R.I.P.

R IN PHYSICS

BAPTISTE AUGUIÉ

SNAP workshop
13 April 22

from Matlab to R
... and on to
Julia

WHAT DO I HAVE TO SAY

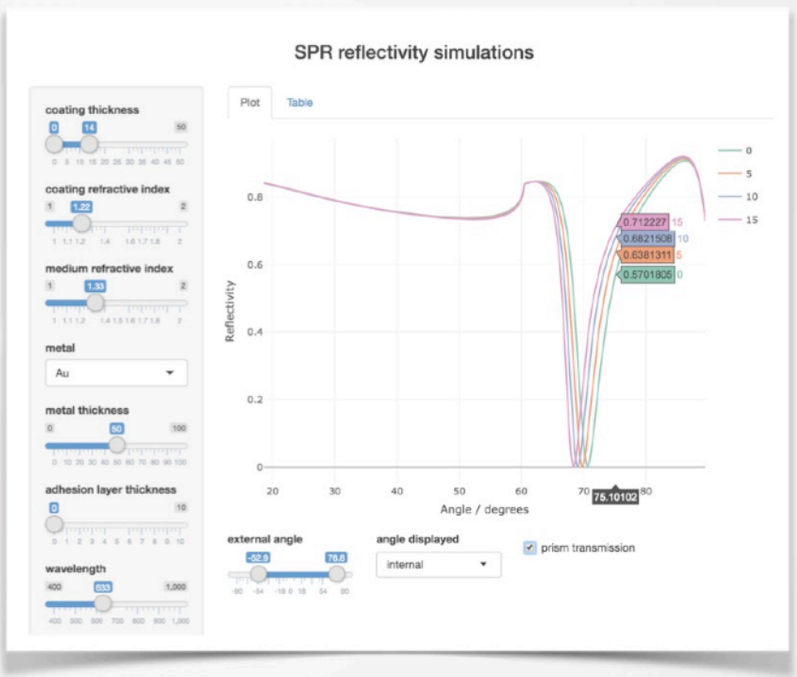
- 15 years using R
- packages

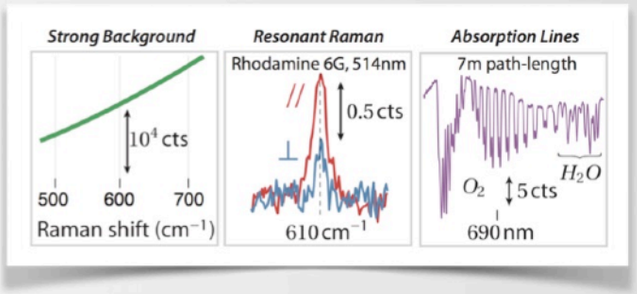
  graphics – gridExtra, `egg`, `ggflags`, …

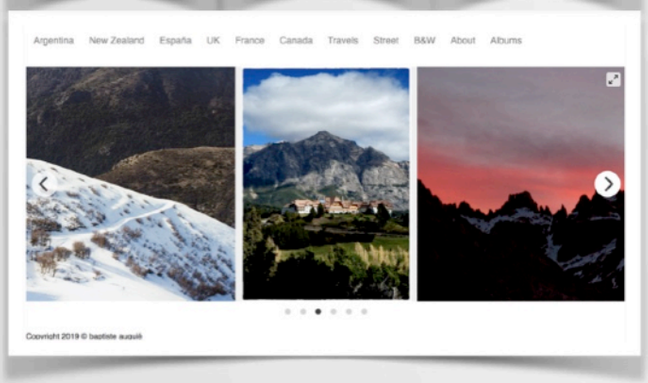
  physics – `cda`, `planar`, `mie`, `dielectric`, …

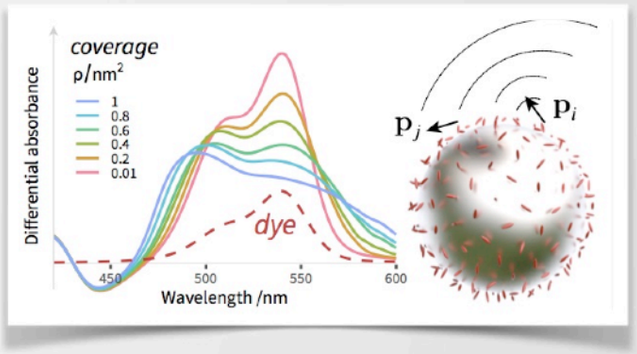
  misc. – `RcppFaddeeva`, `minixcali`, …
- contributions to `ggplot2`, `grid`, `knitr`, `Rcpp`, …
- geeky hobbies

but... what do you use R for?









GANDALF THE GREY

Wizard • pointy-hatted • pipe smoker
Maia, bearer of Narya
Born before Arda was created

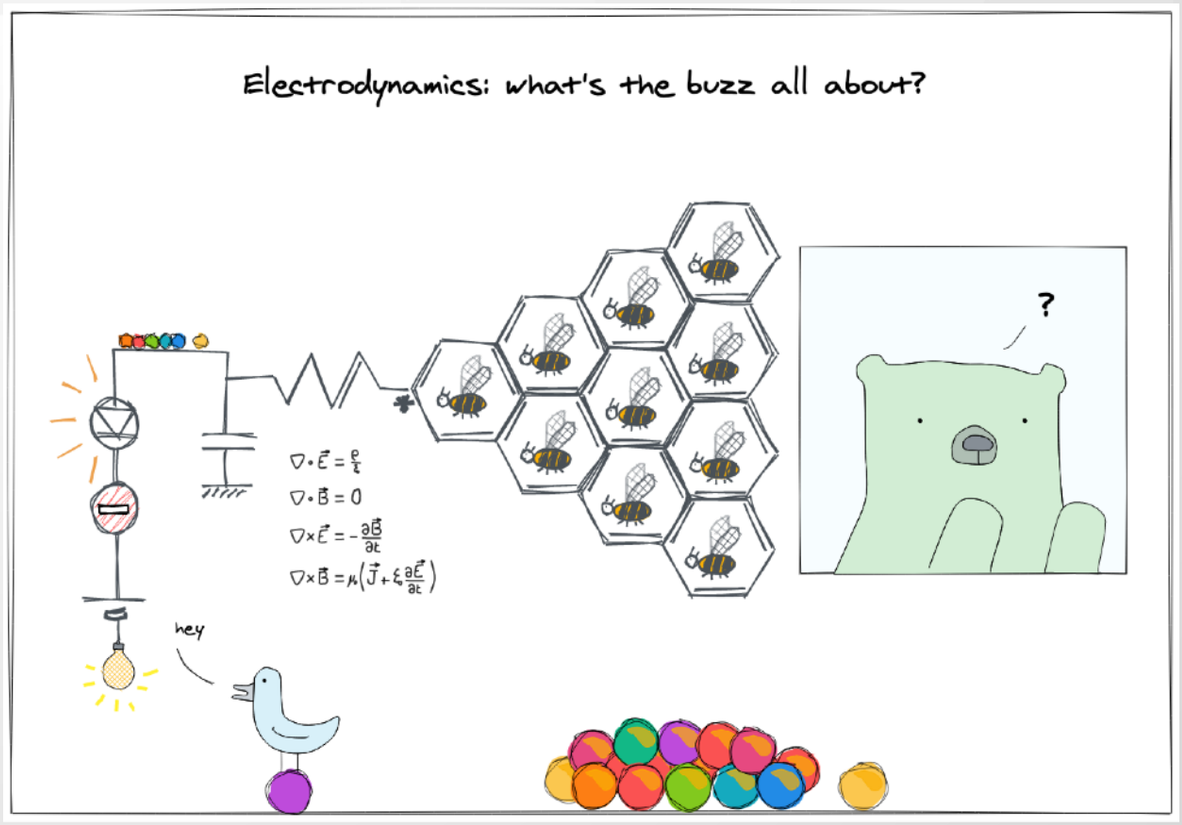
LOCATION	Valinor, Arda
MOBILE	flying moths
EMAIL	mithrandir@istari.me
SKYPE	gandalf
WEBSITE	lotr.wikia.com/wiki/gandalf

Sent by the Valar to combat the threat of Sauron upon Middle-Earth. Out of activity since the Third Age. A true wizard when it comes to fireworks, dragons and Balrogs, I also enjoy a good smoke. When things get too hot even for me, I know to delegate.

