R4Photobiology

A Suite of R Packages

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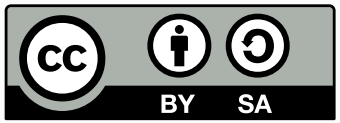


Outline

Background

Examples

Resources

Acknowledgements

Background

Photobiology: Definition, tasks, problems

- **Photobiology** is the study of responses to visible and ultraviolet radiation in living organisms.
- Typical tasks:
  - Describe and quantify the light environment.
  - Describe and quantify the responses of organisms to light.
  - Compute summary radiation quantities meaningful for different processes.
  - Compute day and night length and/or the position of the sun.
- Many calculations are conceptually simple but computations complex.
- (Similar data and calculations are used in photochemistry, biochemistry, medicine, radiation physics, meteorology, etc.)

Light-related spectra

What is common to all these spectra?

- A variable **wavelength**, λ, (or equivalent quantity) is always present
- Some other quantity either *expressed per unit wavelength* or as a ratio is also present

- Wavelength is a continuous variable, but measurements are taken at discrete and rather frequently arbitrary positions along this axis.
- The response variables are also continuous (or almost).
- Weighting functions used for the calculation of effective "quantities" are not always continuous.
- Calibrations applied to both wavelength and measured variable.

Aims: User friendly ‘programmatic’ interface

- Hide the need of interpolation from users.
- Integration not affected by irregular spacing of wavelengths.
- Use operators for operations among spectra.
- Easy to plot different types of spectra.
- Easy to annotate such plots.
- Exchange of spectral data (import/export).
- (Direct acquisition of spectral data.)
- *Reasonably* fast performance.

Aims: Support reproducible research

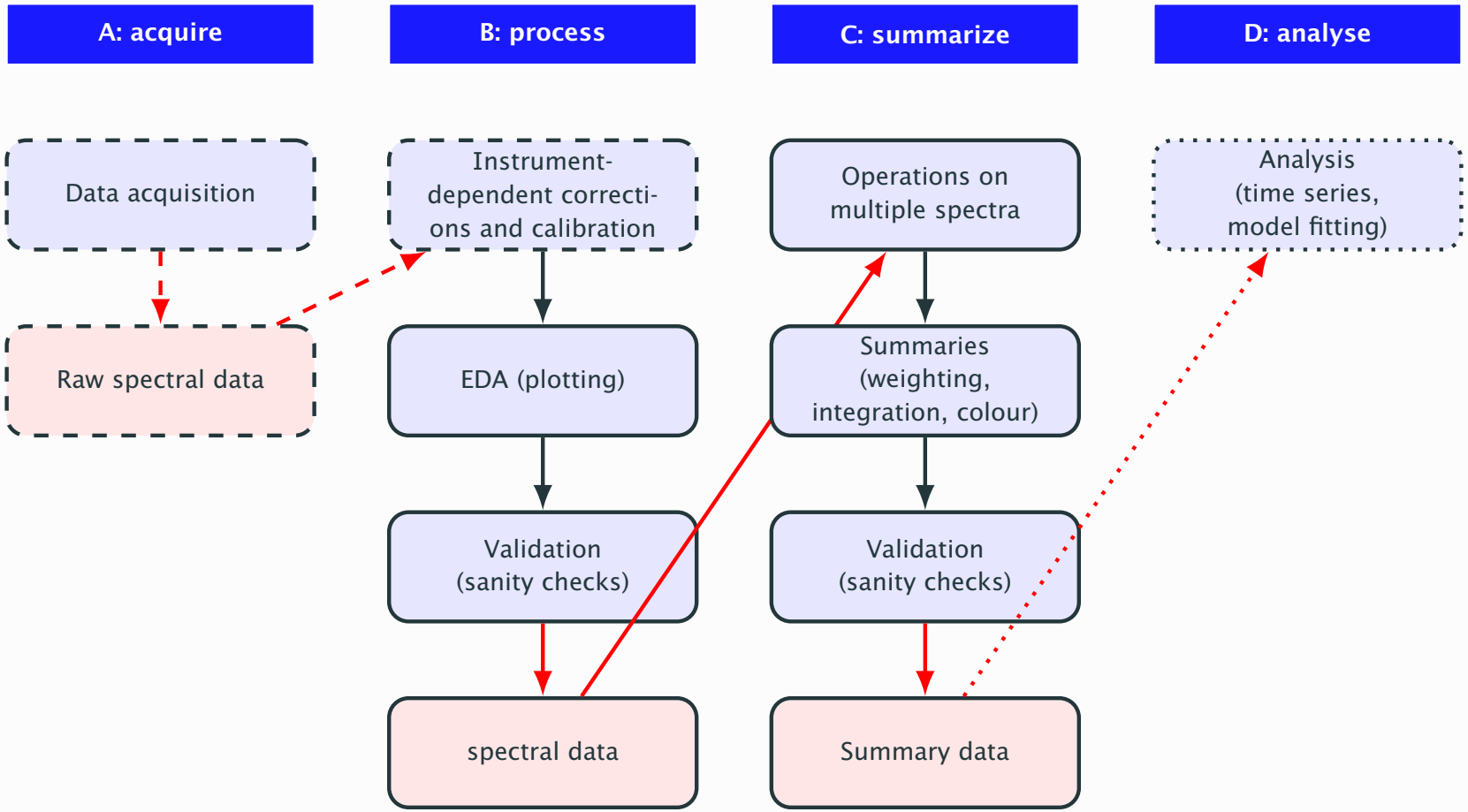
- A class system for different types of spectral data.
- Functions for conversions among bases of expression.
- Functions for conversions among related quantities.
- Store data and metadata in the same object.
- Propagate (and merge) metadata contained in objects.
- A set of “reference” data for comparisons.
- Automated testing of package code.

