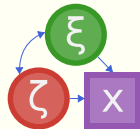


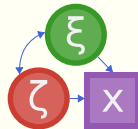
Extensible Software for Research

principles and an example in julia



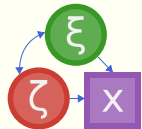
Contents

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



Research Software Personas

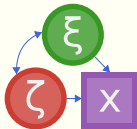
- research software engineers
- statistics researcher
- applied user



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

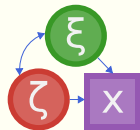
❏ to test → prototype

❏ to make it available → deploy

What's the fastest way to get there?

existing software

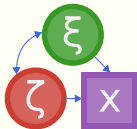
It would be nice if they could extend existing software



But ...

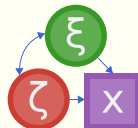
- **understand** 1000s of lines of code
- make **changes**, possibly breaking stuff
- get maintainers to **adopt** their changes

these hurdles are often too high!





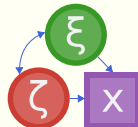
A day in the live of ...

- 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



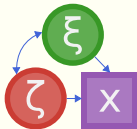
My Experience

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



Culture

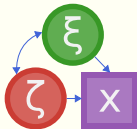
- care about extensibility
- developer documentation
- assume their code is read



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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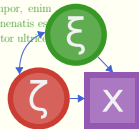
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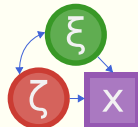


Why julia?

In Julia, everything has a type:

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

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

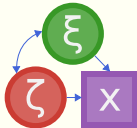


Why julia?

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:

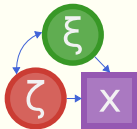
```
typeof(1.0) # Float64
```

```
typeof(1) # Int64
```

```
@code_llvm 6.0*7.0
```

```
@code_llvm 6*7
```

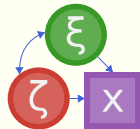
```
methods(*)
```



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
```

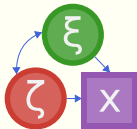


Goal achieved

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?

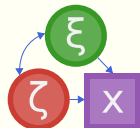
I want to multiply sparse matrices of clock times

```
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)
```

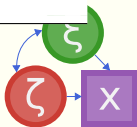
```
b[3,9] = 1
```

```
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
```

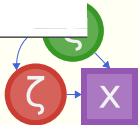
```
BenchmarkTools.Trial: 10000 samples with 1 evaluation.
```

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

```
Time (median): 57.111 μs
```

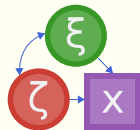
```
Time (mean ± σ): 59.411 μs ± 18.922 μs
```

```
Memory estimate: 23.75 KiB
```



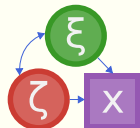
A few days in a methods researchers life

- ❖ 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.



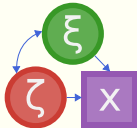
An hour in our life

- 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.



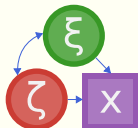
Two hours in our life

- ❏ 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.



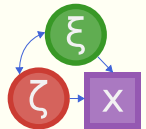
Why?

- 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

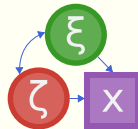
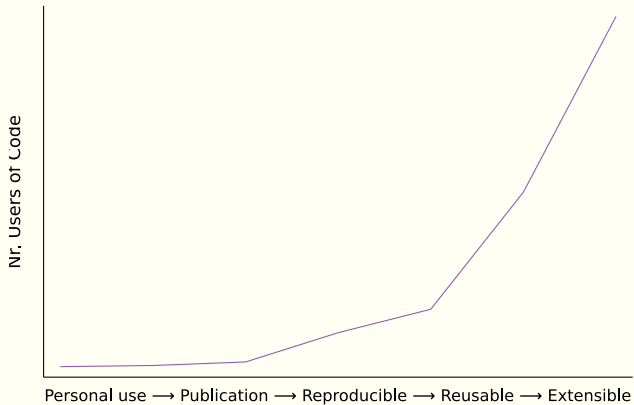


But why?

convenience

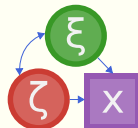


The leverage of extensible software

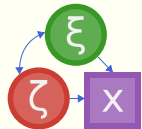
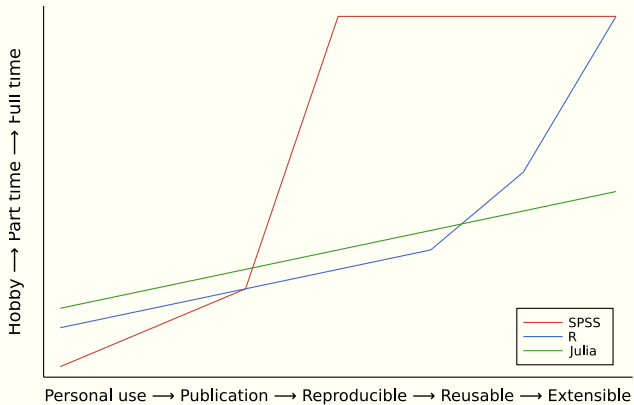


How to improve convenience?

1. Extensible Software
2. Dokumentation
3. User Interface

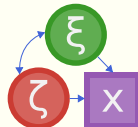


Time is limited



Dokumentation

- Dokumentation for users
- Dokumentation for contributors/developers



User Interface

- Frictionless
- Connected to prior knowledge