WORK EXPERIENCE

Before Ëa — **ILÚVATAR & CO., OUT OF THIS WORLD** — PHILOSOPHER, MUSIC ENTHUSIAST
- Participated in the music that shaped the universe (Ainur orchestra • duration: eons)
- Co-created all the riches in the world
- Countered dissonant views with more harmonious music
- Admired what might come to be

First Age — **MANWË'S ASSISTANT, VALINOR** — MAIA, ISTARI
- Participated in the shaping of Middle-Earth
- Helped building lamps, growing trees, teaching elves



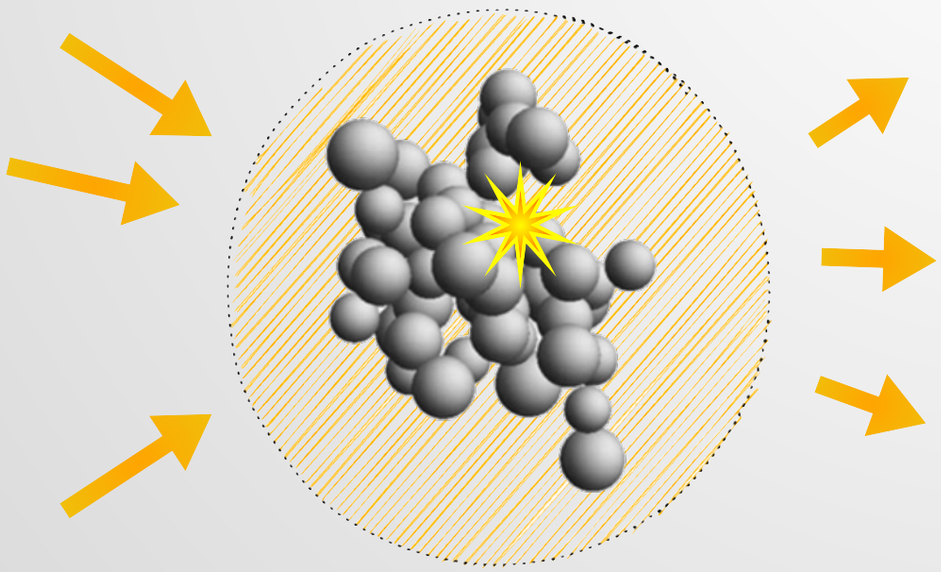
NUMERICAL MODELLING

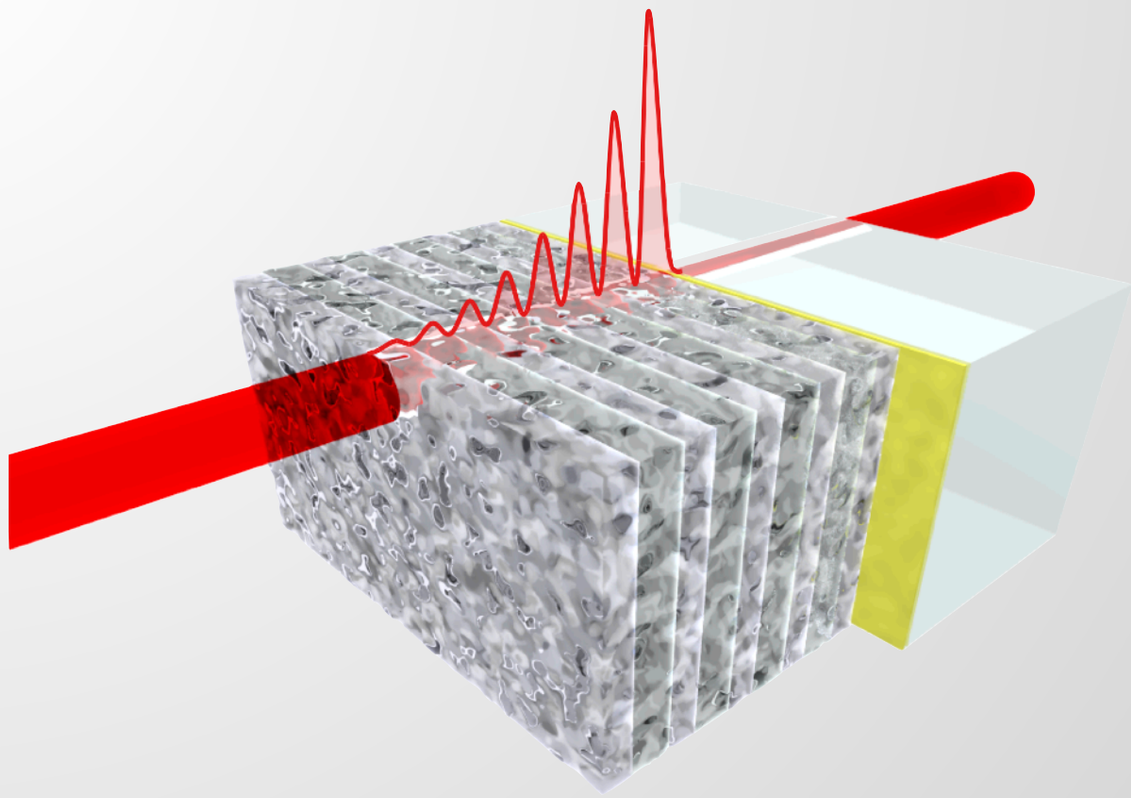
My research:

- Electromagnetic waves
- Light-matter interaction

at the nanoscale

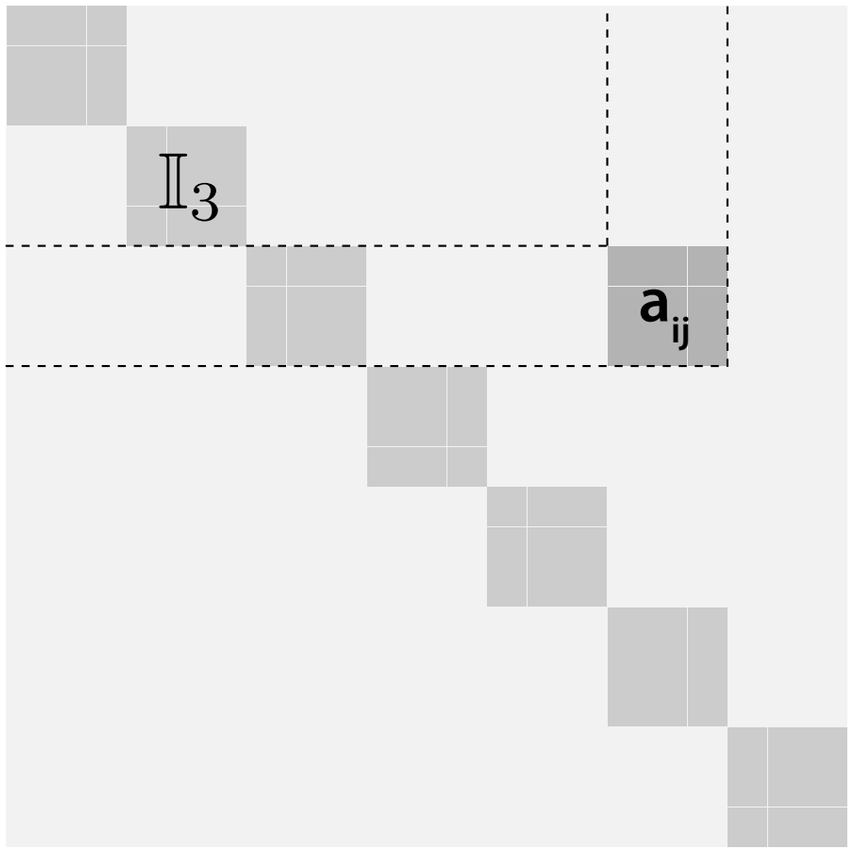
- ☑ complex, linear algebra, …
- ☑ standard syntax
- ☑ interactive, debugger, …
- ☑ **tidy data**
- ☑ **functional programming**
- ☒ fast loops
- ☒ **quirks**





