Graphical Interaction in Spectroscopic Data Analysis

Sebastian Mellor[1], Claudia Beleites[2,*], Colin Gillespie[1], Christoph Krafft[2], and Jürgen Popp[2,3]

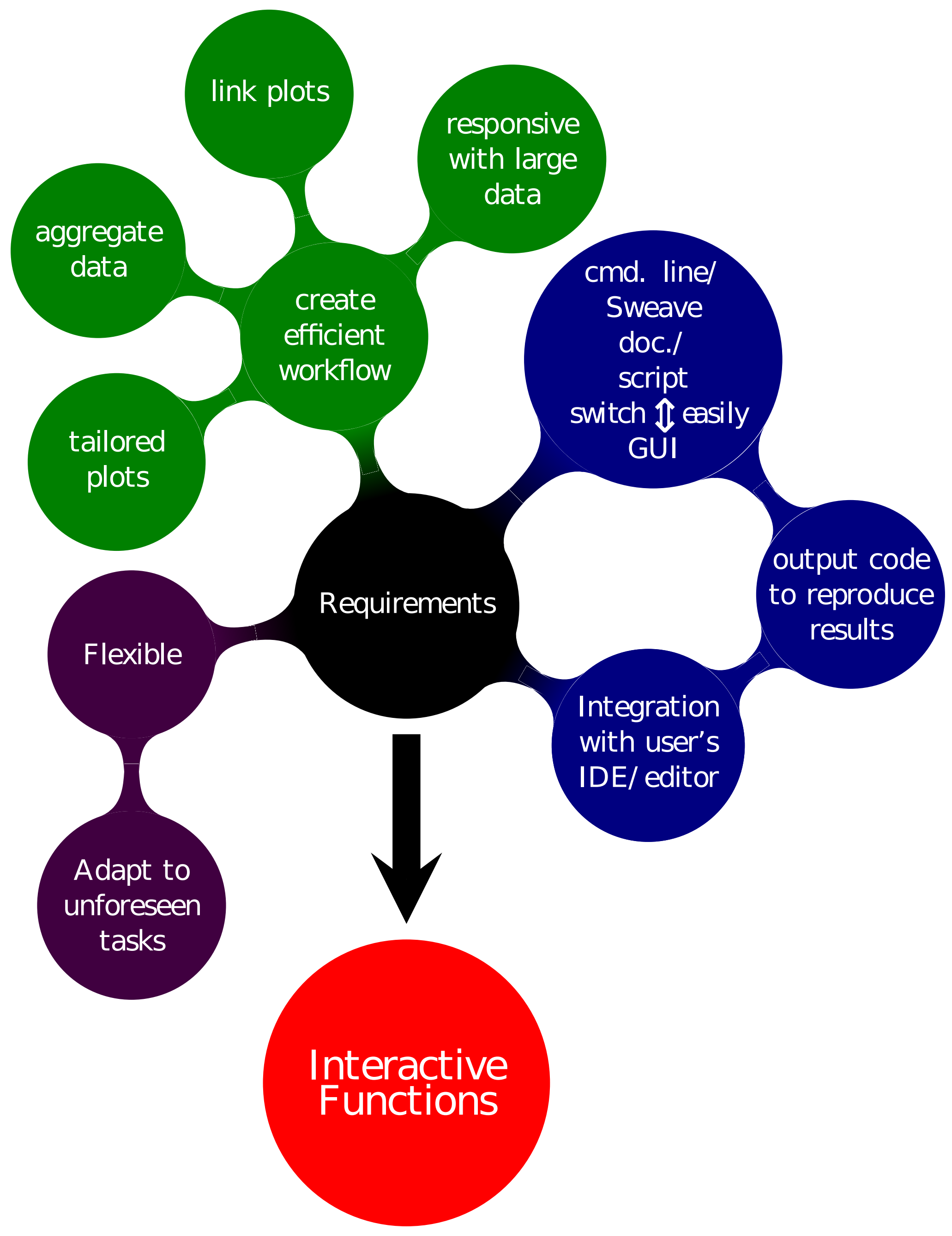
[1] School of Mathematics & Statistics, Newcastle University, Newcastle/UK.
[2] Institute of Photonic Technology, Jena/Germany.
[3] Institute of Physical Chemistry and Abbe Center of Photonics, University Jena/Germany.
[*] Corresponding author: Claudia.Beleites@ipht-jena.de