Packages in the r4photobiology suite

R package	Type	Contents
photobiology	funs + classes	functions, class definitions and methods
photobiologyInOut	functions	data import/export
photobiologyWavebands	definitions	quantification of radiation
ggspectra	methods	plotting of spectral data
photobiologySun	data	solar and daylight
photobiologyLamps	data	emission by light bulbs
photobiologyLEDs	data	emission by LEDs
photobiologyFilters	data	transmission of filters
photobiologySensors	data	response of sensors
photobiologyReflectors	data	reflection by materials
photobiologyPlants	funs + data	plants' responses
rOmniDriver	driver API	Ocean Optics spectrometers
ooacquire	data acquisition	Ocean Optics spectrometers

Examples

Data flow: First look



B: Example data, Spectral irradiance of sunlight

```
sun.spct
```

```
## Object: source_spct [522 x 2]
## Wavelength range 280 to 800 nm, step 0.9230769 to 1 nm
## Label: sunlight, simulated
## Measured on 2010-06-22 09:51:00 UTC
## Measured at 60.2091078 N, 24.9647355 E
## Time unit 1s
##
## # A tibble: 522 x 2
##   w.length s.e.irrad
##      <dbl>     <dbl>
## 1     280.        0.
## 2     281.        0.
## 3     282.        0.
## 4     283.        0.
## # ... with 518 more rows
```

`w.length` = wavelength in nanometres.

`s.e.irrad` = spectral energy irradiance in $\mathrm{W\,m^{-2}\,nm^{-1}}$.