TOO SLOW? RCPP(ARMADILLO)

```
// nested for loop over N dipoles
for(jj=0; jj<N; jj++)
{
  alphajj =  AlphaBlocks.slice(jj);

  for(kk=jj+1; kk<N; kk++)
  {
    alphakk =  AlphaBlocks.slice(kk);

    rk_to_rj = R.col(jj) - R.col(kk) ;
    rjk = norm(rk_to_rj, 2);
    rjkhat = rk_to_rj / rjk;
    rjkrjk =  rjkhat * rjkhat.st();

    Ajk = exp(i*kn*rjk) / rjk *  (kn*kn*(rjkrjk - I3) +
      (i*kn*rjk - arma::cx_double(1,0)) / (rjk*rjk) * (3*rjkrjk - I3)) ;

    // assign blocks
    A.submat(jj*3,kk*3,jj*3+2,kk*3+2) = Ajk * alphakk;
    A.submat(kk*3,jj*3,kk*3+2,jj*3+2) = Ajk.st() * alphajj;

  } // end kk
} // end jj

return(A);
```



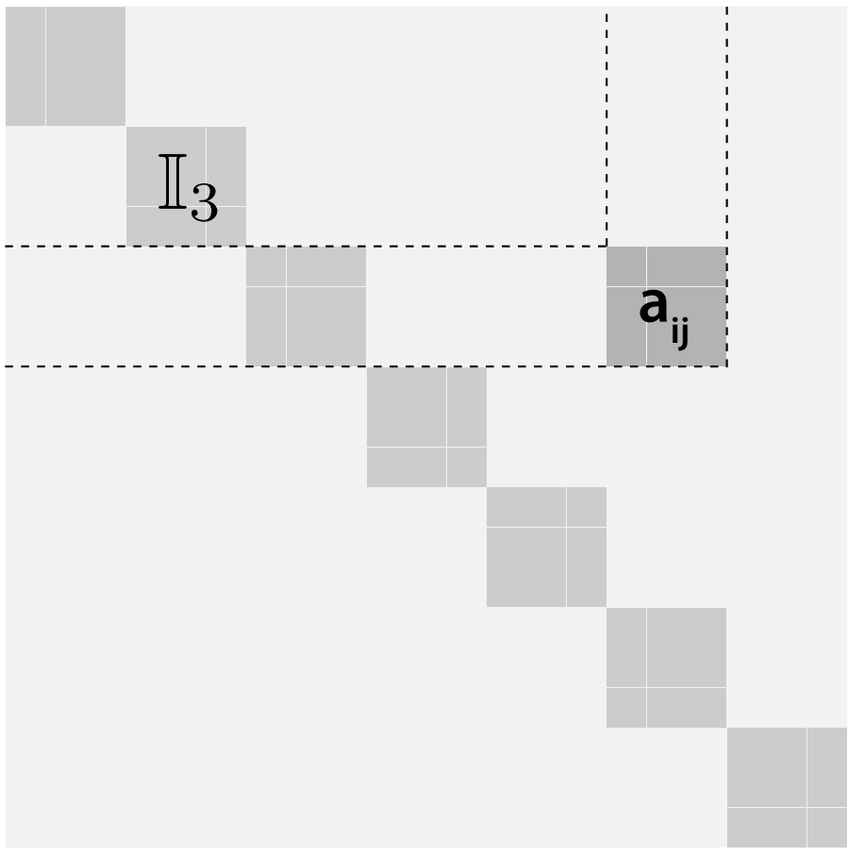
$$\frac{e^{ik_1 r}}{r_{ij}}\left\{k_1^2\left[\mathbb{I}-\mathbf{r}_{ij}\otimes\mathbf{r}_{ij}\right]-\left(\frac{1}{r_{ij}^2}-\frac{ik_1}{r_{ij}}\right)\left[\mathbb{I}-3\mathbf{r}_{ij}\otimes\mathbf{r}_{ij}\right]\right\}$$

... but two languages

JULIA: FOR LOOPS 👍

```julia
function propagator!(A, kn, R, AlphaBlocks)

    N = length(R)
    for jj = 1:N
        for kk = (jj+1):N

            rk_to_rj = R[jj] - R[kk]
            rjk = norm(rk_to_rj, 2)
            rjkhat = rk_to_rj / rjk
            rjkrjk = rjkhat * transpose(rjkhat)

            Ajk = exp(im * kn * rjk) / rjk * (
                kn * kn * (rjkrjk - I) +
                (im * kn * rjk - 1.0) / (rjk * rjk) * (3 * rjkrjk - I)
            )

            # assign blocks
            A[3jj-2:3jj, 3kk-2:3kk] = Ajk * AlphaBlocks[kk]
            A[3kk-2:3kk, 3jj-2:3jj] = transpose(Ajk) * AlphaBlocks[jj]

        end
    end

    return A
end
```

$$\frac{e^{ik_1 r}}{r_{ij}}\left\{k_1^2\left[\mathbb{I}-\mathbf{r}_{ij}\otimes\mathbf{r}_{ij}\right]-\left(\frac{1}{r_{ij}^2}-\frac{ik_1}{r_{ij}}\right)\left[\mathbb{I}-3\mathbf{r}_{ij}\otimes\mathbf{r}_{ij}\right]\right\}$$



