The Julia programming language in the Quantum Community

An overview of the Julia programming language and its applications in quantum software

Xiuzhe (Roger) Luo

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Outline

1. From Punch Card to JIT Compiler
2. Introduction of Selected Packages
3. The Quantum "Gang" in Julia Community

From Punch Card to JIT Compiler

Fortran 1957 - The Punch Card Language

Fortran ***1957***

punch cards

- uppercase only
- goto statements
- multi-dimensional arrays
- …

I WOULD LIKE TO SAY THANKS TO ALL OUR VISITORS! PLEASE KEEP COMING BACK!
MASS:WERK DATA CENTER <masswerk.at>
CDL 0815

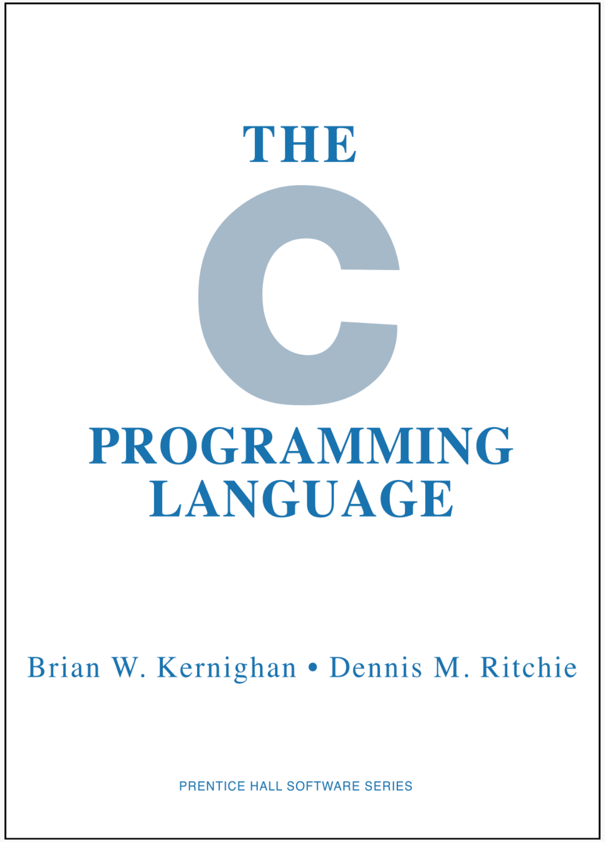
Punch Card generated by Fortran *by Nobert Landsteiner*

C - Compiler Language

C ***1972***

the compiled language

- type system
- pointers
- structs
- …



THE
C
PROGRAMMING LANGUAGE
Brian W. Kernighan • Dennis M. Ritchie
PRENTICE HALL SOFTWARE SERIES

The C Programming Language *by Brian Kernighan and Dennis Ritchie*

Python - Interpreter Language

Python *1991*

the interpreted language

- dynamic typing
- garbage collection
- package manager
- …

Well-known Python Libraries

- NumPy
- SciPy
- Pandas
- Matplotlib
- …

The Python Logo

Compiled vs Interpreted

Compiled

Pros

- no runtime or small runtime
- finer analysis thus more optimizations

Interpreted

Pros

- faster development cycle
- easier to learn
- interactive

Compiled vs Interpreted

Compiled

Pros

- no runtime or small runtime
- finer analysis thus more optimizations

Cons

- slower development cycle
- stiff learning curve
- not interactive

Interpreted

Pros

- faster development cycle
- easier to learn
- interactive

Cons

- slower
- bigger runtime

Why not X for Scientific Computing?

Scientific Computing

- extreme performance requirements
- a lot of deadlines (fast development cycle)
- non-professional programmers (scientists)

Frontier - The World's Fastest Supercomputer (2023).

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More and more complicated HPC

- heterogeneous hardware (CPU, GPU, …)
- distributed systems (cluster, cloud, …)
- …

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- fast development cycle
- easy to learn
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Are we looking for a silver bullet?