B: Example data, Schott glass filter

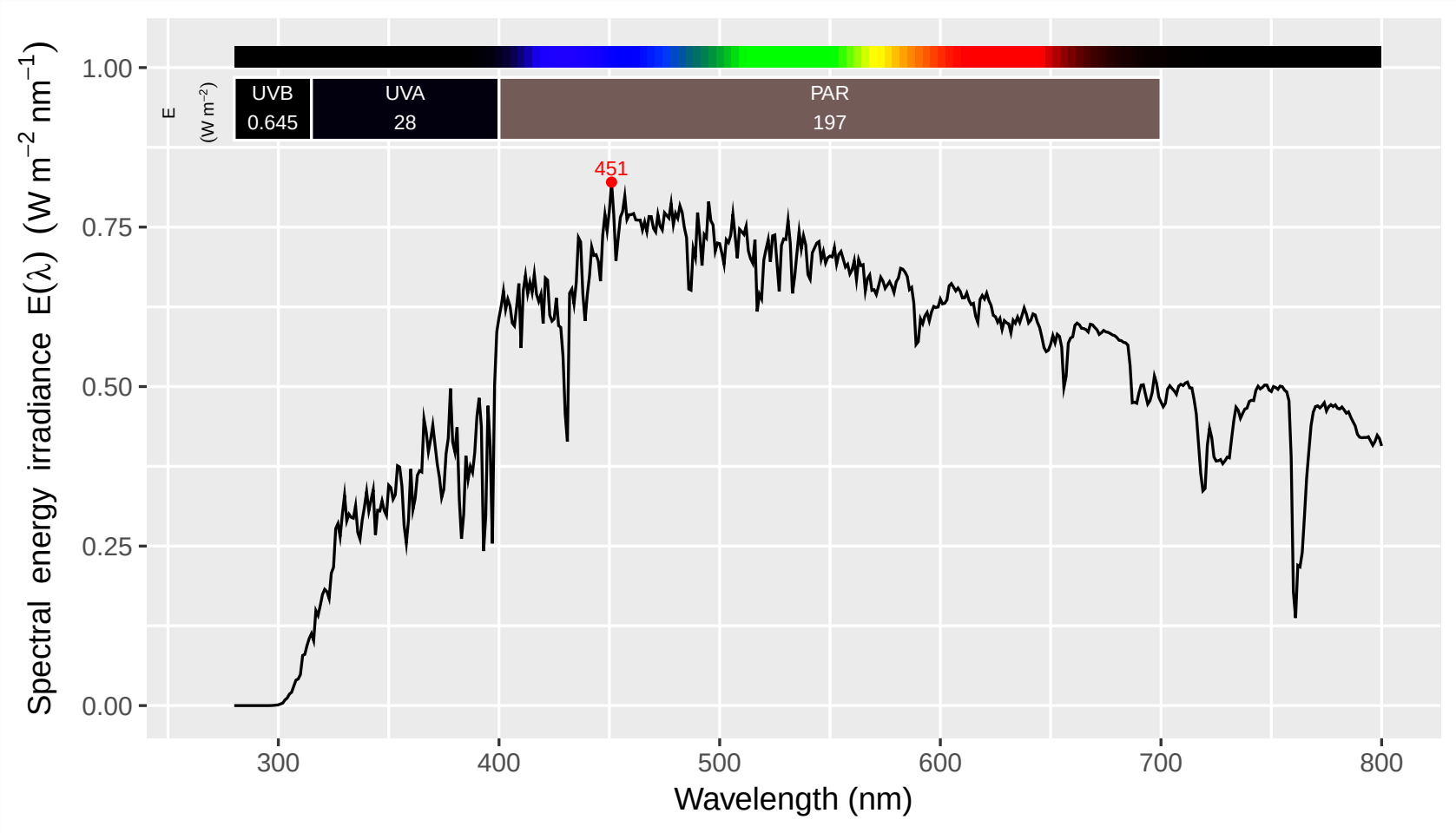
```
filters.mspct$GG435


## Object: filter_spct [1,001 x 2]
## Wavelength range 200 to 5200 nm, step 1 to 50 nm
## Label: SCHOTT GG435, thickness (m): 0.003
##
## # A tibble: 1,001 x 2
##   w.length       Tfr
##      <dbl>     <dbl>
## 1     200. 0.0000100
## 2     201. 0.0000100
## 3     202. 0.0000100
## 4     203. 0.0000100
## # ... with 997 more rows
```

`w.length` = wavelength in nanometres.

`Tfr` = spectral transmittance as a fraction of one.

