TIMPGUI: A graphical user interface for the package TIMP

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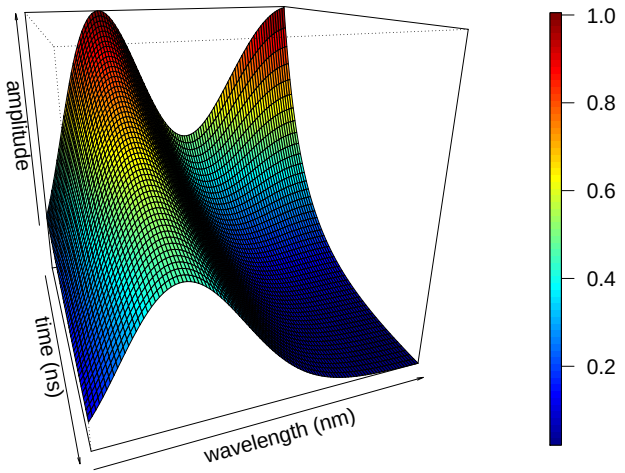
TIMP is a package for fitting superposition models that has been applied to measurements arising in

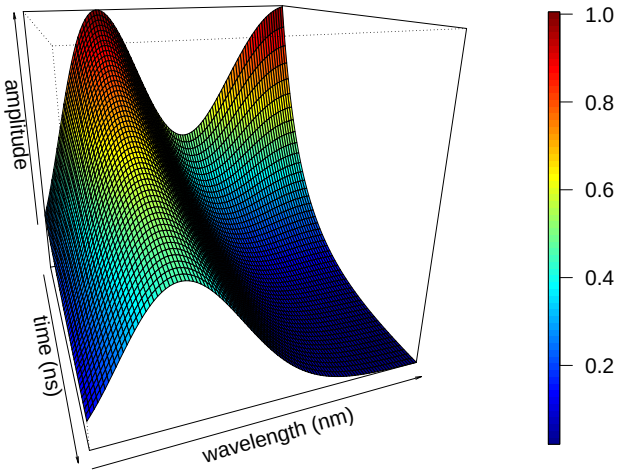
- time (and/or temperature, polarization, pH)-resolved spectroscopy
- fluorescence lifetime imaging microscopy (FLIM)
- time-resolved mass spectrometry data

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

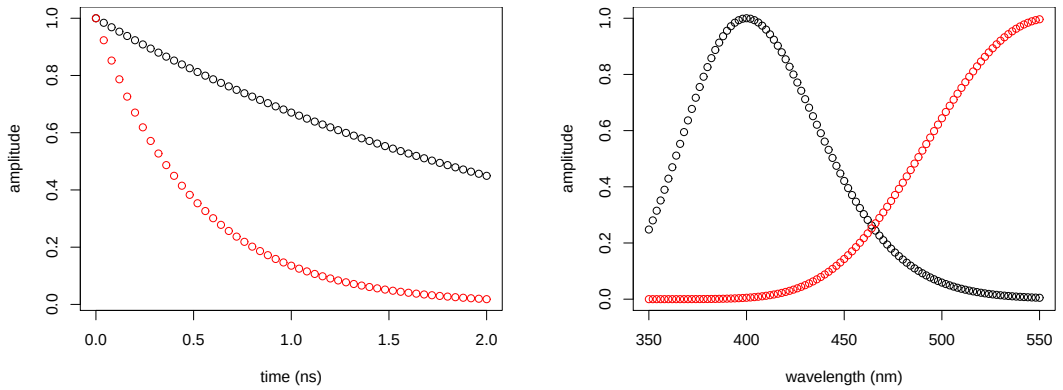


[Parameter estimation problem]