GUIs and Spectroscopic Data

- data are complex
- variety of statistical models used
- are often large: typically 10^2 - 10^5 spectra x 10^2 - 10^3 wavelengths, can reach hundreds of GB.

+ some tasks need visual interaction, see the example of spike filtering.
+ good for exploring complex data and models

Interactive Functions


link plots
responsive with large data
aggregate data
create efficient workflow
tailored plots
cmd. line/ Sweave doc./ script switch ⇕ easily GUI
output code to reproduce results
Requirements
Integration with user's IDE/ editor
Flexible
Adapt to unforeseen tasks
Interactive Functions

Obtaining hyperSpec+GUI

? homepage:
⇨ *hyperspec.r-forge.r-project.org*

? hyperSpec:
- latest stable from CRAN
  ⇨ install.packages ("hyperSpec")
- latest nightly build (dev. version)
  ⇨ `install.packages("hyperSpec", repos="http://R-Forge.R-project.org")`

? hyperSpecGUI:
- latest nightly build (dev. version)
  ⇨ `install.packages("hyperSpecGUI", repos="http://R-Forge.R-project.org")`

References

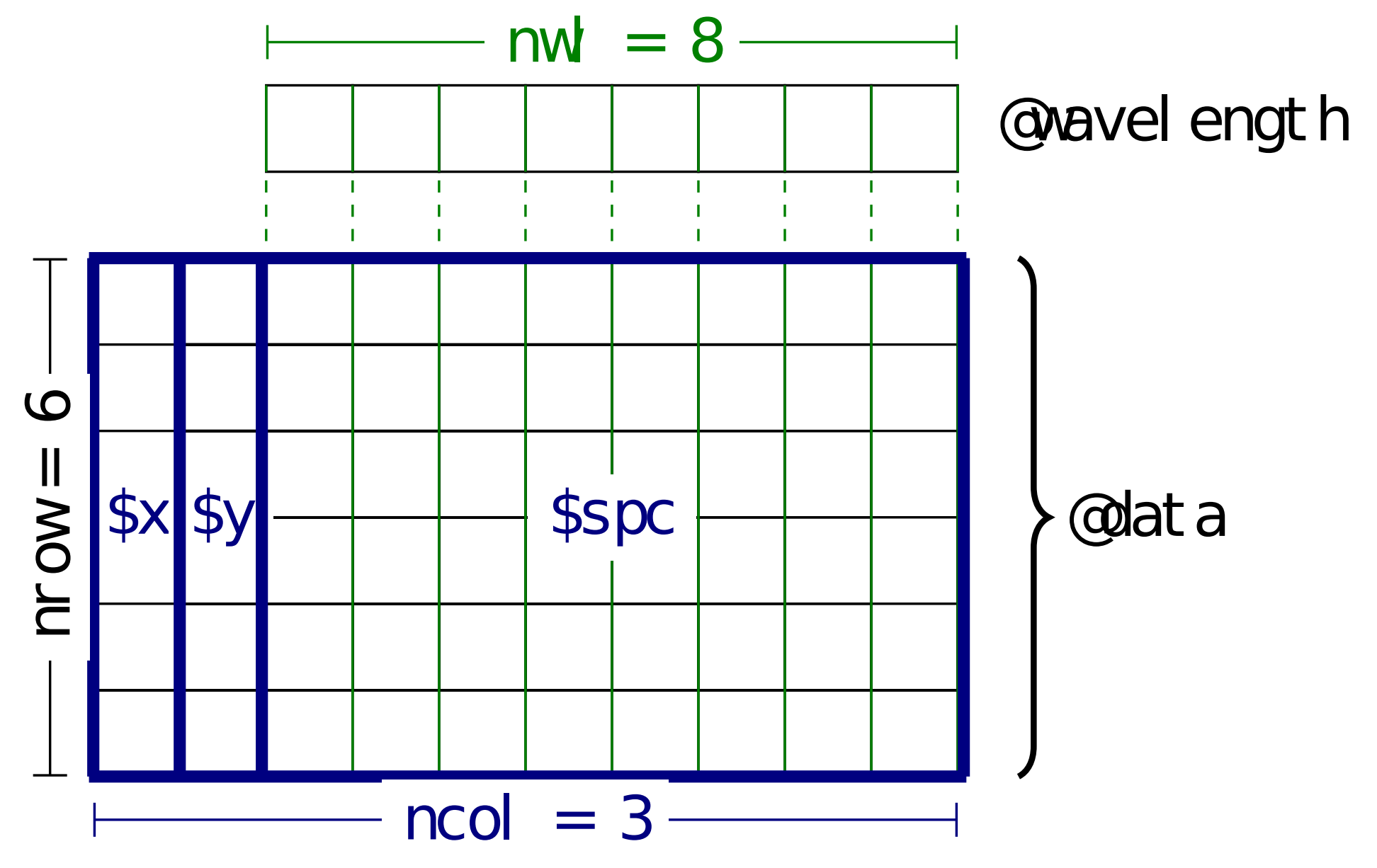
[1] Beleites, C. hyperSpec (*http://hyperspec.r-forge.r-project.org/*)