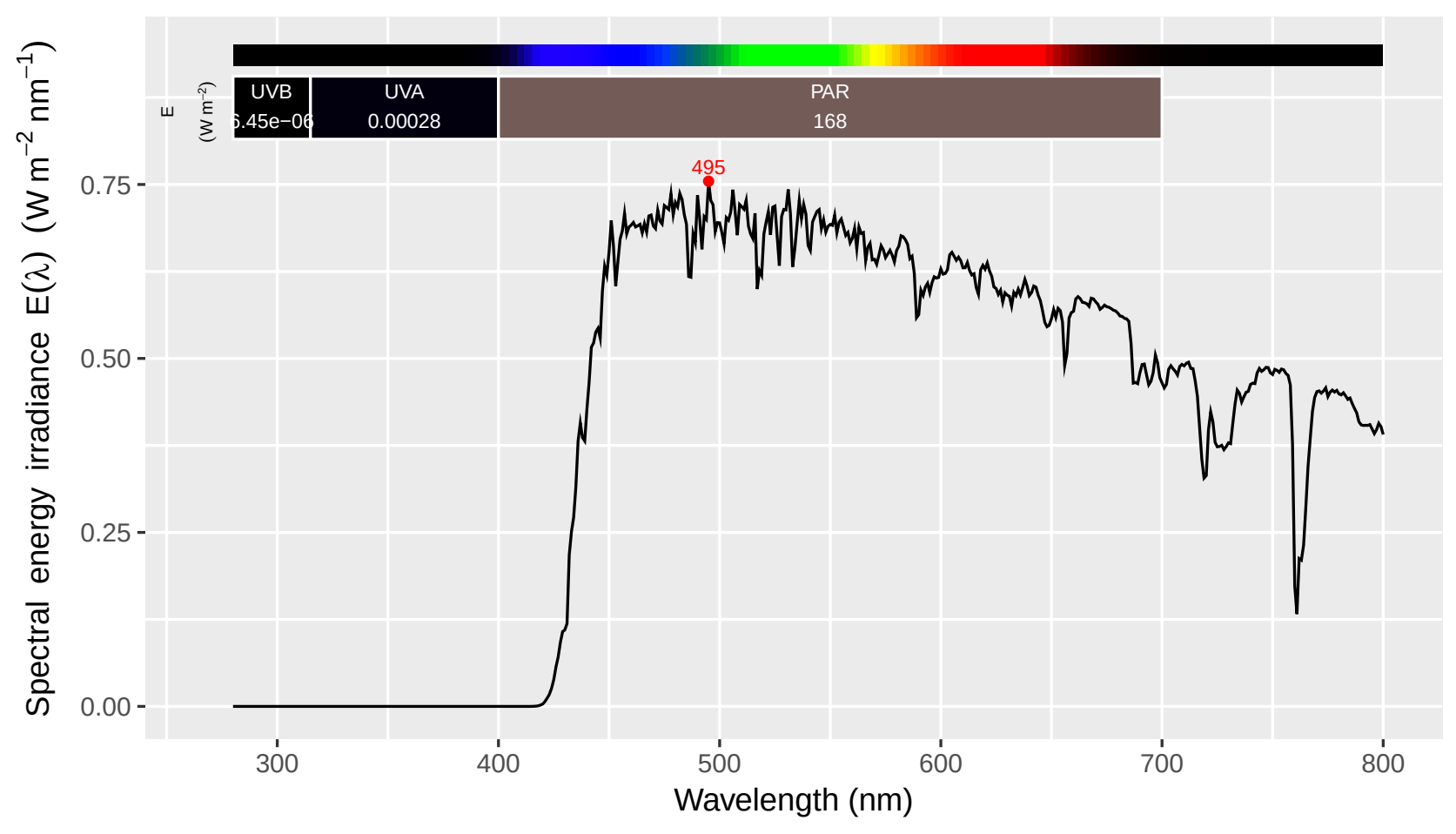
B: plot methods for spectra

```
plot(sun.spct)
```



C: Convolution, filtered sunlight

```
plot(sun.spct * filters.mspct$GG435)
```



C: Summaries of spectra

```
summary(sun.spct)
```

```
## Summary of object: source_spct [522 x 2]
## Wavelength range 280 to 800 nm, step 0.9230769 to 1 nm
## Label: sunlight, simulated
## Measured on 2010-06-22 09:51:00 UTC
## Measured at 60.2091078 N, 24.9647355 E
## Time unit 1s
##
##     w.length       s.e.irrad
##  Min.   :280.0   Min.   :0.0000
##  1st Qu.:409.2   1st Qu.:0.4115
##  Median :539.5   Median :0.5799
##  Mean   :539.5   Mean   :0.5160
##  3rd Qu.:669.8   3rd Qu.:0.6664
##  Max.   :800.0   Max.   :0.8205
```

C: Summaries of spectra

```
range(sun.spct)

## [1] 280 800

color_of(sun.spct)

## source CMF
##  "#544F4B"

color_of(sun.spct * filters.mspct$RG645)

## source CMF
##  "#260000"
```

C: Summaries of spectra

Irradiance (integral over wavelengths): total

$$I_{\lambda_{\text{min}}\cdots\lambda_{\text{max}}} = \int_{\lambda=\lambda_{\text{min}}}^{\lambda=\lambda_{\text{max}}} I(\lambda)\mathrm{d}\lambda \tag{1}$$

```
e_irrad(sun.spct)
```

```
##    Total
## 269.1249
## attr(,"time.unit")
## [1] "second"
## attr(,"radiation.unit")
## [1] "energy irradiance total"
```

C: Non-weighted irradiance

Irradiance (integral over wavelengths): ultraviolet-A

```
e_irrad(sun.spct, UVA())
```

```
##  UVA.ISO
## 27.98421
## attr(,"time.unit")
## [1] "second"
## attr(,"radiation.unit")
## [1] "energy irradiance total"
```