from the data



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

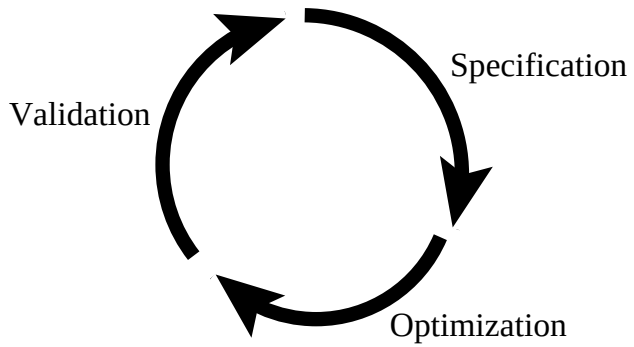


$$\Psi = C(\theta)E^T$$

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

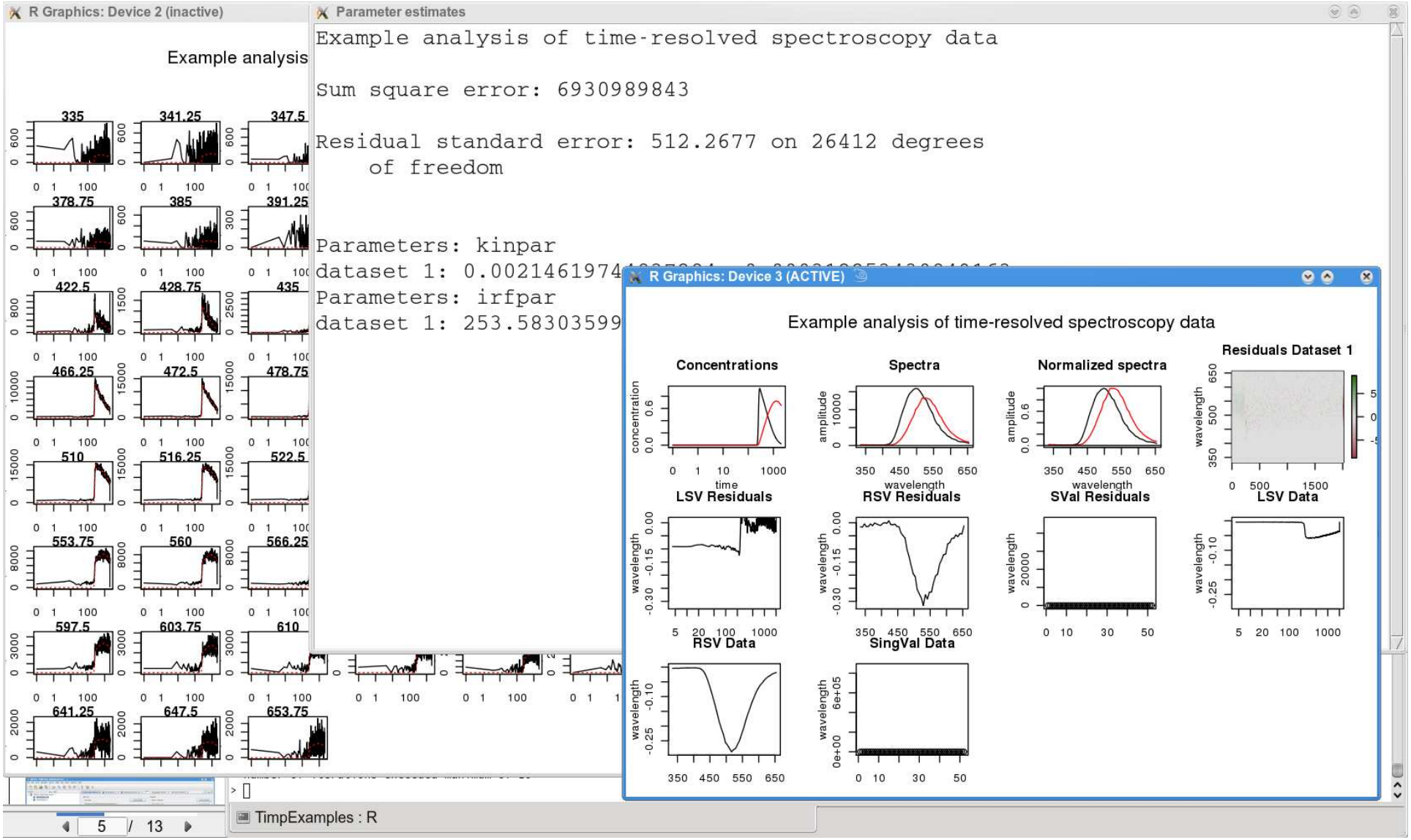
- test many different models
- evaluate the estimated parameters for physical interpretability
- explore the data and fit interactivity