[2] Verzani, J. gWidgets (*http://cran.r-project.org/web/packages/gWidgets/index.html*)

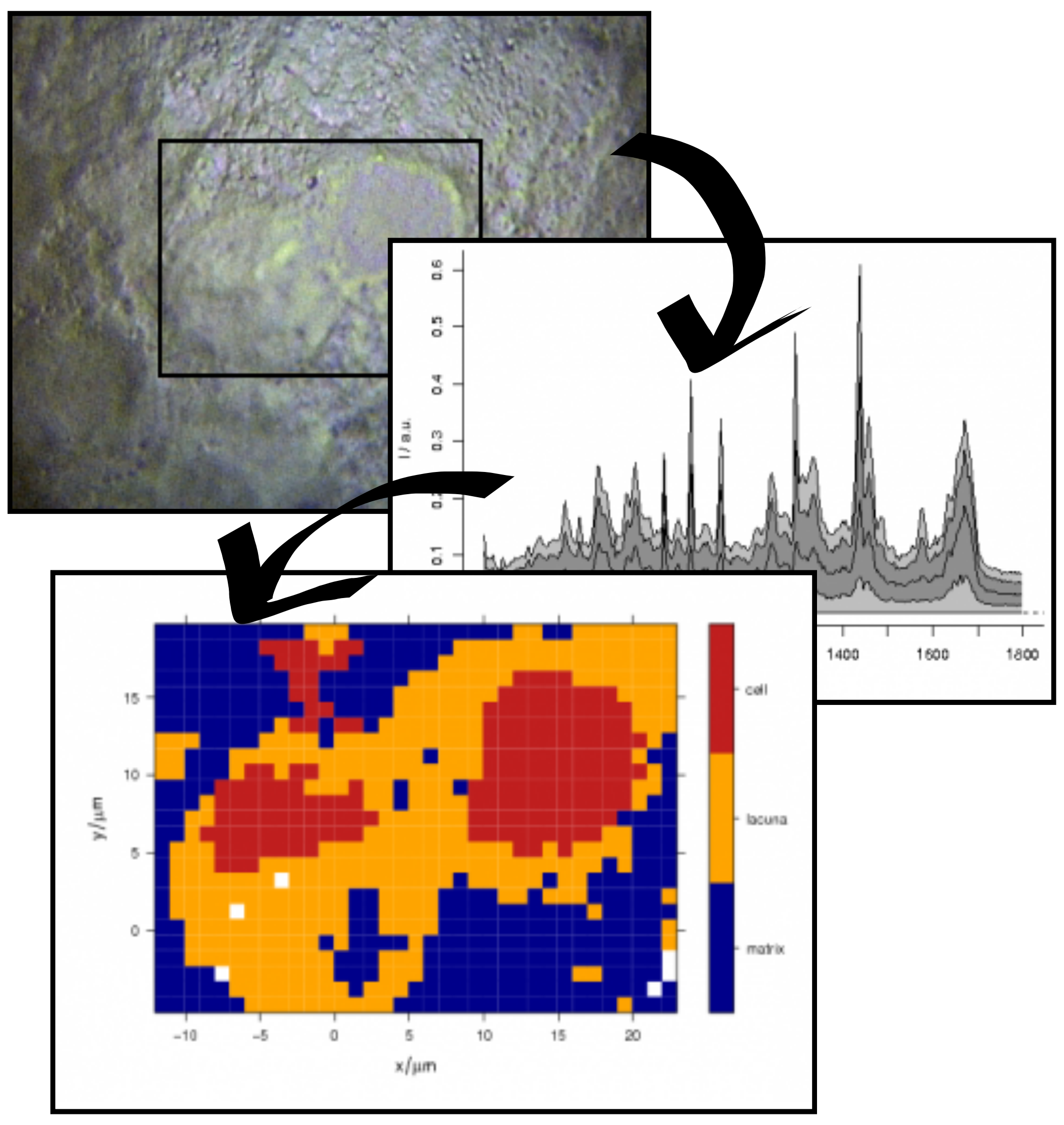
hyperSpecGUI can also be found at *http://hyperspec.r-forge.r-project.org/*.