C: CIE-weighted irardiance

```
e_irrad(sun.spct, CIE())
```

```
##  CIE98.298.tr.lo
##       0.08181583
## attr(,"time.unit")
## [1] "second"
## attr(,"radiation.unit")
## [1] "energy irradiance total"
```

C: Irradiance for multiple bands

```
e_irrad(sun.spct, VIS_bands())
```

```
##  Purple.ISO    Blue.ISO   Green.ISO
##    47.75529    37.55207    49.26860
##  Yellow.ISO  Orange.ISO     Red.ISO
##    13.67971    12.00432    79.38159
## attr(,"time.unit")
## [1] "second"
## attr(,"radiation.unit")
## [1] "energy irradiance total"
```

C: Photon irradiance for “slices”

```
# in moles m-2 s-1
q_irrad(sun.spct, split_bands(c(400, 500, 600, 700)) )
```

```
##  range.400.500  range.500.600
##   0.0002633485   0.0003141467
##  range.600.700
##   0.0003166400
## attr(,"time.unit")
## [1] "second"
## attr(,"radiation.unit")
## [1] "photon irradiance total"
```

C: Irradiance for collections of spectra

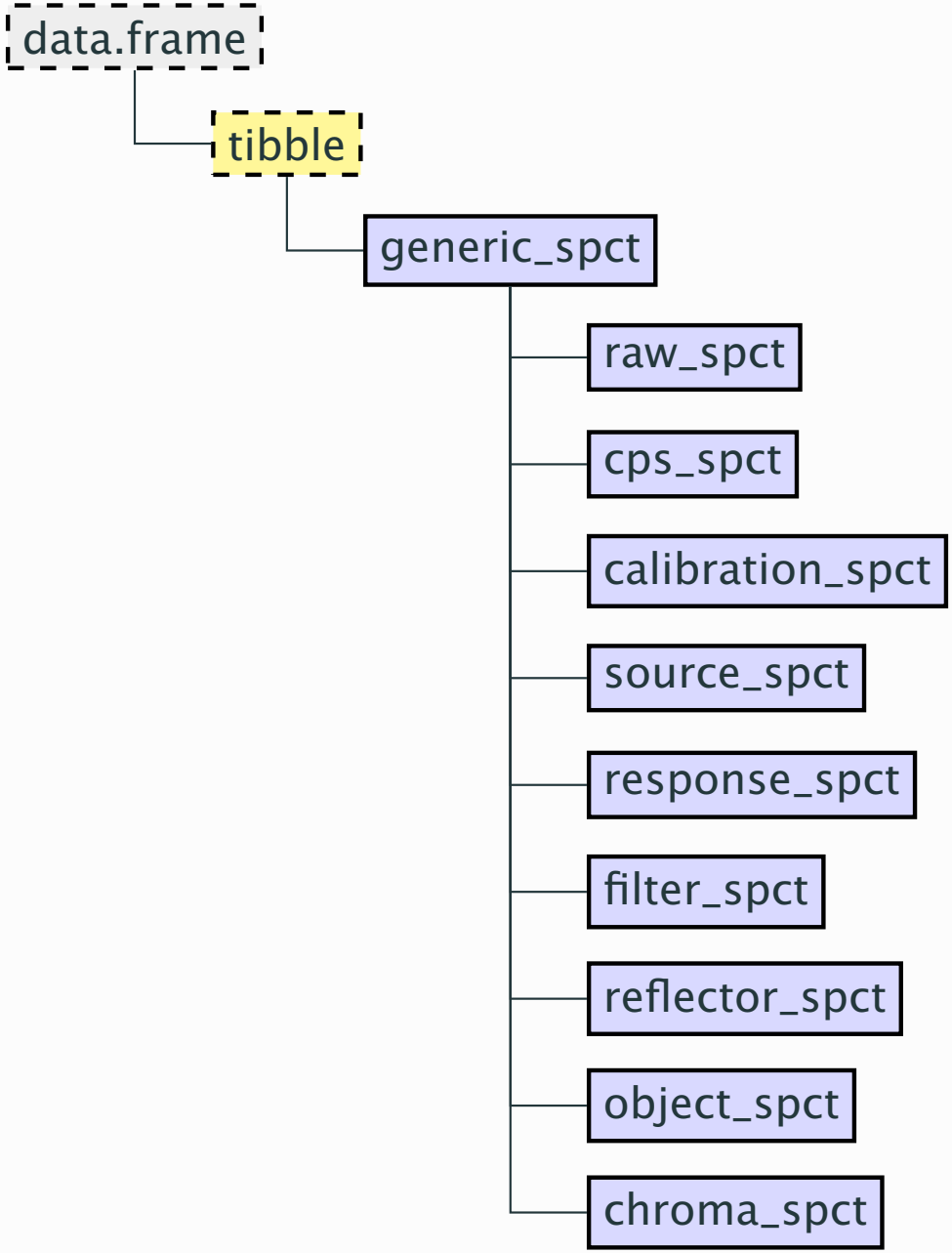
```
e_irrad(convolve_each(sun.spct,
                      filters.mspct[c("GG400","OG530","RG715")]),
        list(Red(), Blue()))
```

```
## # A tibble: 3 x 3
##   spct.idx e_irrad_Red.ISO
##   <fct>                <dbl>
## 1 GG400                 77.9
## 2 OG530                 77.9
## 3 RG715                 19.5
## # ... with 1 more variable:
## #   e_irrad_Blue.ISO <dbl>
```