Julia - the Language for JIT

Julia

the language designed for JIT

how to make python run faster
Julia
Look what they need just to
mimic a fraction of our power!

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Julia

the language designed for JIT

What is JIT?

Just-In-Time compilation

- compile code at runtime
- ship the interpreter along with a compiler
- optimize only frequently executed code

how to make python run faster
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bonus: compiler can know more about your code by running interpreter

how to make python run faster
Julia
Look what they need just to mimic a fraction of our power!

Julia - the Language for Science

Designed for Science

- nice syntax for scientific tasks

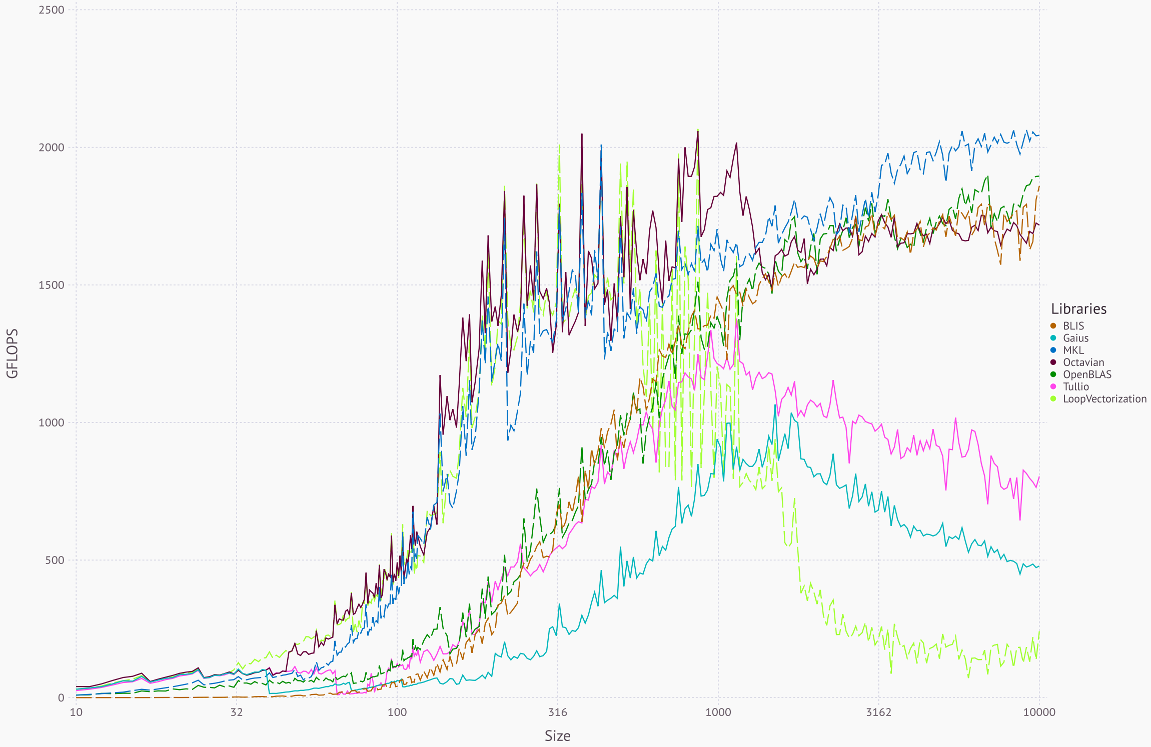
```
# broadcasting
sin.(A)
A .+ B .+ C

[1, 2, 3]        # Vector
[1 2 3;2 3 4]    # Matrix
[1 2 3;2 3 4;;; # Tensor
 1 1 1;2 2 2]
```

Julia - the Language for Science

Designed for Science

- nice syntax for scientific tasks
- comparable performance to highly-optimized C & Assembly



Native Julia GEMM vs OpenBLAS & MKL

Julia - the Language for Science

Designed for Science

- nice syntax for scientific tasks
- comparable performance to highly-optimized C & Assembly
- a rich ecosystem of matrices & arrays with unified interface

- Dense Arrays (builtin)
- SparseMatrix (builtin)
- Heterogeneous Arrays (CUDA, OpenCL, AMD, Metal, ...)
- Special Matrices (Permutation, Tridiagonal, Gaussian, ...)
- ...