hyperSpectral Data = Spectroscopic Data + Extra Dimensions

hyperSpec handles hyperspectral data:



```
R> chondro
hyperSpec object
   875 spectra
   4 data columns
   300 data points / spectrum
wavelength: Delta * tilde(nu)/cm^-1 [numeric] 602 606 ... 1798
data:  (875 rows x 4 columns)
   1. y: y/(mu * m) [numeric] -4.77 -4.77 ... 19.23
   2. x: x/(mu * m) [numeric] -11.55 -10.55 ... 22.45
   3. clusters: clusters [factor] matrix matrix ... lacuna + NA
   4. spc: I / a.u. [matrix300] 501.8194 500.4552 ... 169.2942
```



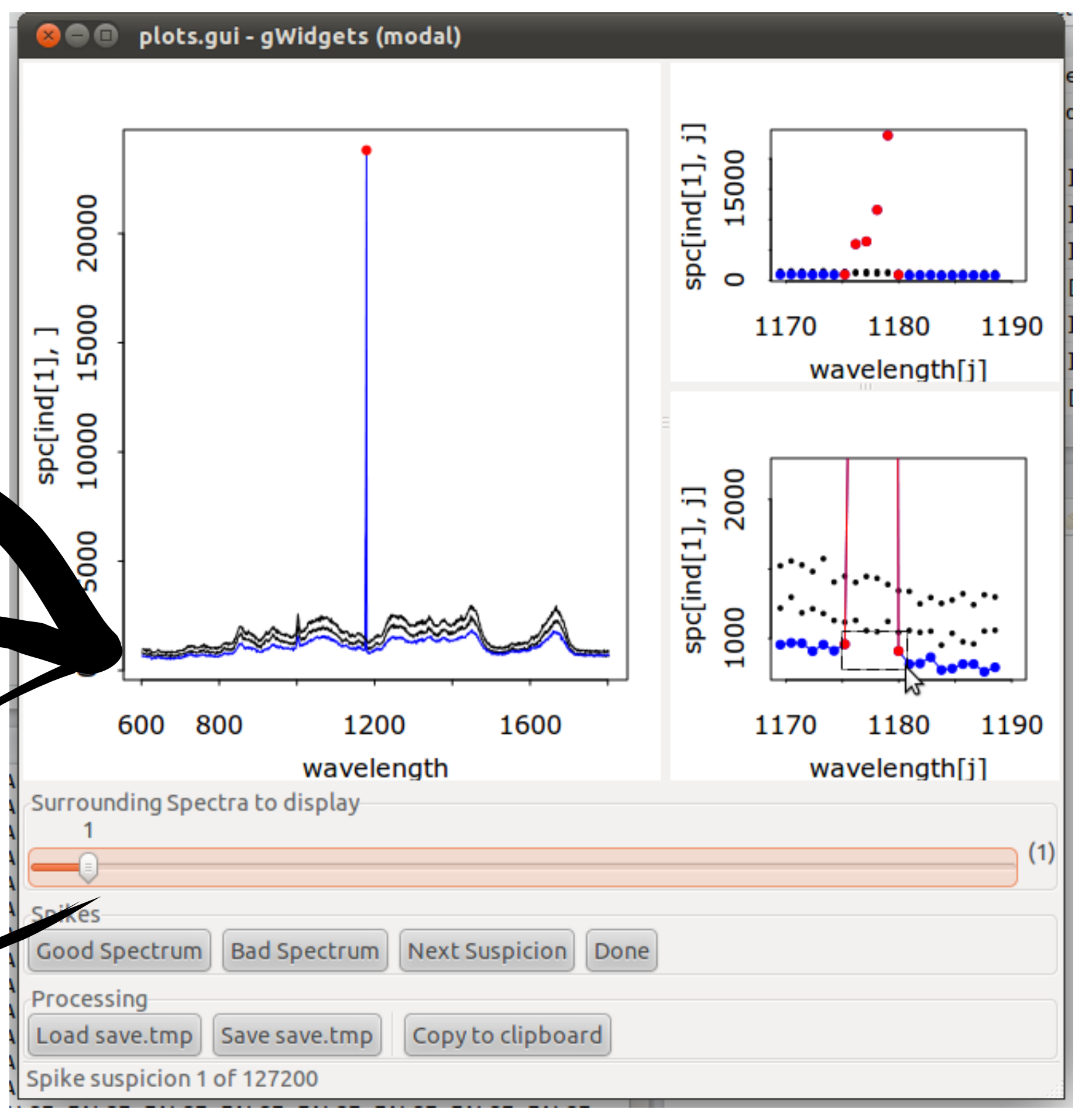
Example: Interactive Spike Filtering

- cosmic rays hit the detector
  ⇨ spikes are observed in the Raman spectra

- several stategies exist for automated detection

+ works well with high, sharp spikes
! broader artifacts confused with sharp Raman bands
! and vice versa
! borders of broader artifacts difficult to detect
⇨ manual control and adjustment necessary