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:

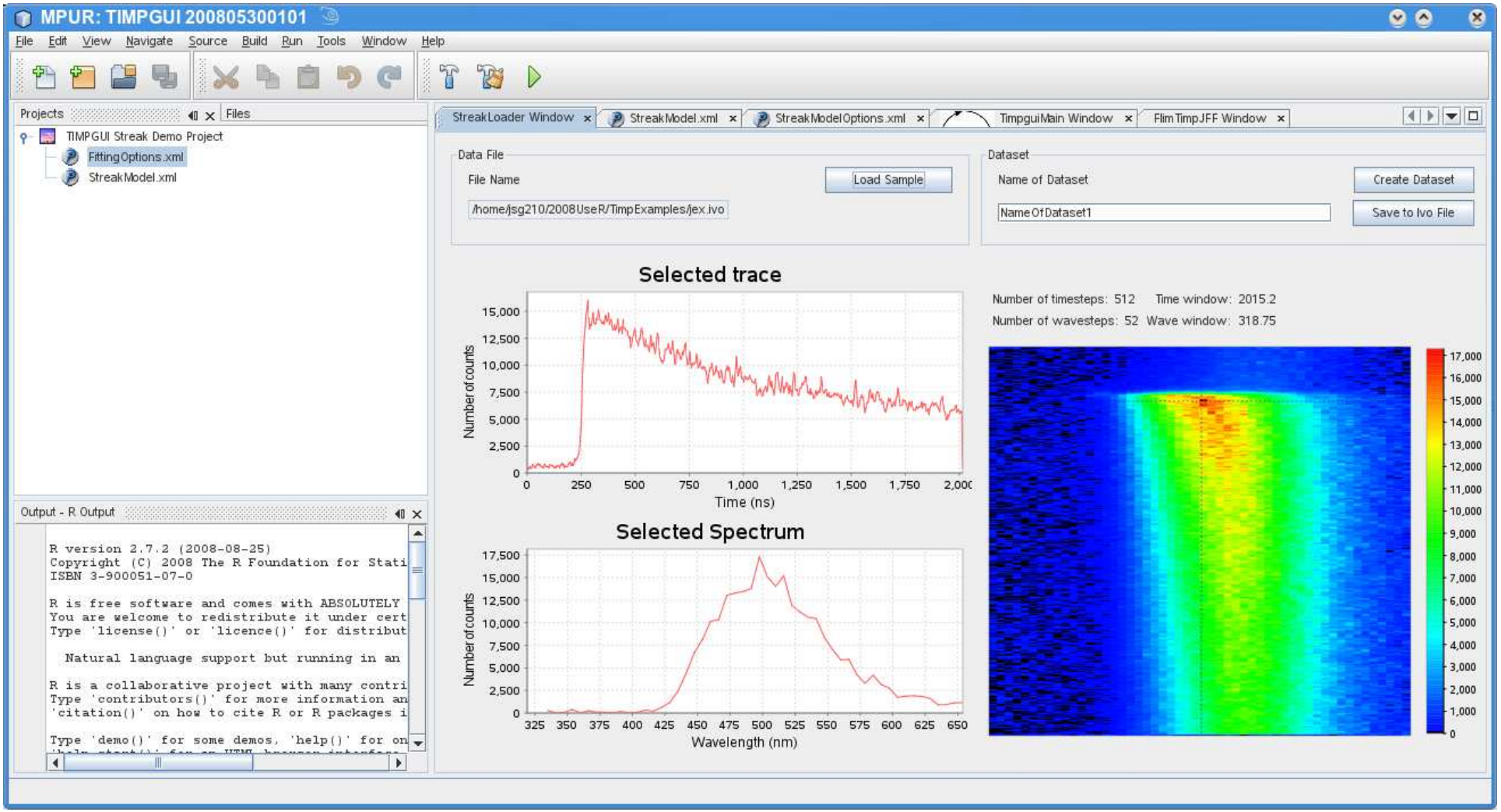
- possibilities for model specification via a graphical user interface (GUI)
- cross-platform software, to allow collaboration between Linux/Unix, MS Windows, and Mac OS users
- possibilities for interactive exploration of data and fit

