# Extensible Software for Research

principles and an example in julia

Center for Lifespan Psychology, Max Planck Institute for Human Development
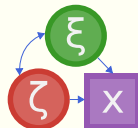
Maximilian Ernst
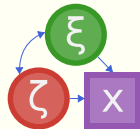
# Contents

- Why should you care?

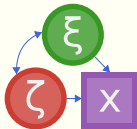- How do you get there?
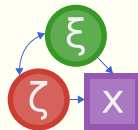
# Research Software Personas

- research software engineers

- statistics researcher

- applied user

# A day in the live of …

a statistics researcher

- **work with a specific type of model**
  - linear regression, deep learning, …

- **have an idea**

- **test it**

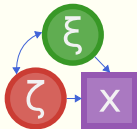- **make it available to applied researchers**

# Now we need software

- to test → prototype

- to make it available → deploy
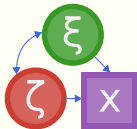
What's the fastest way to get there?

existing software

**It would be nice if they could extend existing software**

# But …

- **understand** 1000s of lines of code

- make **changes**, possibly breaking stuff

- get maintainers to **adopt** their changes

**these hurdles are often too high!**

# A day in the live of …

- to test: barebone, minimal reimplementation
    - waste of time
    - not well tested
    - hard to reproduce

- to deploy: put their code on github
    - bad user interface, no documentation
    - missing features
    - incompatible to existing software
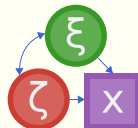
# My Experience

- from R → **julia**

- most R packages are very hard to extend

- most **julia** packages are very easy to extend
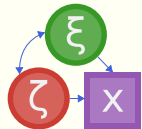
# Culture

- care about extensibility

- developer documentation

- assume their code is read

# Software Design

You need to be able to add new features...

- without understanding existing code
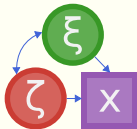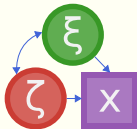
- without changing existing code

- syntactical requirements need to be clear and easy communicable!

# Two modes of extension

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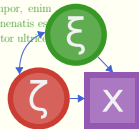
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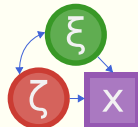
In Julia, everything has a type:

```
a = 1.0
typeof(a) # Float64

b = "hello"
typeof(b) # String
```
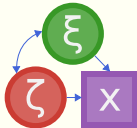
# Why julia?

You can define your own types:

```julia
struct ClockTime{T}
    time::T
end

my_time = ClockTime(5.0) # ClockTime{Float64}(5.0)
my_time.time # 5.0
```
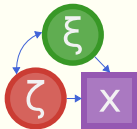
# Why julia?

A function is a collection of methods:

```julia
typeof(1.0) # Float64
typeof(1) # Int64

@code_llvm 6.0*7.0
@code_llvm 6*7

methods(*)
```
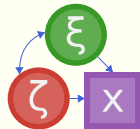
# Why julia?

We can write our own addition:

```julia
import Base: +

function +(x::ClockTime{T}, y::ClockTime{T}) where{T}
    return ClockTime((x.time + y.time) % T(24))
end

my_time = ClockTime(11.2)
your_time = ClockTime(18.4)

our_time = my_time + your_time
```
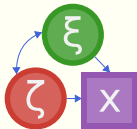
# Goal achieved

We have just written extensible code.

*I have memory problems, and I only care about full hours.*

```
my_time = ClockTime(UInt8(5))
your_time = ClockTime(UInt8(8))

our_time = my_time + your_time
```
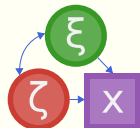
# Why julia?

*I want to multiply sparse matrices of clock times*

```julia
using SparseArrays

import Base: zero, *

function *(x::T, y::ClockTime{T}) where T
    return ClockTime((x * y.time) % T(24))
end

zero(x::ClockTime{T}) where T = ClockTime(zero(T))
zero(::Type{ClockTime{T}}) where T = ClockTime(zero(T))
```

# Why julia?

Let's define some matrices!

```julia
a = zeros(ClockTime{Float64}, 20, 20)

a[1,1] = ClockTime(5.0)
a[1,2] = ClockTime(11.673)
a[6,9] = ClockTime(17.23)
a[16,4] = ClockTime(20.87)

a_sparse = sparse(a)

b = zeros(20, 20)
b[3,9] = 1
b[6,9] = sqrt(2)
b[19,1] = π
b[4,5] = e

b_sparse = sparse(b)
```
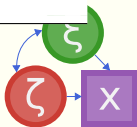
# Why julia?

```julia
using BenchmarkTools

@benchmark b_sparse*a_sparse

BenchmarkTools.Trial: 10000 samples with 199 evaluations.
 Range (min … max):  422.864 ns …  12.295 μs
 Time  (median):     453.877 ns
 Time  (mean ± σ):   566.627 ns ± 648.451 ns
Memory estimate: 2.22 KiB

@benchmark b*a

BenchmarkTools.Trial: 10000 samples with 1 evaluation.
 Range (min … max):  56.683 μs …  1.323 ms
 Time  (median):     57.111 μs
 Time  (mean ± σ):   59.411 μs ± 18.922 μs
 Memory estimate: 23.75 KiB
```
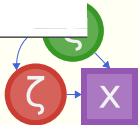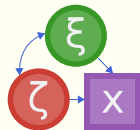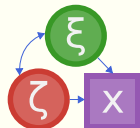
# A few days in a methods researchers life

- Do you have any ideas why this does not converge?

- Staring puzzled at the theory (should work?!).

- Staring very puzzled at the implementation in C++.

- Rinse and repeat for a couple of days and researchers.

# An hour in our life

- Look at the formula: $ridge(x, \lambda) = \lambda \sum_{j=1}^{p} x^2$

- Implement in Julia: `ridge(x, λ) = λ * sum(x.^2))`

- add 30 lines of API (formal requirements)

- Enjoy.

# Two hours in our life

- Original simulation takes weeks on a dedicated workstation.

- Original simulation freezes our cluster due to bad parrelization.

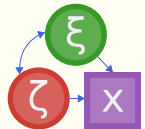- Simulation in Julia takes 2 hours on my laptop.
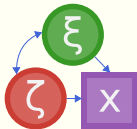
# Why?

- Some investments in extensibility

- division of labor:
  - optimizing linear algebra is done by Intel
  - numerical optimization is done by dedicated experts
  - differentiation is automated
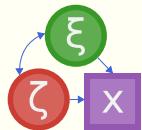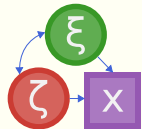
- modern infrastructure
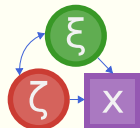
usability

# The effectiveness of usability

- usability $\neq$ lazyness

- enables quick prototyping

- allows domain experts to contribute their expertise

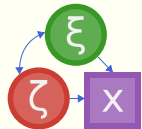- theorethical and technical development move in lockstep

# How to improve usability?

1. Extensible Software
2. Dokumentation
3. User Interface

# Dokumentation

- Dokumentation for Users

- Dokumentation for Contributors

# User Interface

- Frictionless

- Connected to prior knowledge