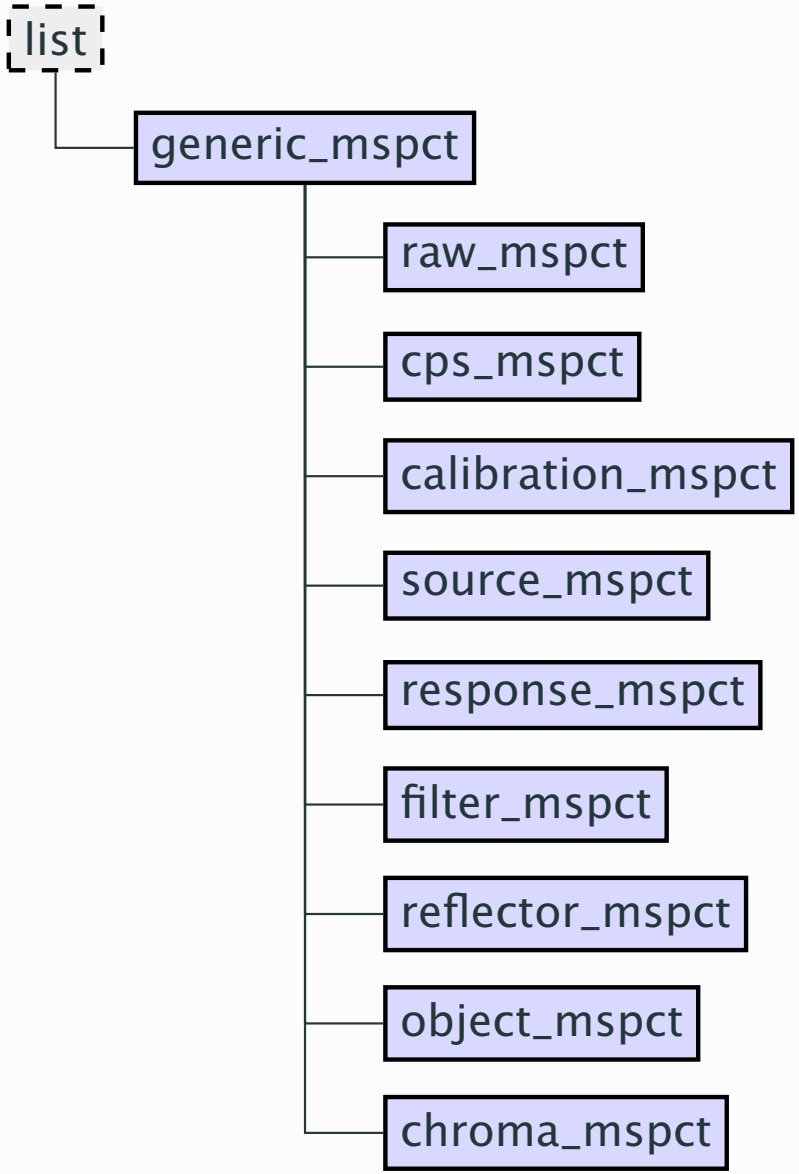
C: Photon ratios for collections of spectra

```
q_ratio(convolve_each(sun.spct,
                      filters.mspct[c("GG400","OG530","RG715")]),
        list(Red(), Blue()), VIS())


## # A tibble: 3 x 3
##   spct.idx `q_ratio_Red.ISO:VIS.ISO(q:~
##   <fct>                           <dbl>
## 1 GG400                           0.429
## 2 OG530                           0.642
## 3 RG715                           1.000
## # ... with 1 more variable:
## #   `q_ratio_Blue.ISO:VIS.ISO(q:q)` <dbl>
```