we developed the java-based graphical user interface **TIMP**GUI

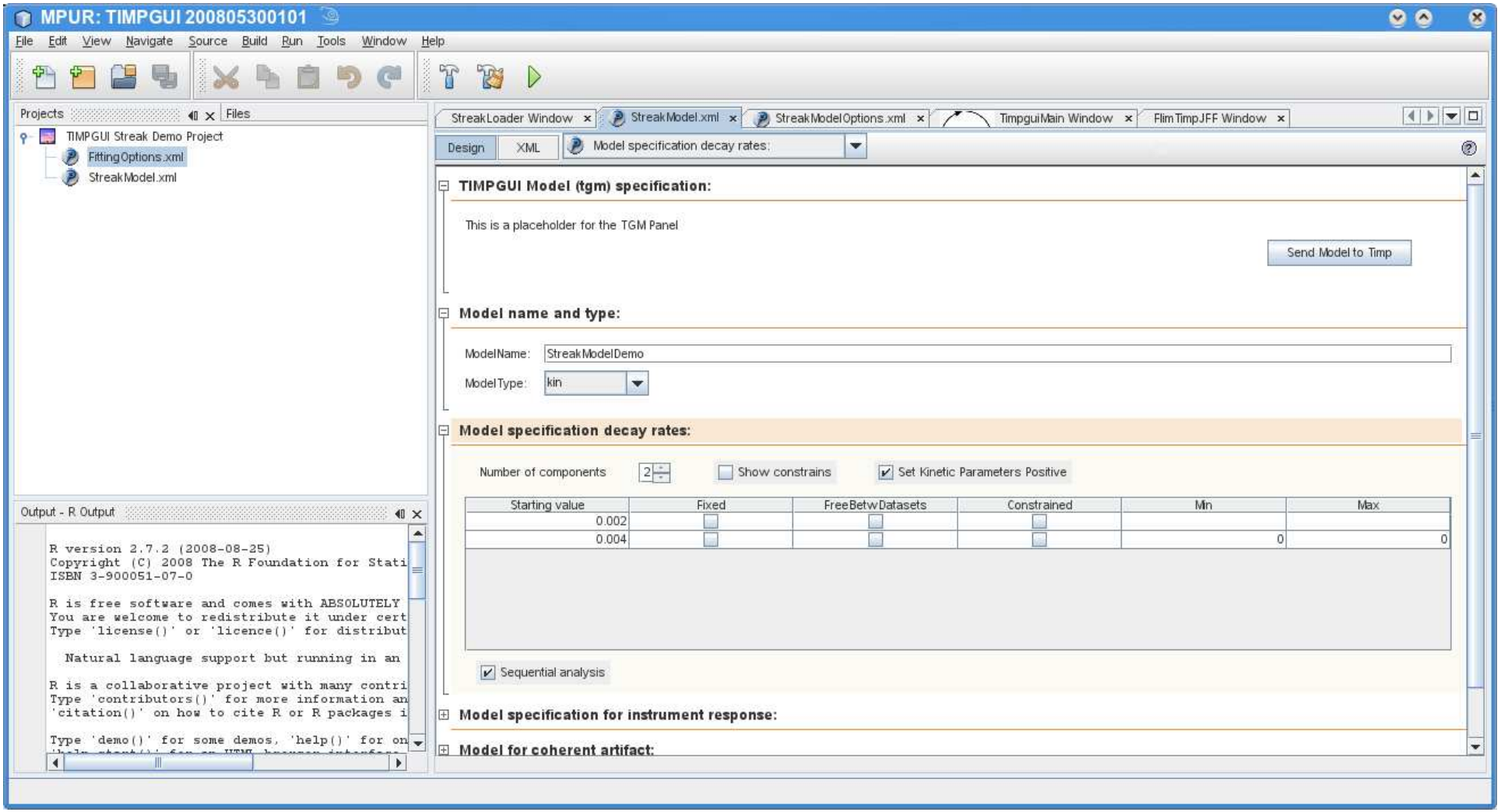
- built on top of the Netbeans platform
- calls **TIMP** via **JRI** from RoSuDa
- persistant storage of models and fitting options via XML files

The results are also best explained by example ...