Shiny apps – nano-optics.ac.nz/apps

Mie scattering simulations

sphere radii

5 50 200

1 21 41 61 81 101 121 141 161 181 200

material

Au

wavelength

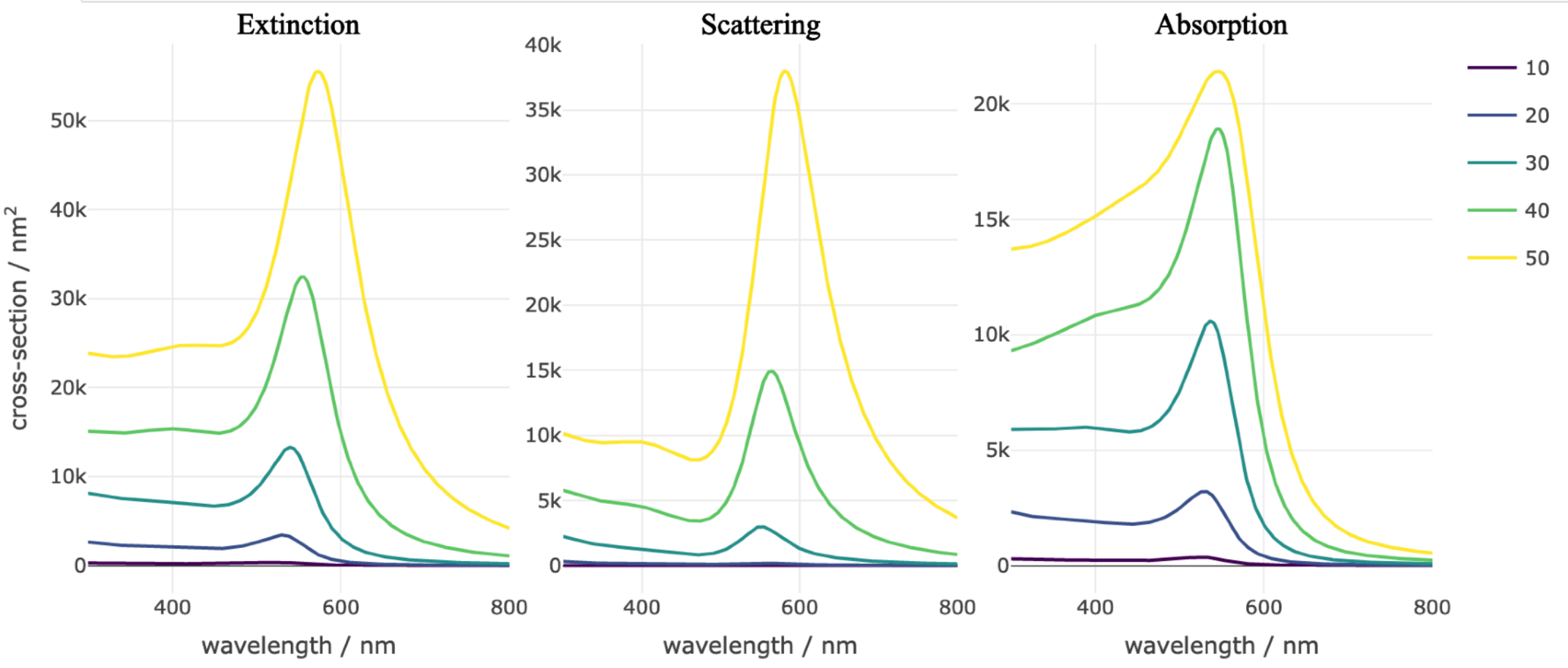
300 800 2,000

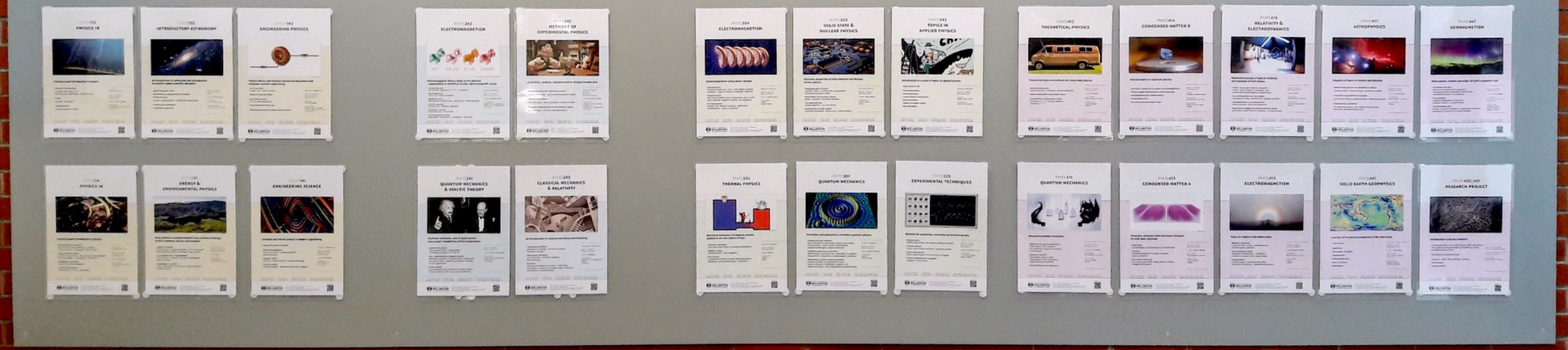
200 400 600 800 1,000 1,400 1,800

medium refractive index

1.33

Plot Table





PHYS222
ELECTRONS & PHOTONS

Electronic and optical properties of materials

- **ELECTROSTATICS**
  Gauss' law • electric potential
- **ELECTRIC CIRCUITS**
  Kirchhoff's laws • RLC circuits
- **OPTICS**
  electromagnetic waves • interference • diffraction
- **SPECTROSCOPY & LASERS**

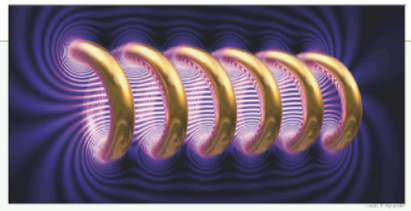
Required for: PHYS major

15 points • trimester 2
36 lectures/tutorials

Lecturers:
Govorniov, Meyer, Darby

Pre-requisites*
MATH142, MATH151
PHYS113/PHYS115
or equivalent

PHYS304
ELECTROMAGNETISM



Electromagnetism using vector calculus

- **ELECTROSTATICS**
  Coulomb & Gauss' laws • div *E* • curl *E* • electric potential • conductors • Laplace's equation • multipoles • dielectrics
- **MAGNETOSTATICS**
  Biot-Savart & Ampère's laws • Lorentz force • div *B* • curl *B* • vector potential • magnetic materials • ferromagnetism
- **ELECTRODYNAMICS**
  Faraday's law • Maxwell's equations • plane waves • Poynting vector • waves in conductors

Required for: PHYS major

15 points • trimester 2
36 lectures/tutorials

Lecturers: Ingham, Augusé

Pre-requisites*
MATH243
PHYS222, PHYS223

PHYS415
ELECTROMAGNETISM

Advanced classical electromagnetism

- **MAXWELL'S EQUATIONS**
  in vacuum and in media • conservation laws • electromagnetic potentials
- **ELECTROMAGNETIC WAVES**
  absorption and dispersion • polarisation • reflection and transmission • guided waves
- **RADIATION AND SCATTERING**
  moving charges • dipole radiation • introduction to electromagnetic scattering

15 points • trimester 1
24 lectures/tutorials

Lecturers: Le Ru, Grand

Pre-requisites*
BSC IV PHYSICS or equivalent

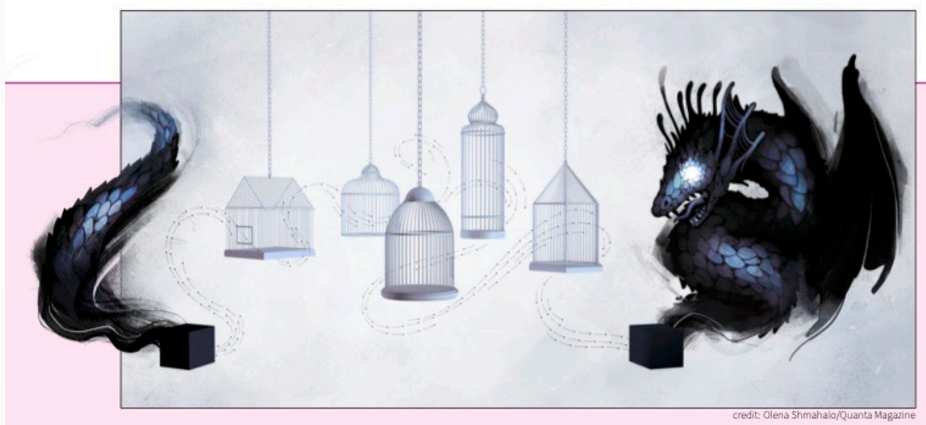
Recommended
PHYS304
MATH243

POSTERS, LECTURE SLIDES, FLYERS, CV, …

```
---
discipline: "phys"
code: "411"
title: "quantum mechanics"
shortdescription: "Advanced quantum mechanics"
credit: "Olena Shmahalo/Quanta Magazine"
trimester: "1"
points: "15"
format: "**24** lectures/tutorials"
lecturers: ["***Ruck***, **Majić**"]
prereqs: "**BSc in physics** or equivalent"
recommended: ["**phys307**, **phys309**", "**math243**"]
highlight: "phys411"
lastchecked: "16-02-2022"
---

## Principles of quantum mechanics
Hilbert spaces • Dirac notations •
the postulates of quantum mechanics •
interpretations

## Advanced concepts
mixed states • density matrix •
entanglement • Bell's inequalities •
systems of identical particles

## Relativistic quantum mechanics
```

PHYS411

QUANTUM MECHANICS



credit: Olena Shmahalo/Quanta Magazine

Advanced quantum mechanics

- **PRINCIPLES OF QUANTUM MECHANICS**
  Hilbert spaces • Dirac notations •
  the postulates of quantum mechanics •
  interpretations
- **ADVANCED CONCEPTS**
  mixed states • density matrix •
  entanglement • Bell's inequalities •
  systems of identical particles
- **RELATIVISTIC QUANTUM MECHANICS**

15 points • trimester 1
24 lectures/tutorials

Lecturers: ***Ruck***, **Majić**

Pre-requisites*
BSc IN PHYSICS or equivalent

Recommended
PHYS307, PHYS309
MATH243

PHYS115 PHYS132 ENGR142	PHYS242 PHYS245	PHYS304 PHYS345	PHYS412 PHYS414 PHYS416 PHYS417
PHYS114 PHYS131 ENGR141	PHYS241 PHYS243	PHYS305 PHYS307	**PHYS411** PHYS413 PHYS415 PHYS490

