DEVELOPMENT OF A HIGH PERFORMANCE

DEVELOPMENT OF A HIGH PERFORMANCE HYDROLOGICAL MODEL

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eurac research

THE GOAL: INTRODUCE MYSELF (& THE PROJECT)

The Plan: The Five Ws and the How

WHO?

BACKGROUND: THEORETICAL PHYSICS

I graduated with a thesis in HEP (phenomenology, hadron spectroscopy) at the University of Bari

EMBEDDED SYSTEM DEVELOPER

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Embedded Systems ≈ HPC

knowledge of the hardware, limited resource and relevance of computational time

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Embedded Systems ≠ HPC

numerical algorithms, open-source development environment and higher level languages

SUBSTITUTE TEACHER (PHYS & MATH)

Funny enough, thanks to a script:

```
# Sending MADs with Python!
for indx, s in schools.iterrows():
    print("Sending to {}, {}".format(s.Istituto, s.Comune))
    code = indx.lower()
    send_email(code, "pec")
```

(You can find the whole script here)

More to the point, long interest in OSS and CS

WHAT?

- I got a HPC-TRES fellowship
- I am now a student of the MHPC
- I will work on GEOtop

MHPC

a program that prepares students for careers in the fast-growing field of HPC

GEOTOP

an integrated hydrological model that simulates the heat and water budgets at and below the soil surface

WHEN?

- The MHPC lectures will last until june (approx)
- Then I will work on my thesis on GEOtop

WHERE?

Trieste (SISSA and ICTP) and Bolzano (Eurac)

EURAC RESEARCH

a private research institute based in Bolzano and with a strong focus on the alpine environment

WHY?

GEOtop, scientifically advanced, but codebase & documentation **need a fix**

(not uncommon among scientific software packages)

THE AIM

- ease further development
- increase usability
- integration with other packages
- {pre,post}-processing tools
- better performance

WHAT HPC REALLY MEANS FOR GEOTOP?

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High Performance Computing

WHAT HPC REALLY MEANS FOR GEOTOP?

High ~~Performance~~ Computing

WHAT HPC REALLY MEANS FOR GEOTOP?

High Productivity Computing

So the title of this presentation should really be:

DEVELOPMENT OF A HIGH PRODUCTIVITY HYDROLOGICAL MODEL

HOW?

REFACTORING?

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See previous talk...

REENGINEERING?

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- Replacing custom linear algebra routines with BLAS/LAPACK: multithreading for free

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REENGINEERING?

- Replacing custom linear algebra routines with BLAS/LAPACK: multithreading for free
- Removing useless IO code
- Modularizing the codebase

REWRITING?

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GEOtop as library?

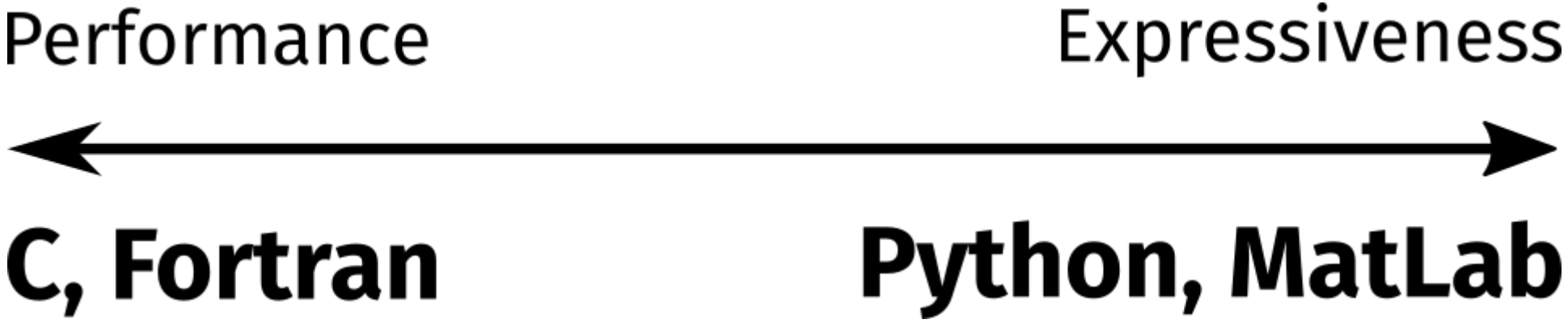
REWRITING?

GEOtop as library?