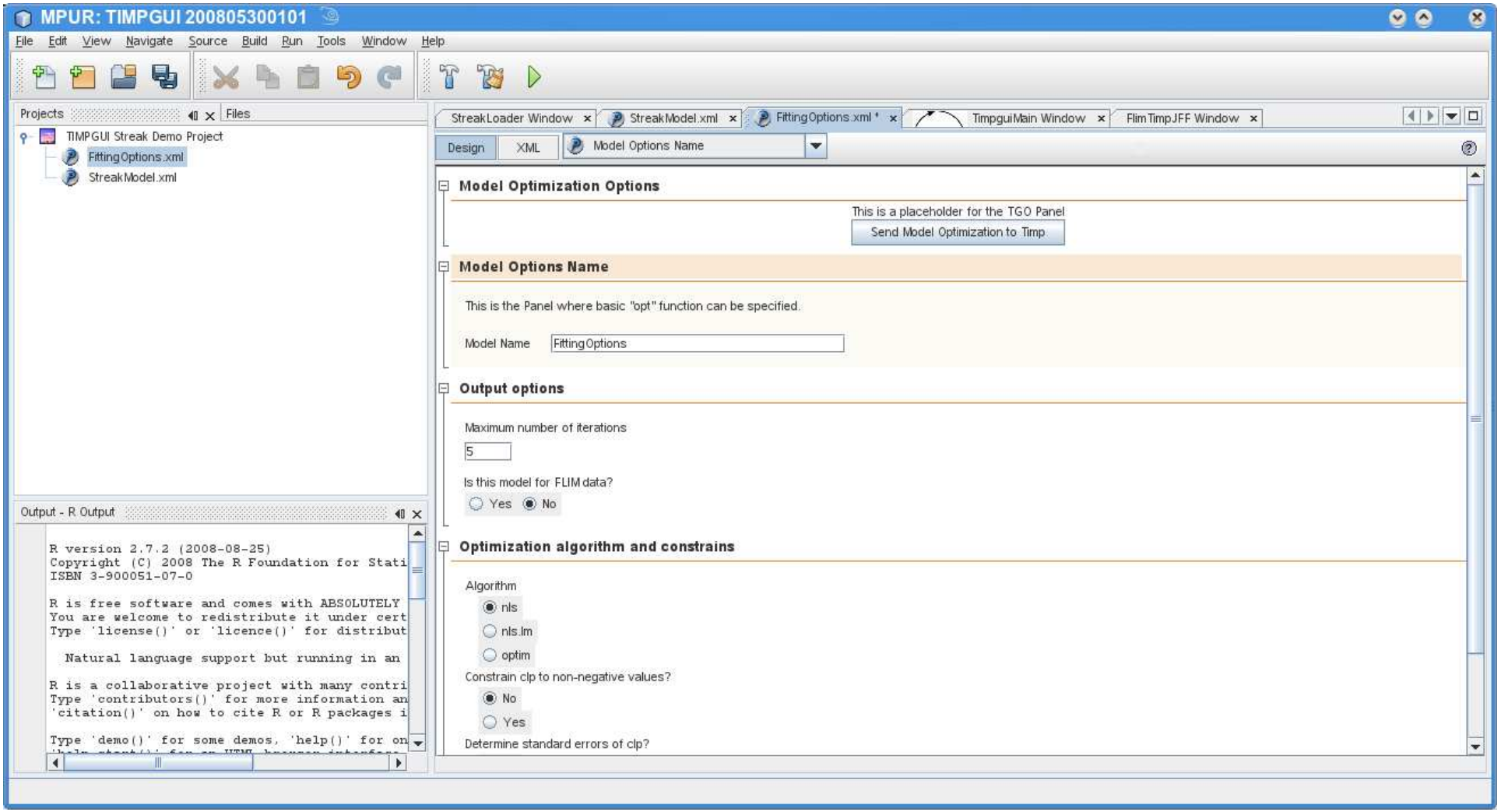
[LIVE DEMO SCREENSHOT: loading data]