VICTORIA UNIVERSITY OF WELLINGTON TE HERENGA WAKA

SCHOOL OF CHEMICAL & PHYSICAL SCIENCES • TE WĀNANGA MATŪ
FACULTY OF SCIENCE • TE WĀHANGA PŪTAIAO
Victoria University of Wellington, PO Box 600, Wellington 6140, New Zealand
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* MORE INFO:

	year	contribution	event
1	2021	talk	Electromagnetic and Light Scattering conference ELS XIX, Russia (online)
2	2021	talk	NZIP conference, Wellington
3	2021	talk	NZIP/Physikos Physics Teachers Conference, Wellington
4	2020	talk	Invited seminar at LMU Munich, Germany (online)
5	2019	organiser \& talk	Inaugural MacDiarmid Institute hui on _Light and Spectroscopy_, Kerikeri
6	2019	invited talk	MacDiarmid Institute _Future Leaders_ (postgrads) workshop, Wellington
7	2019	talk	18th Electromagnetic and Light Scattering conference, Hangzhou, China
8	2019	talk	Progress in Electromagnetics Research Symposium, Rome, Italy
9	2018	talk	General audience presentation of the 2018 Nobel prize, Wellington
10	2018	talk	Presentation of the 2018 Nobel prize to secondary school teachers, Auckland
11	2018	talk	15th Near-Field Optics conference, Troyes, France
12	2017	talk	Dodd-Walls Centre meeting on sensing
13	2017	talk	12th International Conference on Optics of Surfaces and Interfaces, Dublin, Ireland
14	2017	talk	Australian and New Zealand Conference on Optics and Photonics, Queenstown
15	2016	talk	Dodd-Walls Centre symposium
16	2016	talk	Presentation of the T-matrix method, Auckland
17	2016	talk	MacDiarmid Institute cluster hui, Christchurch
18	2016	invited talk	MacDiarmid Institute Development Programme, Christchurch
19	2016	talk	Dodd-Walls Centre annual meeting, Queenstown
20	2015	invited talk	MacDiarmid Emerging Scientists workshop, Kaikōura
21	2015	talk	Quantum Optics workshop, Otago University
22	2015	talk	Adv. Materials & Nanotech. (AMN7) conference, Nelson
23	2014	poster	Nano 2014 meeting, Argentina
24	2014	talk	International Meeting on Chemical Sensors, Argentina
25	2014	outreach	Science and Technology week (local secondary schools), Argentina
26	2013	talk & chair	AMN6 conference, Auckland
27	2013	seminar	Post-graduate summer series, Victoria University
28	2012	poster	Quantum Nano Optics workshop, Barcelona, Spain
29	2012	talk & poster	Near-Field Optics conference (NFO), San Sebastián, Spain

BAPTISTE AUGUIÉ

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MOBILE +64(0)223052277
EMAIL augurieba@gmail.com
SKYPE baptiste.auguie
WEBSITE nano-optics.ac.nz • bapt.xyz

PhD in physics • Senior Lecturer
French, NZ permanent resident
Born in 1982

My research interests revolve around light's interaction with nanoscale materials. I combine experimental approaches, including novel spectroscopy techniques and original nanostructures, and theoretical studies that have led to new insights and computational tools for the nano-optics community. In 2017 I was awarded a Rutherford Discovery Fellowship, leading me to rejoin Victoria University as Senior Lecturer and start my own research group. I have since fully embraced other facets of the profession, contributing to our programme's re-design and to the academic environment well above expectations.

PROFESSIONAL EXPERIENCE

2017–today **Senior lecturer** • *Te Herenga Waka – Victoria University*
Rutherford Discovery Fellowship (Royal Society Te Apārangi • 5 years, $800,000)
Associate Investigator with the MacDiarmid Institute and the Dodd-Walls Centre
Associate Investigator in MBIE-funded *Smart Ideas* project in collaboration with GNS
Group leader • research, teaching and admin responsibilities

2016 **Researcher** • *Engender technologies, Auckland (4 months)*
Optical design & experiments, electromagnetic modelling, reporting
Contributed to the Photon Factory's research and teaching environment

2015–2016 **Research and teaching fellow** • *Te Herenga Waka – Victoria University*
Lectured at 300-level
Contributed to a study of absorption in turbid media published in *Nature Photonics*
Developed open-source programs for electromagnetic simulations

2013–2015 **Research fellow** • *Centro Atómico Bariloche, Argentina*
Proposed and demonstrated a novel optical sensor, initiating a new collaboration

2011–2013 **Post-doctoral fellow** • *Te Herenga Waka – Victoria University*
Developed a new technique enabling Raman spectroscopy of highly fluorescent dyes
Combined SPR and SERS spectroscopy with an original microscopy setup

2010–2011 **Post-doctoral fellow** • *University of Vigo, Spain*
Conducted pioneering research in chiral plasmonics

2009, 2010 **Invited Research Fellow** • *Instituto de Óptica–CSIC, Madrid, Spain*
Elucidated incompatible results on supported arrays of metal nanoparticles

QUALIFICATIONS

2005–2009 **PhD in physics** • *Exeter University, UK*
Thesis: *Optical properties of gold nanostructures* (Advisor: Prof William L. Barnes)
First-author publication in the prestigious journal *Physical Review Letters*

2004–2005 **Masters in Physics** • *Montréal, Canada | Rennes, France*
Year abroad at École Polytechnique, Montréal
Thesis: *Ultralow chromatic dispersion measurement in optical fibres*, 1 publication

2000–2005 **Engineering degree in Physics** • *National Institute of Applied Sciences, Rennes, France*
Core topics: physics, technology, materials science
Specialised in modern optics and nano-technology

2000 Baccalauréat scientifique, highest honours (*mention très bien*) • *France*

knitr pandoc lua pandoc xelatex

yaml + Rmd ↳ yaml + md ↳ AST ↳ AST ↳ tex ↳ pdf

WEBSITES — NANO-OPTICS.AC.NZ/TERMS

terms 1.0.0 Keywords Examples Technical notes News

TERMS

TERMS stands for **T**-matrix for **E**lectromagnetic **R**adiation with **M**ultiple **S**catterers — it is a Fortran program to simulate the near-field and far-field optical properties of collections of particles. TERMS solves rigorously the Maxwell equations via the superposition *T*-matrix method, where incident and scattered fields are decomposed into a basis of multipolar electric and magnetic spherical waves.

In a multiple-scattering problem the net field exciting a given particle is composed of the incident field plus the scattering contribution from neighbouring particles, restulting in a coupled system of equations to be solved for the total fields. TERMS implements several algorithms to describe the self-consistent electromagnetic interaction between multiple scatterers, and from there compute optical properties such as absorption, scattering, extinction, circular dichroism, as well as near-field intensities and the local degree of optical chirality.

By describing the incident and scattered fields in a basis of spherical waves the *T*-matrix framework lends itself to analytical formulas for orientation-averaged quantities such as far-field cross-sections and near-field intensities, greatly reducing the computational time needed to simulate particles and systems of particles in random orientation.

