counts

Wavelength (nm)

Number of timesteps: 512 Time window: 2015.2

Number of wavesteps: 52 Wave window: 318.75

Output - R Output

```
R version 2.7.2 (2008-08-25)
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ISBN 3-900051-07-0

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Natural language support but running in an English locale

R is a collaborative project with many contributors.
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Type 'demo()' for some demos, 'help()' for on-line help, or
'help.start()' for an HTML browser interface to help.
Type 'q()' to quit R.
```

[LIVE DEMO SCREENSHOT: specification of model]

The screenshot displays the TIMPGUI software interface. The main window is titled "MPUR: TIMPGUI 200805300101". The menu bar includes File, Edit, View, Navigate, Source, Build, Run, Tools, Window, and Help. The toolbar contains various icons for file operations and execution. The left sidebar shows a project tree for "TIMPGUI Streak Demo Project" with files "FittingOptions.xml" and "StreakModel.xml". The main workspace is titled "Model specification decay rates:" and contains several sections:

- TIMPGUI Model (tgm) specification:** A placeholder for the TGM Panel with a "Send Model to Timp" button.
- Model name and type:**
 - ModelName: StreakModelDemo
 - ModelType: kin
- Model specification decay rates:**
 - Number of components: 2
 - Show constrains:
 - Set Kinetic Parameters Positive:

Starting value	Fixed	Free Betw Datasets	Constrained	Mn	Max
0.002	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>		
0.004	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	0	0

 - Sequential analysis:
- Model specification for instrument response:**
- Model for coherent artifact:**

