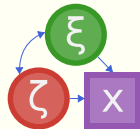


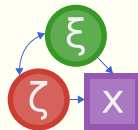
# Extensible Software for Research

principles and an example in julia



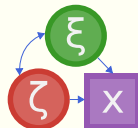
# Contents

- Why should you care?
- How do you get there?



# Research Software Personas

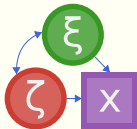
- research software engineers
- statistics researcher
- applied user



# 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

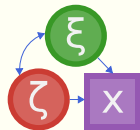
❏ to test → prototype

❏ to make it available → deploy

What's the fastest way to get there?

existing software

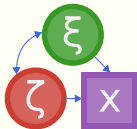
**It would be nice if they could extend existing software**



# But ...

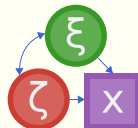
- **understand** 1000s of lines of code
- make **changes**, possibly breaking stuff
- get maintainers to **adopt** their changes

**these hurdles are often too high!**





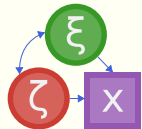
# A day in the live of ...

- ❏ 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

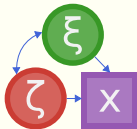
- from R  $\rightarrow$  
- most R packages are very hard to extend
- most  packages are very easy to extend





# Culture

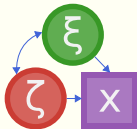
- care about extensibility
- developer documentation
- assume their code is read



# 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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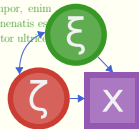
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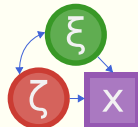


# Why julia?

In Julia, everything has a type:

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

```
b = "hello"  
typeof(b) # String
```

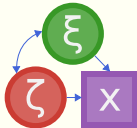


# Why julia?

You can define your own types:

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

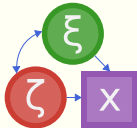
```
my_time = ClockTime(5.0) # ClockTime{Float64}(5.0)
my_time.time # 5.0
```



# Why julia?

A function is a collection of methods:

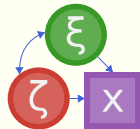
```
typeof(1.0) # Float64  
typeof(1) # Int64  
  
@code_llvm 6.0*7.0  
@code_llvm 6*7  
  
methods(*)
```



# Why julia?

We can write our own addition:

```
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
```

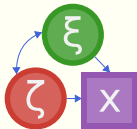


# Goal achieved

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?

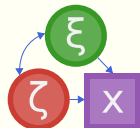
*I want to multiply sparse matrices of clock times*

```
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!

```
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)
```

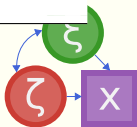
```
b[3,9] = 1
```

```
b[6,9] = sqrt(2)
```

```
b[19,1] =  $\pi$ 
```

```
b[4,5] =  $e$ 
```

```
b_sparse = sparse(b)
```



# Why 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
```

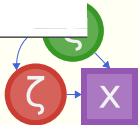
```
BenchmarkTools.Trial: 10000 samples with 1 evaluation.
```

```
Range (min ... max): 56.683 μs ... 1.323 ms
```

```
Time (median): 57.111 μs
```

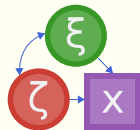
```
Time (mean ± σ): 59.411 μs ± 18.922 μs
```

```
Memory estimate: 23.75 KiB
```



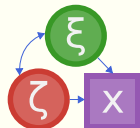
# A few days in a methods researchers life

- ❏ 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.



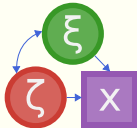
# An hour in our life

- Look at the formula:  $\text{ridge}(x, \lambda) = \lambda \sum_{j=1}^p x^2$
- Implement in Julia: `ridge(x, λ) = λ * sum(x.^2)`
- add 30 lines of API (formal requirements)
- Enjoy.



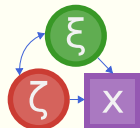
# Two hours in our life

- ❏ Original simulation takes weeks on a dedicated workstation.
- ❏ Original simulation freezes our cluster due to poor parallelization.
- ❏ Simulation in Julia takes 2 hours on my laptop.



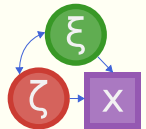
# Why?

- 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



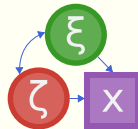
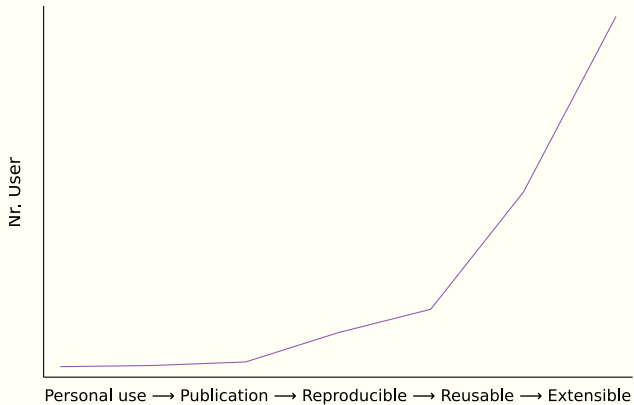
# But why?

convenience



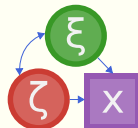


# The leverage of convenience

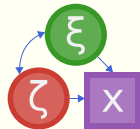
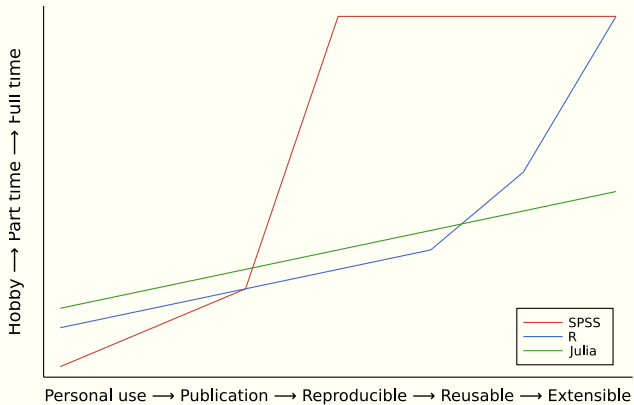


# How to improve convenience?

1. Extensible Software
2. Dokumentation
3. User Interface

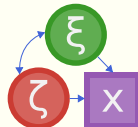


# Time is limited



# Dokumentation

- Dokumentation for users
- Dokumentation for contributors/developers



# User Interface

- Frictionless
- Connected to prior knowledge