Features

The possible computations are divided into three main modes:

- Far-field quantities (absorption, scattering, extinction, circular dichroism) for multiple wavelengths and angles of incidence, as well as orientation-averages
- Near-field calculations for multiple wavelengths and incident angles, also computing the local degree of chirality, as well as orientation-averages
- Stokes parameters and differential scattering cross-sections for multiple incidence or scattering angles

LINKS

Browse source code

Report a bug

Download

LICENSE

Mozilla Public License Version 2.0

CITATION

Citing terms

DEVELOPERS

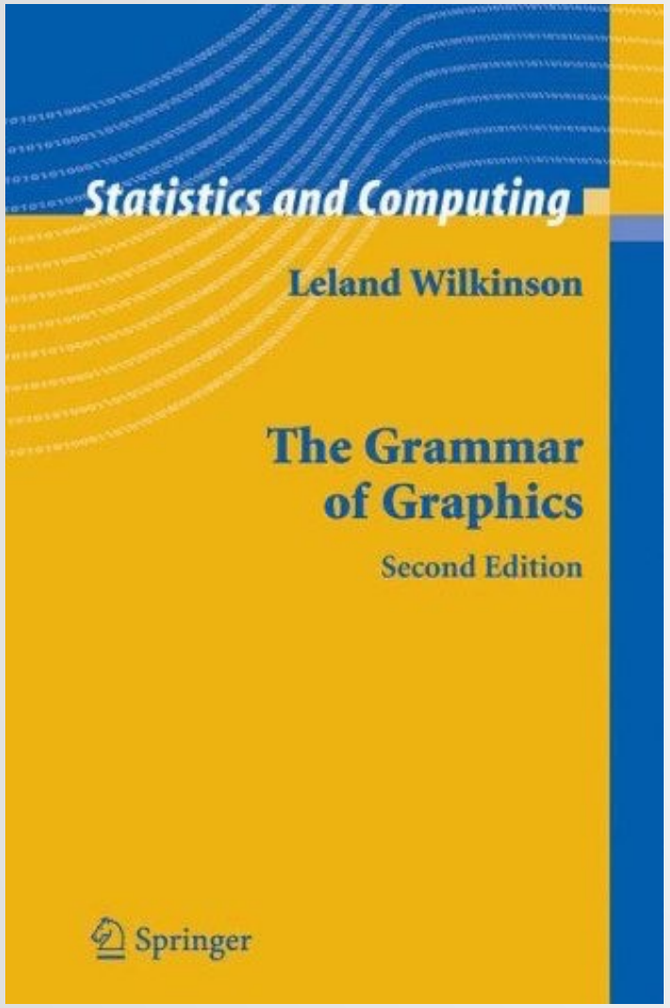
Dmitri Schebarchov
AUTHOR

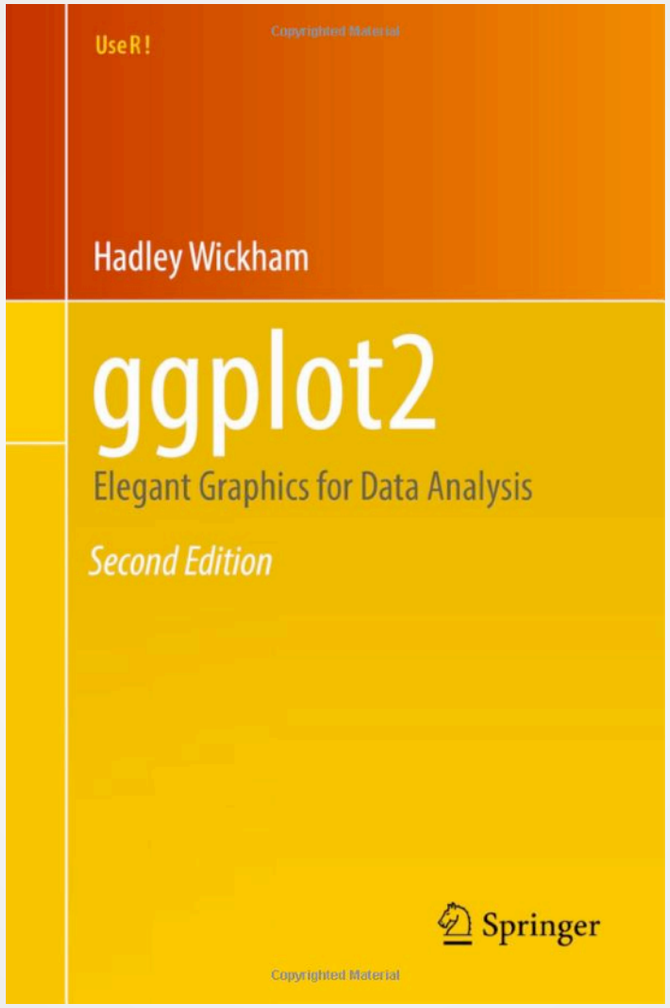
Atefeh Fazel-Najafabadi
AUTHOR

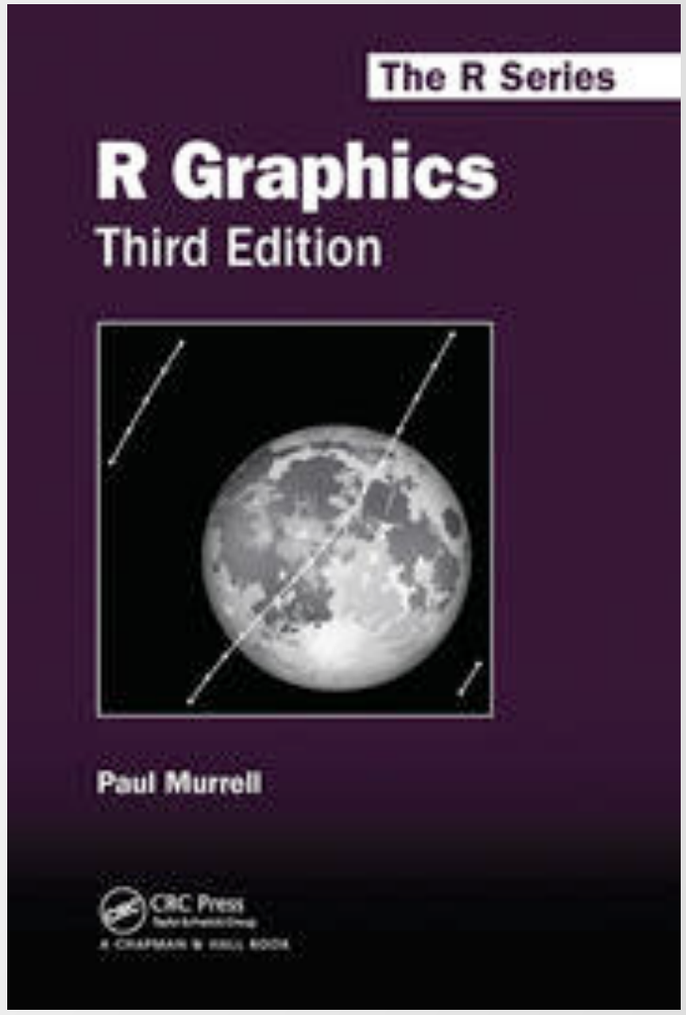
Eric Le Ru
AUTHOR

Baptiste Auguié
AUTHOR, MAINTAINER

R GRAPHICS







packages: gridExtra (17.6M downloads), egg, …

https://cran.rstudio.com/web/packages/gridExtra/

EXPRESSIVITY, LEGIBILITY, REPRODUCIBILITY

Point & Click

Yeah but, no but, yeah but, no but ! ! !