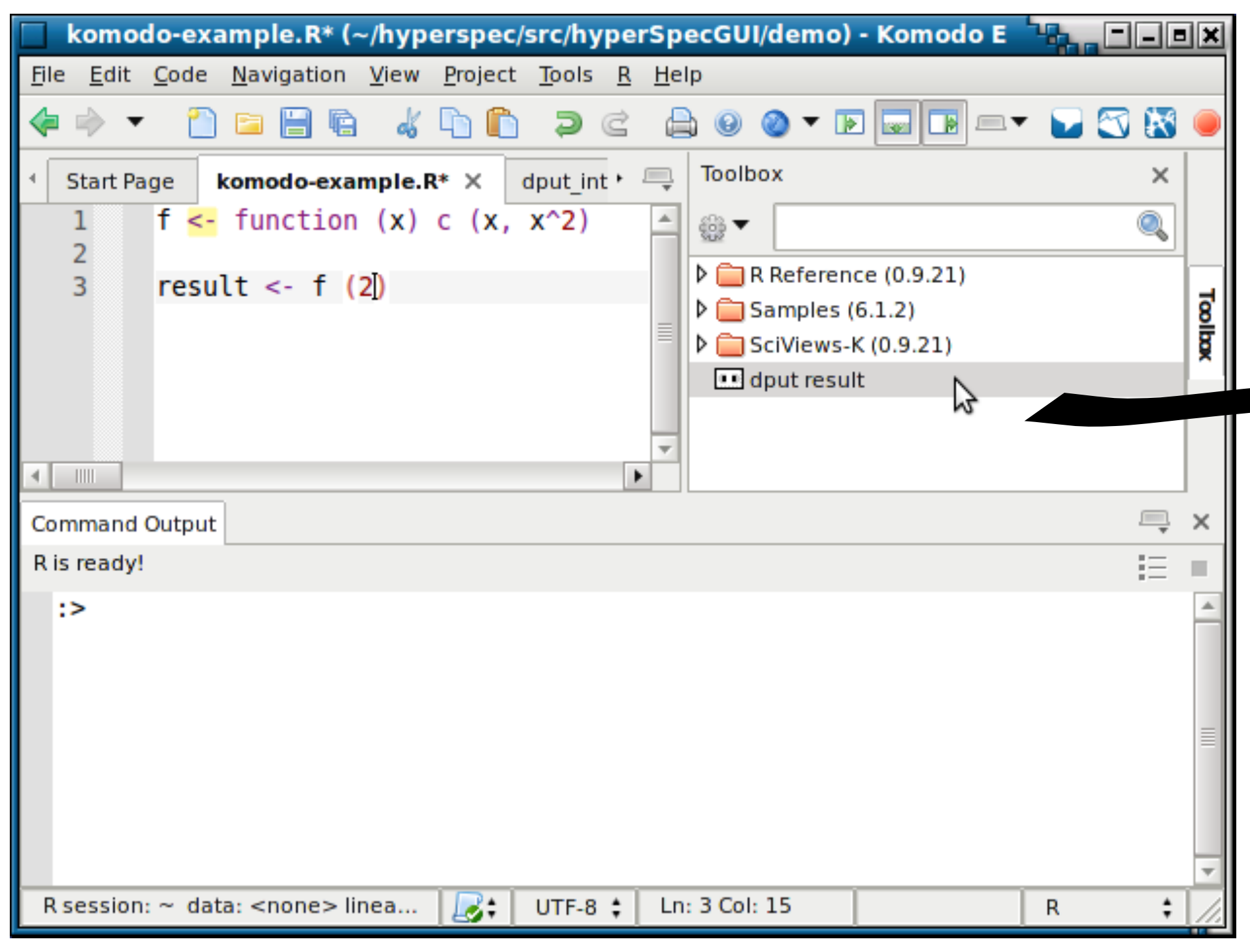
```
R> load("cartilage-raw.RData")
R> tmp <- sweep(cartilage, 1, median, `/`)
R> tmp <- sweep(tmp, 2, median, `-`)
R> scores <- spikefilter2d(spcmatrix=tmp[[]])
R> spikes <- spikes.interactive.GUI(
                  cartilage[1:100],
                  scores[1:100, ])

R> spikes
1175.22 1176.18 1177.13 1178.08 1179.03 1179.98
    577     578     579     580         582
```