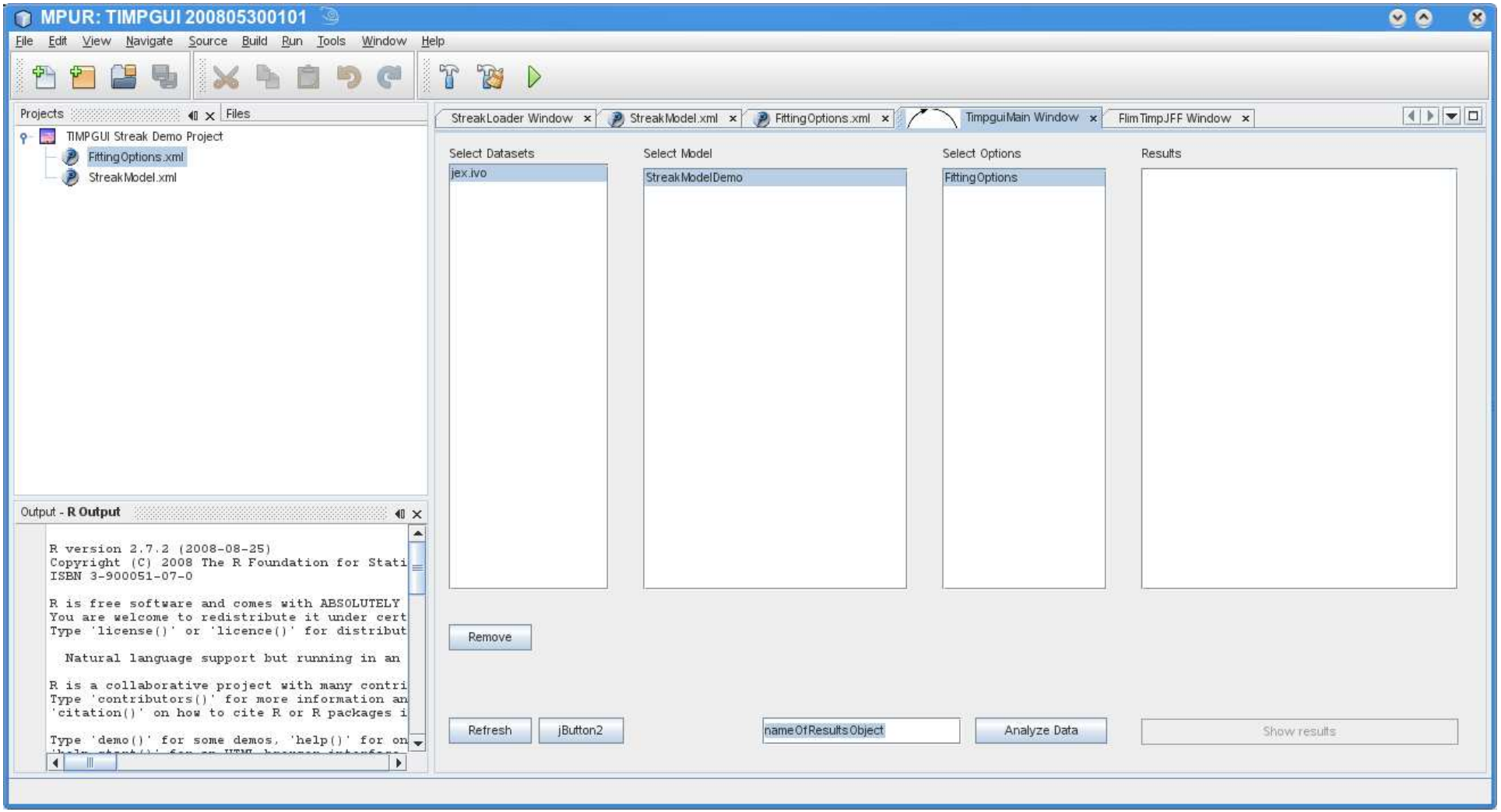
[LIVE DEMO SCREENSHOT: specification of model]