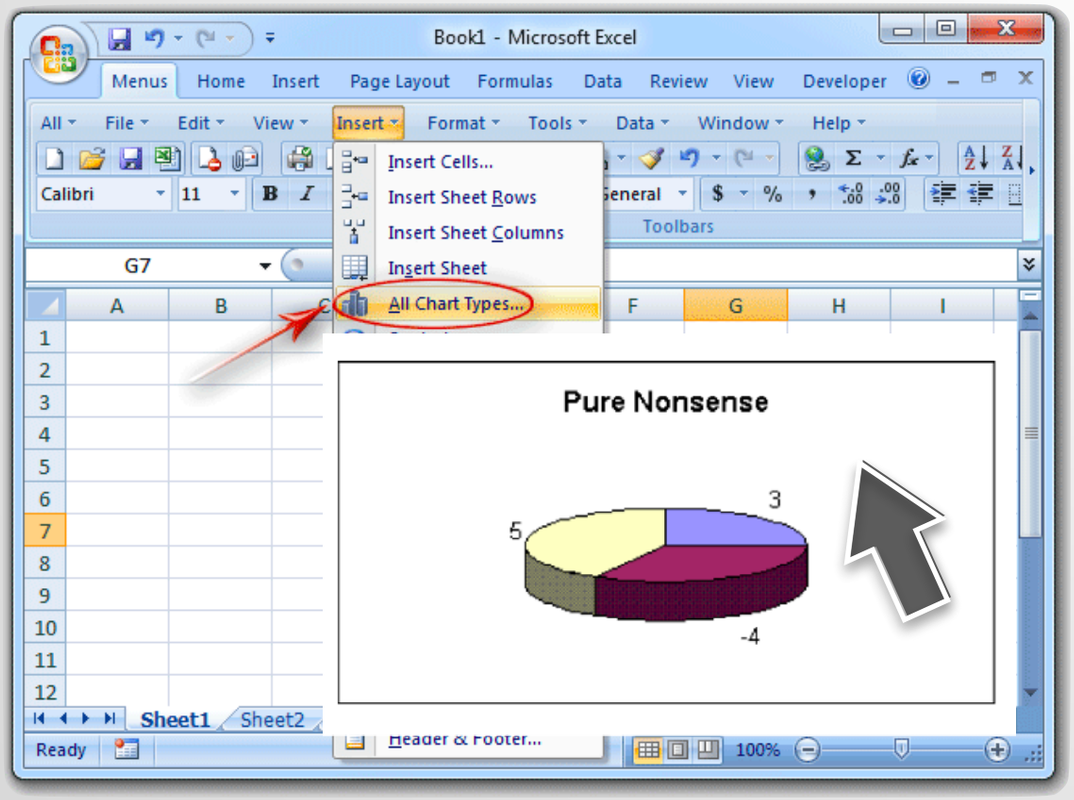
yeah but . . . I swear * * * * * * * ! ! ! ? ! ! !

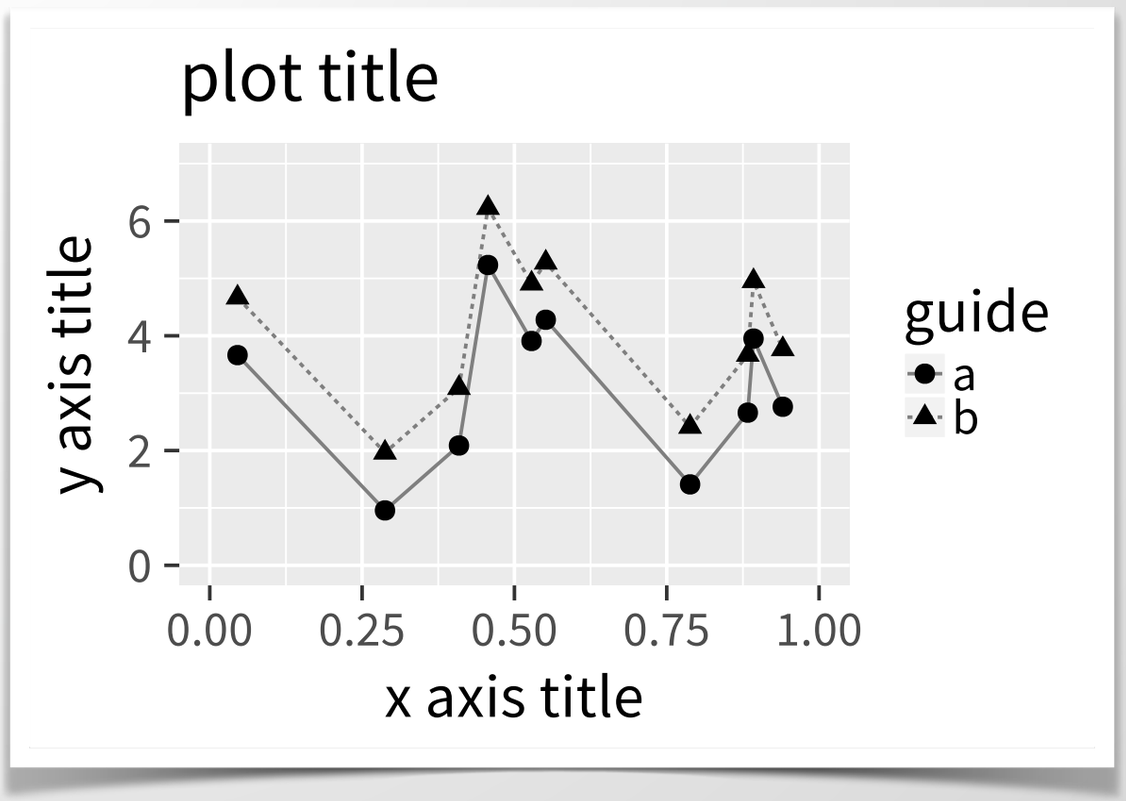
. . . but yeah _(ツ)_/ **COMPUTER SAYS NO**

Grammar of Graphics

```
plot(data, map(x, y)) +
  layer(point, map(colour = z))    +
  layer(line,  map(linetype = t)) +
  theme(fontsize = 12)
```