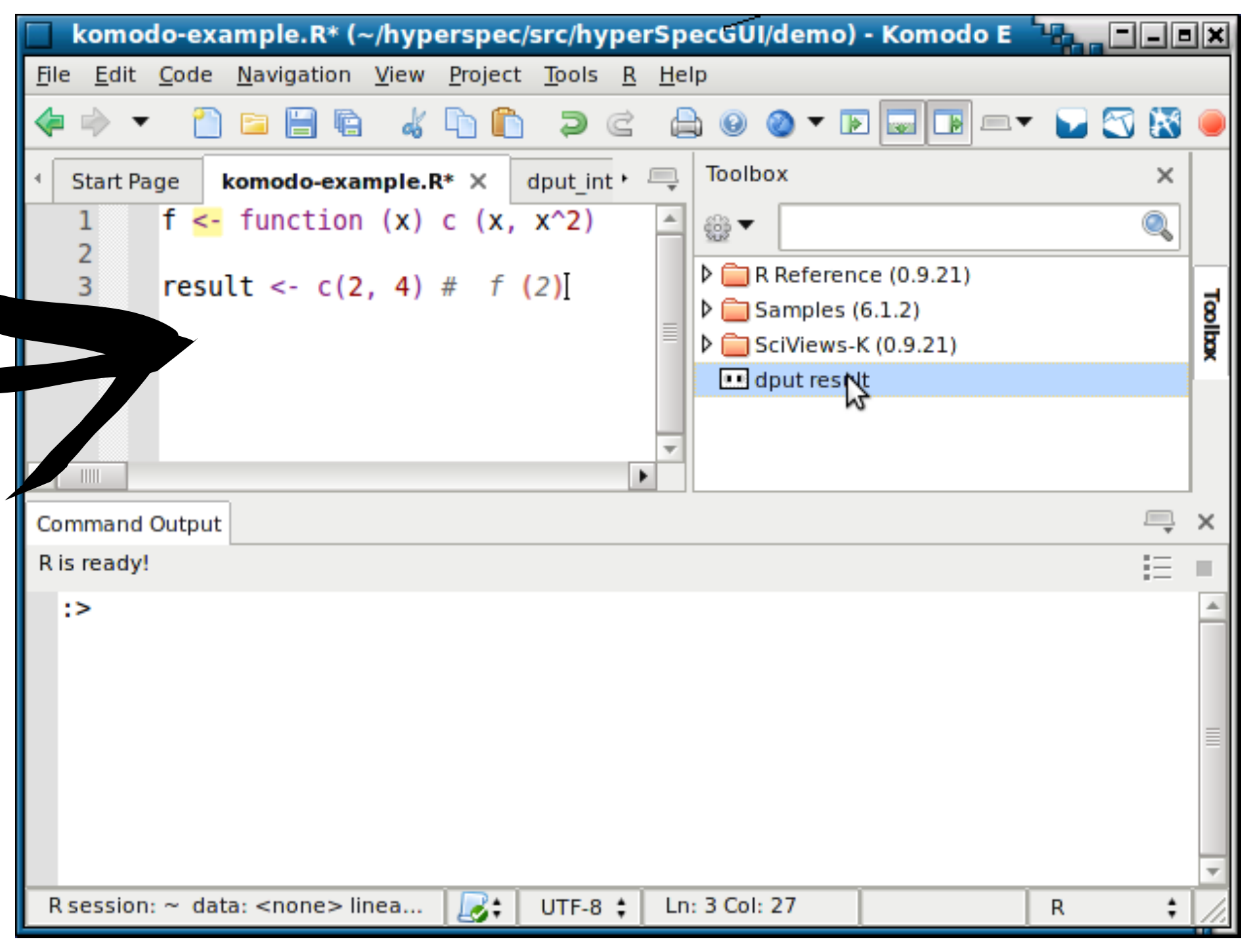
Spike suspicion 1 of 127200

Example: Integration with IDE

- wrapper function replacing function call by "`dput (result)`"



```
f <- function (x) c (x, x^2)

result <- f (2)
```



```
f <- function (x) c (x, x^2)

result <- c(2, 4) #  f (2)
```

⇨ compatible with reproducible research practices
- "poor man's solution": applet copies "`dput (result)`" to clipboard

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