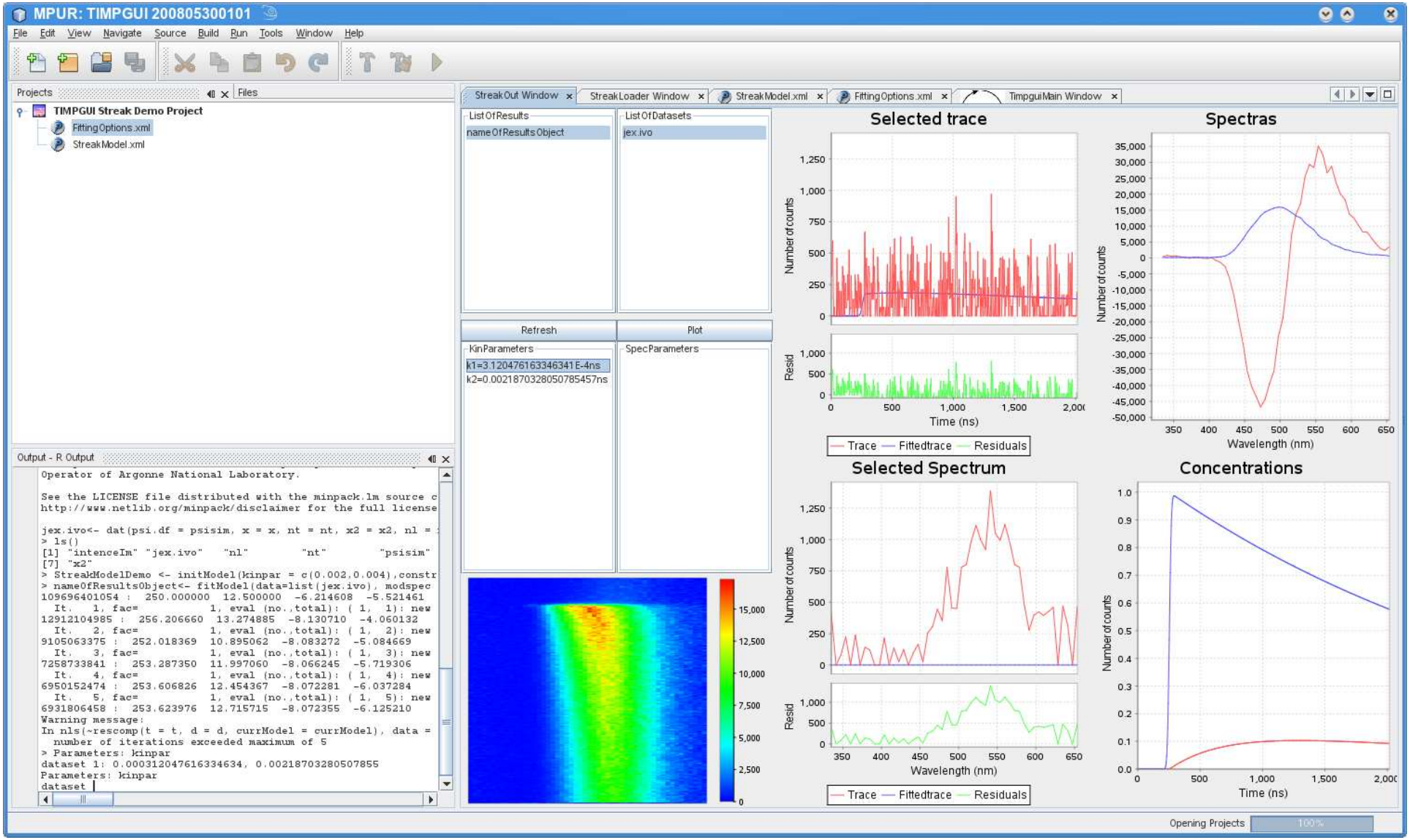
[LIVE DEMO SCREENSHOT: specification of fitting options]



— [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**
- **TIMP**GUI is in very active development and will continue to be extended

outlook:

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

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