Classes for spectra



Classes for collections of spectra



Classes of returned objects

A filtered light source is a light source, not a filter:

```
class_spct(polyester.spct * sun.spct)
```

```
## [1] "source_spct"  "generic_spct"
```

An attenuated light source is still a light source:

```
class_spct(1/3 * sun.spct)
```

```
## [1] "source_spct"  "generic_spct"
```

A stack of two filters is still a filter:

```
class_spct(polyester.spct * yellow_gel.spct)
```

```
## [1] "filter_spct"  "generic_spct"
```

Metadata attributes

```
  getWhereMeasured(sun.daily.spct)
```

```
##        lon      lat
## 1 24.96474 60.20911
##                             address
## 1 kumpula, 00560 helsinki, finland
```

```
  getWhenMeasured(sun.daily.spct)
```

```
## [1] "2012-06-01"
```

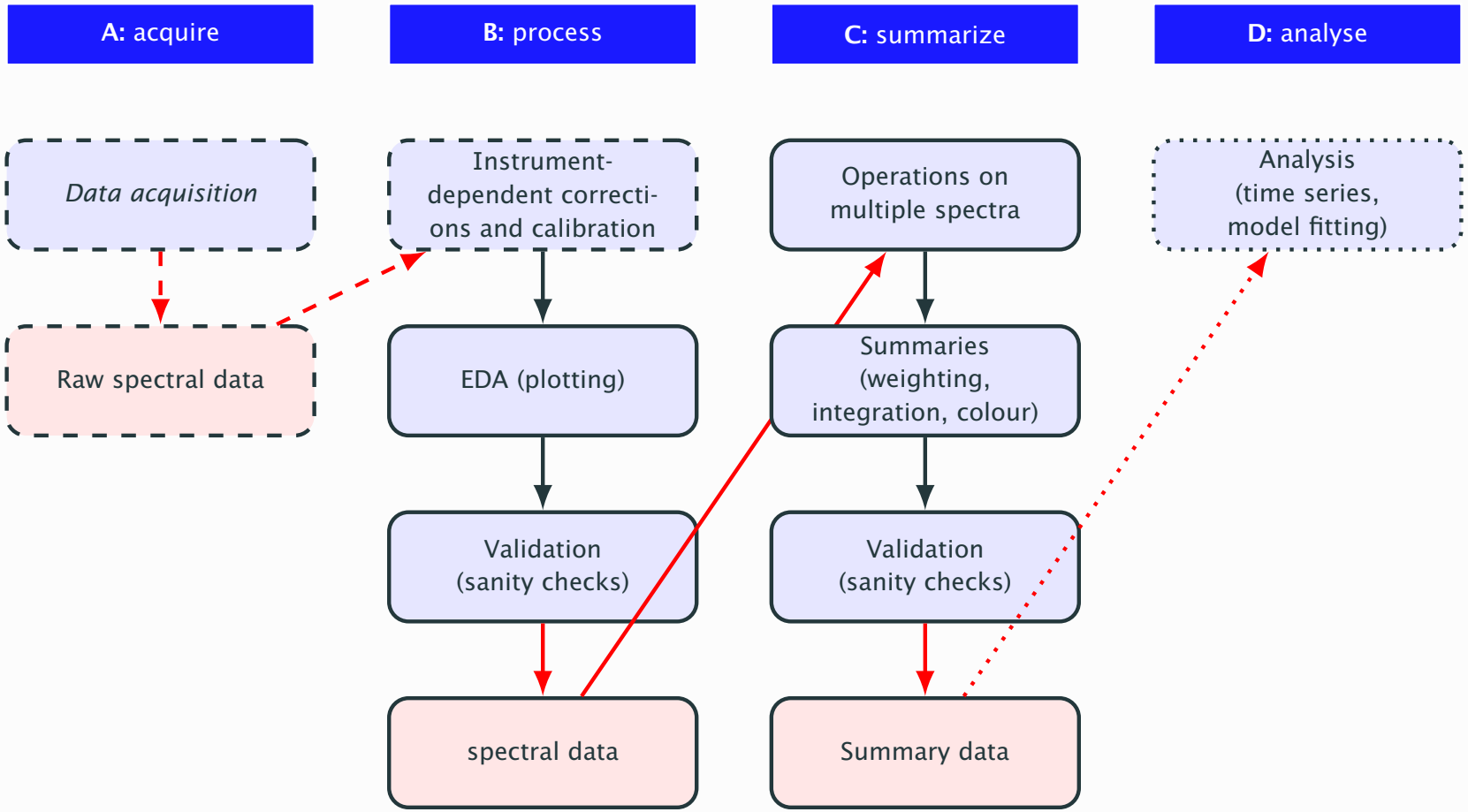
```
  getTimeUnit(sun.daily.spct)
```

```
## [1] "day"
```

```
  getWhatMeasured(sun.daily.spct)
```

```
## [1] "sunlight, simulated"
```