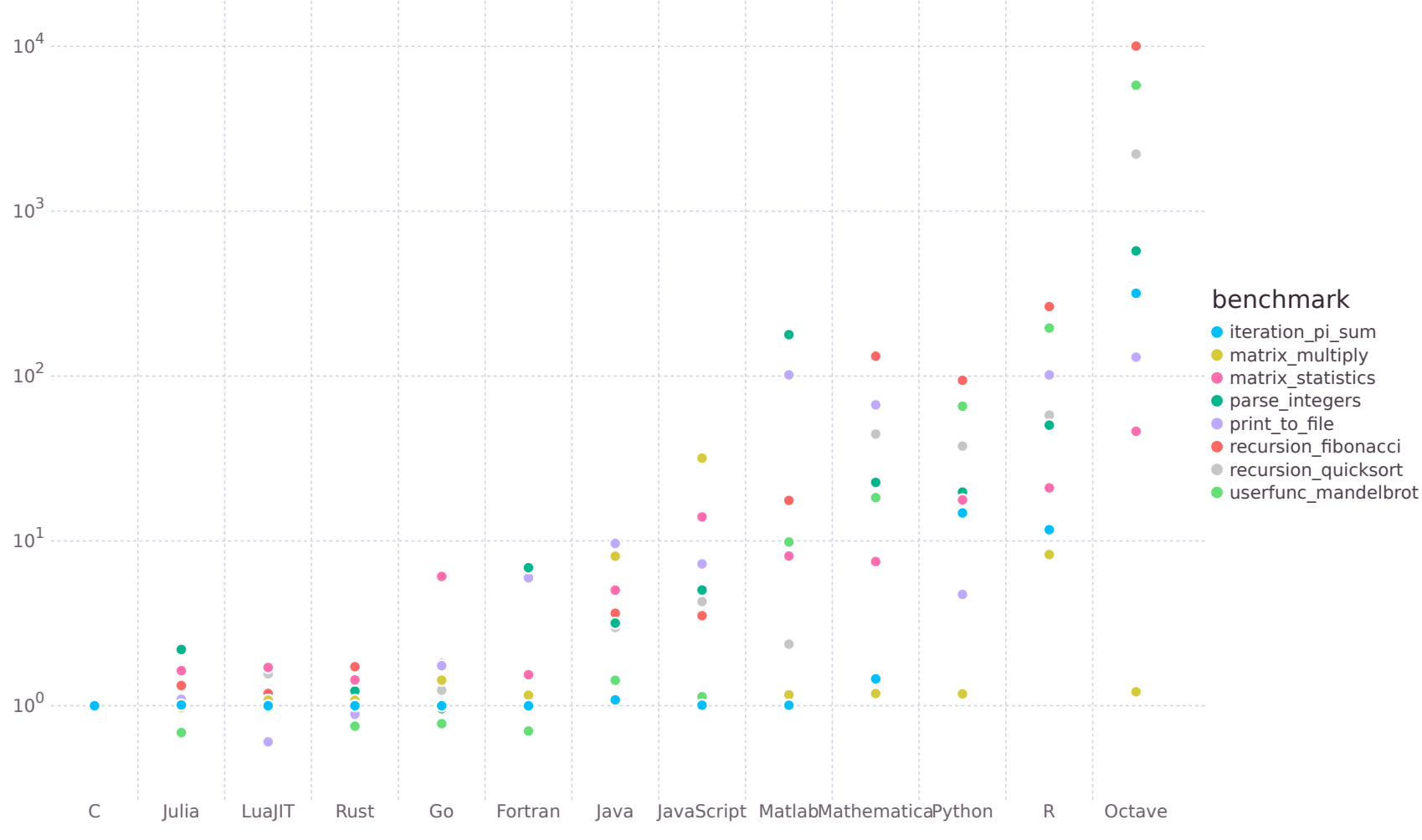
PyGEOtop? GEOtop.jl?

JULIA IN 3 SLIDES

THE 2 LANGUAGE PROBLEM



JULIA: SOME MICROBENCHMARKS



JIT COMPILATION & DYNAMIC MULTIPLE DISPATCH

```
methods(sin) # ex. sin(x), x = 1, 3.14, 1 + 2im, [1 2; 2 1]...
# 12 methods for generic function "sin":
[1] sin(x::BigFloat) in Base.MPFR at mpfr.jl:743
[2] sin(::Missing) in Base.Math at math.jl:1072
[3] sin(a::Complex{Float16}) in Base.Math at math.jl:1020
[4] sin(a::Float16) in Base.Math at math.jl:1019
[5] sin(z::Complex{T}) where T in Base at complex.jl:796
[6] sin(x::T) where T<:Union{Float32, Float64} in Base.Math at
[7] sin(x::Real) in Base.Math at special/trig.jl:53
[8] sin(A::LinearAlgebra.Hermitian{#s616,S} where S<:(Abstract
[9] sin(A::Union{LinearAlgebra.Hermitian{#s617,S}, LinearAlgeb
[10] sin(D::LinearAlgebra.Diagonal) in LinearAlgebra at /build
[11] sin(A::AbstractArray{#s617,2} where #s617<:Real) in Linea
[12] sin(A::AbstractArray{#s617,2} where #s617<:Complex) in Li
```

ACKNOWLEDGMENTS

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JULIA: FOR A FEW SLIDES MORE

UTILITIES FOR SCIENTIFIC COMPUTING

```
using DifferentialEquations, ParameterizedFunctions, Plots

lorenz = @ode_def begin                    # define the system
 dx = σ * (y - x)
 dy = x * (ρ - z) - y
 dz = x * y - β*z
end σ ρ β

u0 = [1.0,0.0,0.0]                         # initial conditions
tspan = (0.0,100.0)                        # timespan
p = [10.0,28.0,8/3]                        # parameters
prob = ODEProblem(lorenz, u0, tspan, p) # define the problem
sol = solve(prob)                          # solve it
plot(sol, vars = (1, 2, 3))                # plot solution
```

"NO BOILERPLATE" PHILOSOPHY

```
function getenv(var::AbstractString)
    val = ccall((:getenv, "libc"),
                Cstring, (Cstring,), var)
    if val == C_NULL
        error("getenv: undefined variable: ", var)
    end
    unsafe_string(val)
end

getenv("SHELL") # "/bin/bash"
```

PARALLEL AND HETEROGENEOUS COMPUTING

```
using CuArrays, CUDAnative

xs, ys = CuArray(rand(1024)), CuArray(rand(1024))
zs = CuArray(zeros(1024))

function kernel_vadd(out, a, b)
  i = (blockIdx().x-1) * blockDim().x + threadIdx().x
  out[i] = a[i] + b[i]
  return
end

@cuda (1, length(xs)) kernel_vadd(zs, xs, ys)
```

HOMOICONICITY

```
macro time(ex)
  return quote
    local t0 = time()
    local val = $ex
    local t1 = time()
    println("elapsed time: ", t1-t0, " seconds")
    val
  end
end

@time sin(3.14) # output: elapsed time 0.000002 seconds
```