The bottom panel shows the "Output - R Output" window with the following text:

```
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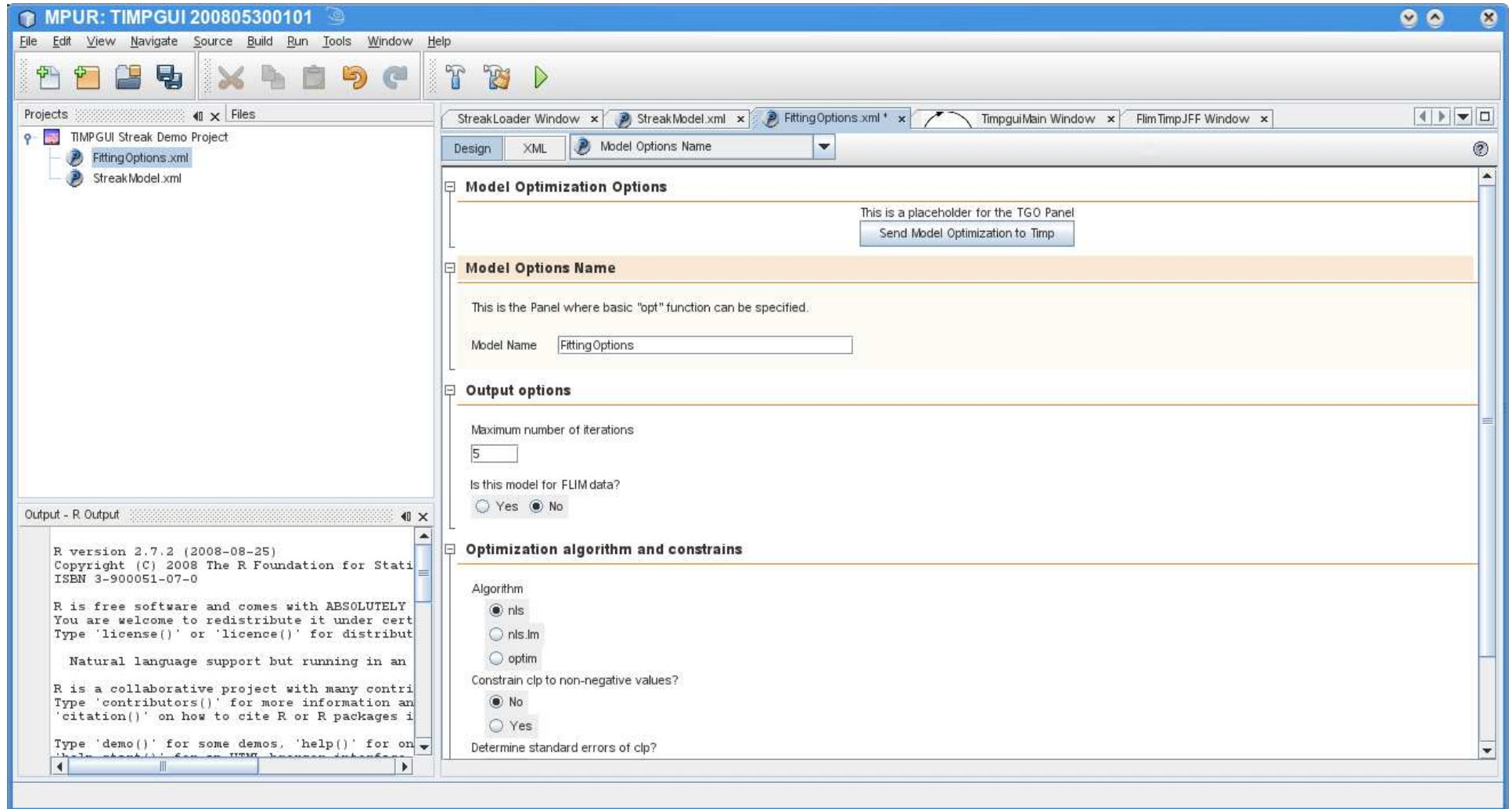
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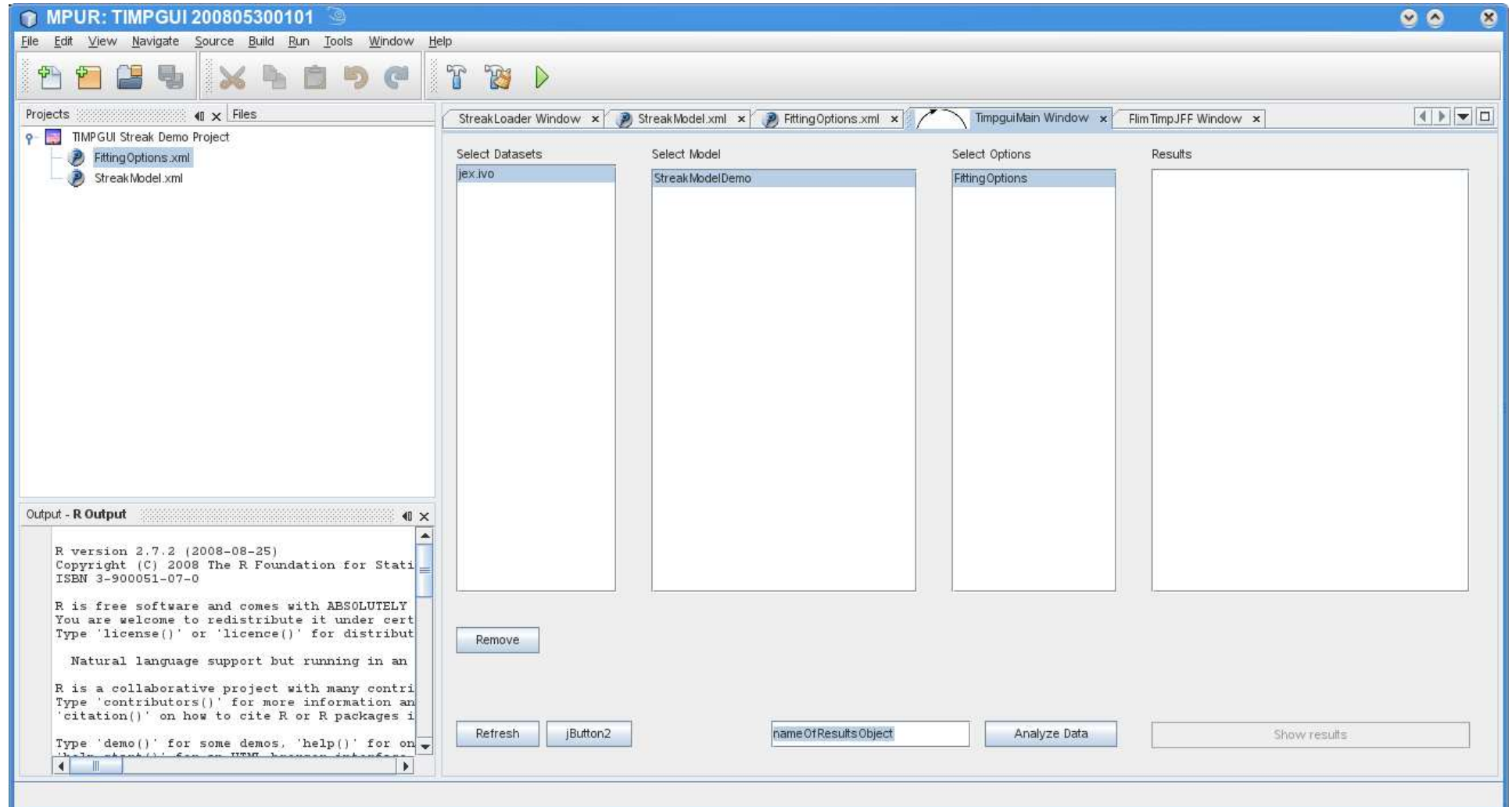
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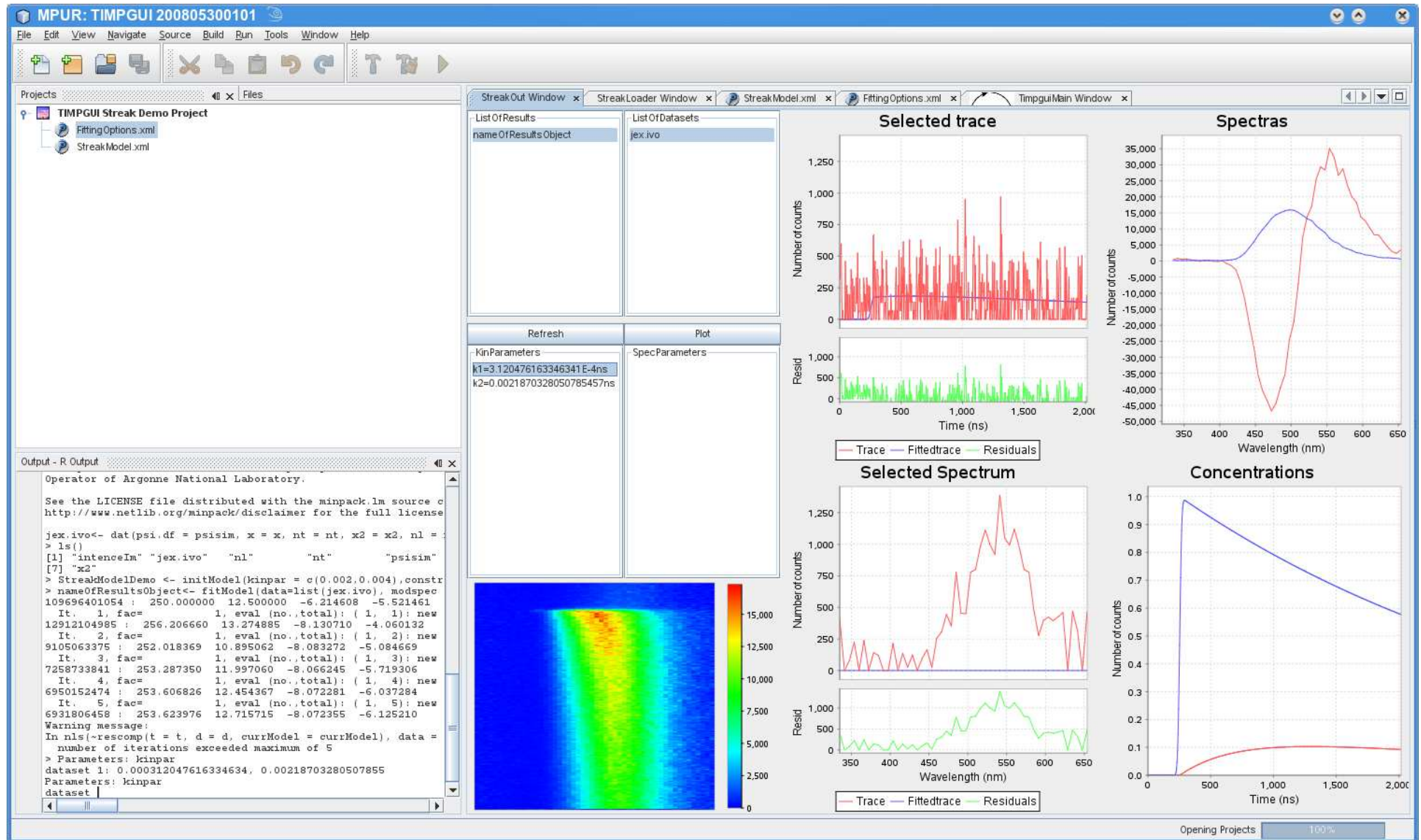

[LIVE DEMO SCREENSHOT: specification of fitting options]



— [LIVE DEMO SCREENSHOT: selection of data, model and fitting options] —



[LIVE DEMO SCREENSHOT: interactive validation of results]



[Conclusions and outlook]

- package **TIMP** fits superposition models to data arising in physics and chemistry
- a java-based GUI has been developed to facilitate interactive model specification, optimization and validation with **TIMP**
- **TIMPGUI** is in very active development and will continue to be extended

outlook:

- develop further **TIMPGUI** options
- publicly release source code
 - source is currently available by request to those willing to participate in testing

[Acknowledgments]

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