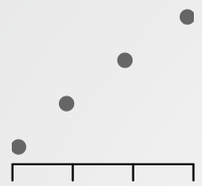
Ctrl-Z

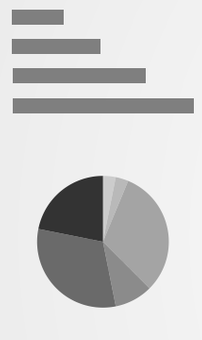


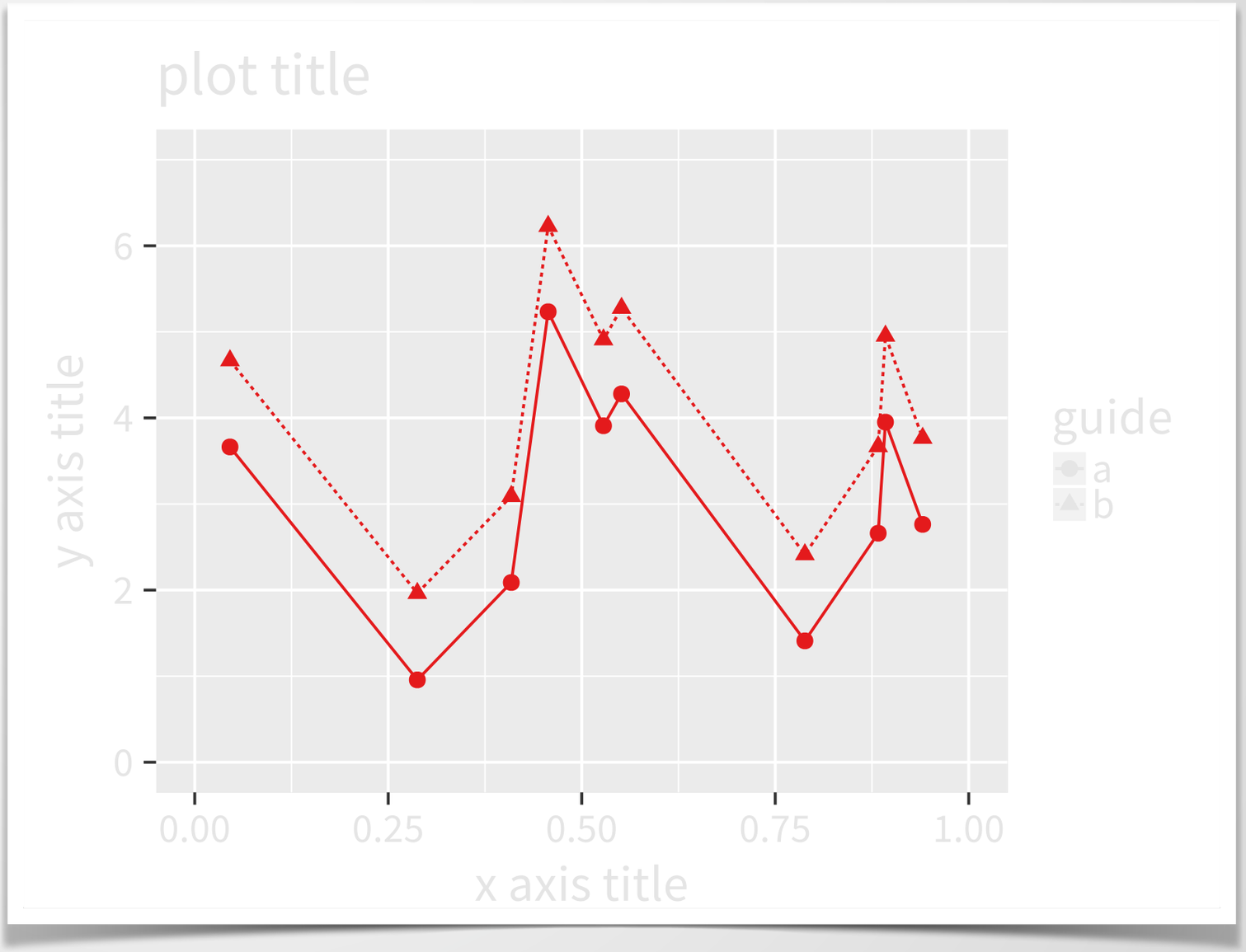


GRAMMAR OF GRAPHICS – MAPPING DATA

- position
- length
- angle
- area
- colour
- shape
- line type, size, time, …



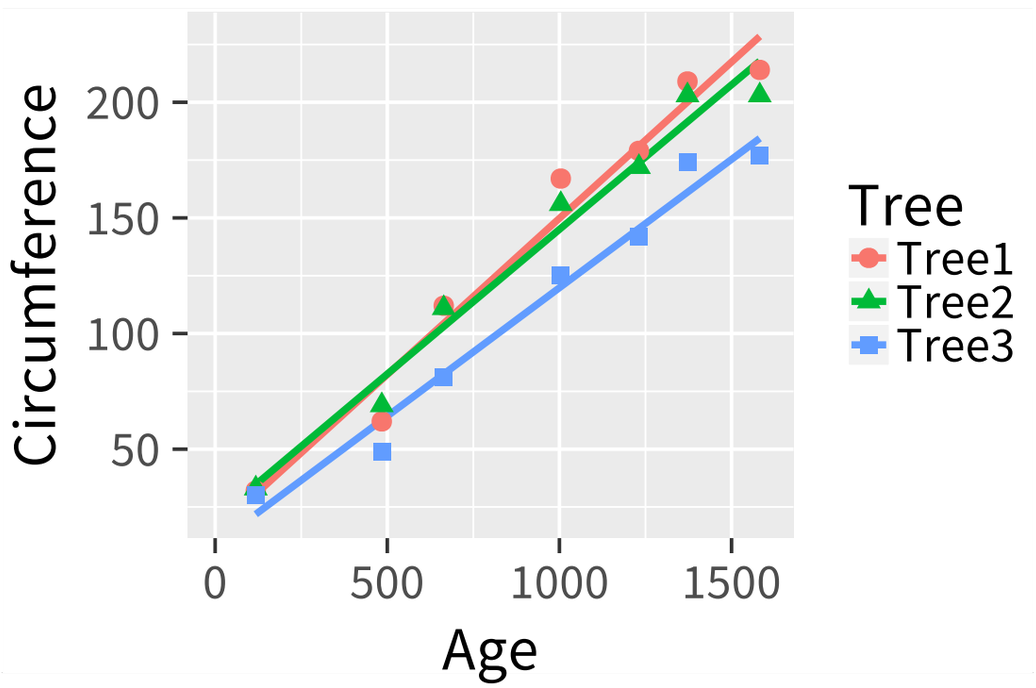




MAPPING DATA TO GLYPHS

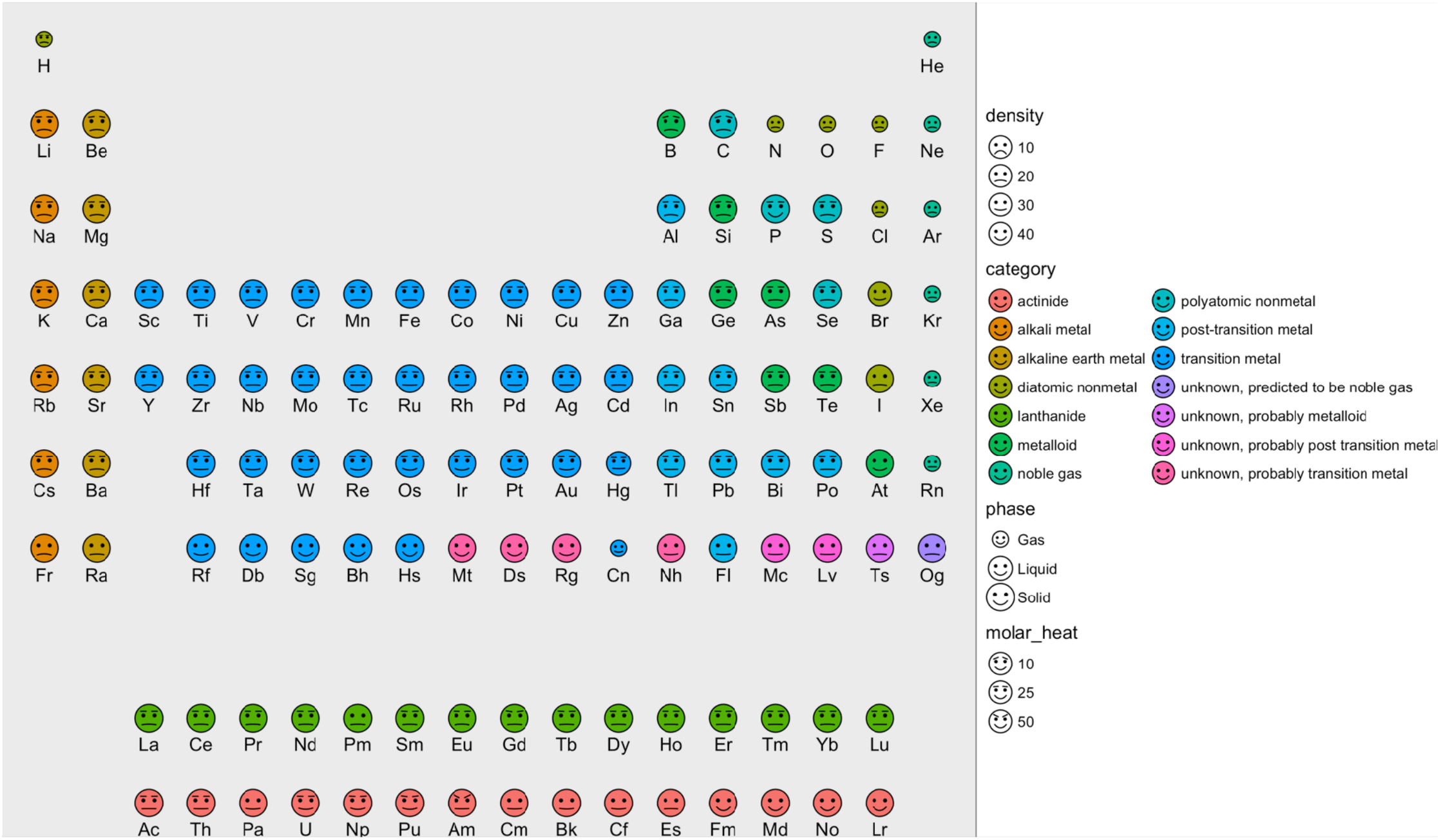
```
plot(data = d,
     mapping = map(x = age,
                   y = circumference)) +
  layer(type = point,
        mapping = map(shape  = Tree,
                      colour = Tree))  +
  layer(type = line,
        mapping = map(colour = Tree))
```

	Tree	age	circ.
1	Tree1	1582	214
2	Tree1	118	32
3	Tree2	118	33
4	Tree2	1372	203
5	Tree3	484	49
6	Tree3	1372	174
7	Tree3	1004	125



SUPPLEMENTARY

MAPPING DATA TO VISUAL ATTRIBUTES



GRAPHICAL EXPLORATIONS

```
last_plot() +
  facet_grid(Tree ~ .) +
  theme_publication
```