Data flow: Second look



Resources

Where to find the suite of packages

- Most packages in CRAN (the “official R repository”.
- mailto:pedro.aphalo@helsinki.fi
- Web site at http://www.r4photobiology.info/
  - Installation instructions
  - Posts (also) RSS feed for package updates
  - Some other related posts and pages
- Book/handbook draft available at http://leanpub.com/r4photobiology/
- Git repository at Bitbucket for development http://bitbucket.org/aphalo/
- Other resources at http://www.uv4plants.org/

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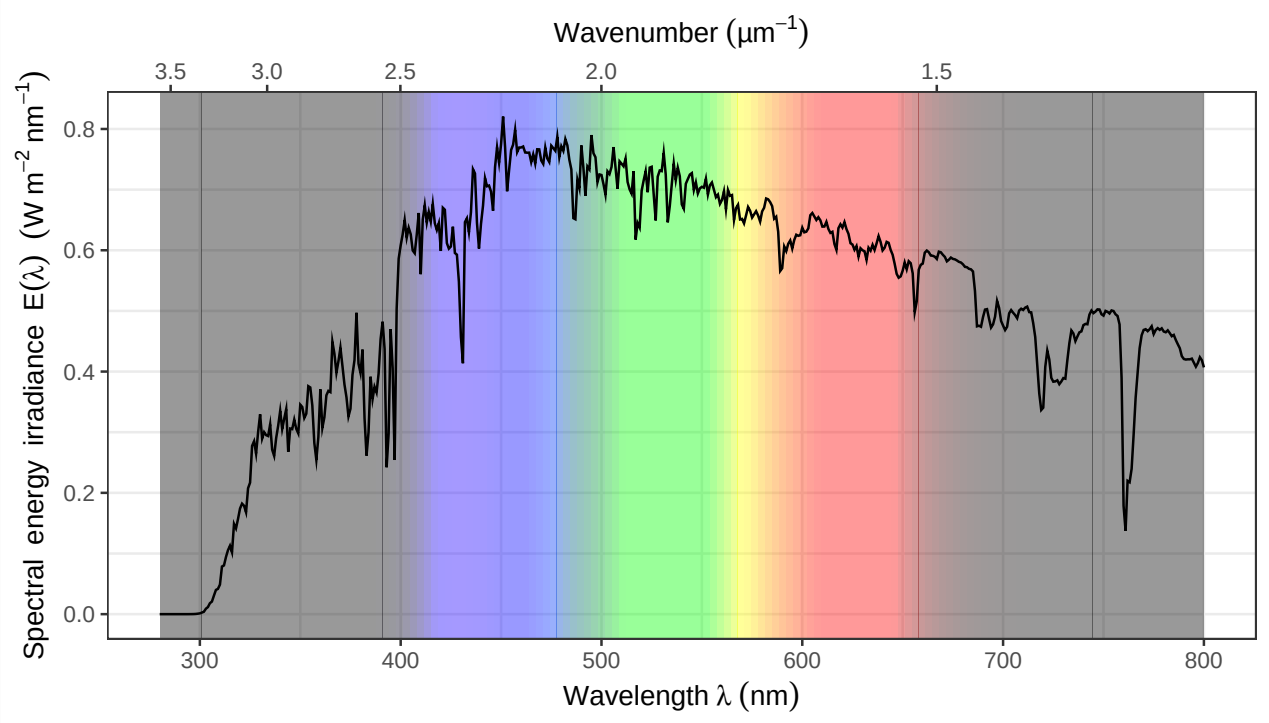
A very special thanks to the R and TEX communities for all the tools, packages, documentation and help that made developing this suite not only possible but also so enjoyable!



Thanks for listening!