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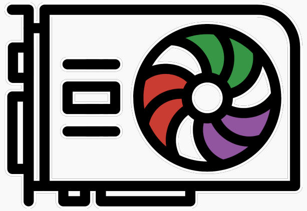

The JuliaGPU organization

- KernelAbstractions.jl - unified interface for GPU programming
- CUDA.jl - high-level and kernel programming with CUDA
- AMDGPU.jl - high-level and kernel programming with AMD GPUs
- Metal.jl - high-level and kernel programming with Apple GPUs

Julia - the Cons

The Technical Price of JIT

- bigger runtime
- slower startup time (warm-up)
- not able to generate small binaries (yet/never)

The Non-Technical Cons

- relatively young and small community (not an ideal language for business)
- evolving ecosystem

Julia - the Cons

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Yes

- (performance) build from scratch & runs > 5s
- (expressiveness) my code has many different cases

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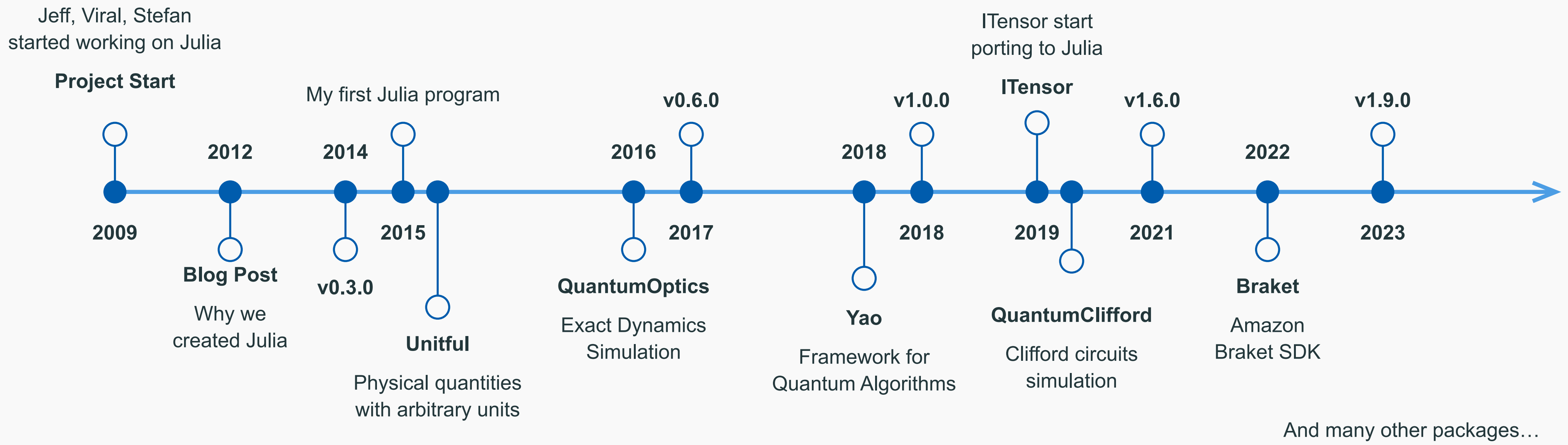
No

- Just wanna write a tiny CLI app (use rust)
- Mainly want to use a package (e.g PyTorch)
- My users are not technical
  - no new language (use python)
  - no code (use web app interface, e.g drag & drop circuit compilation)

A Long History with Quantum



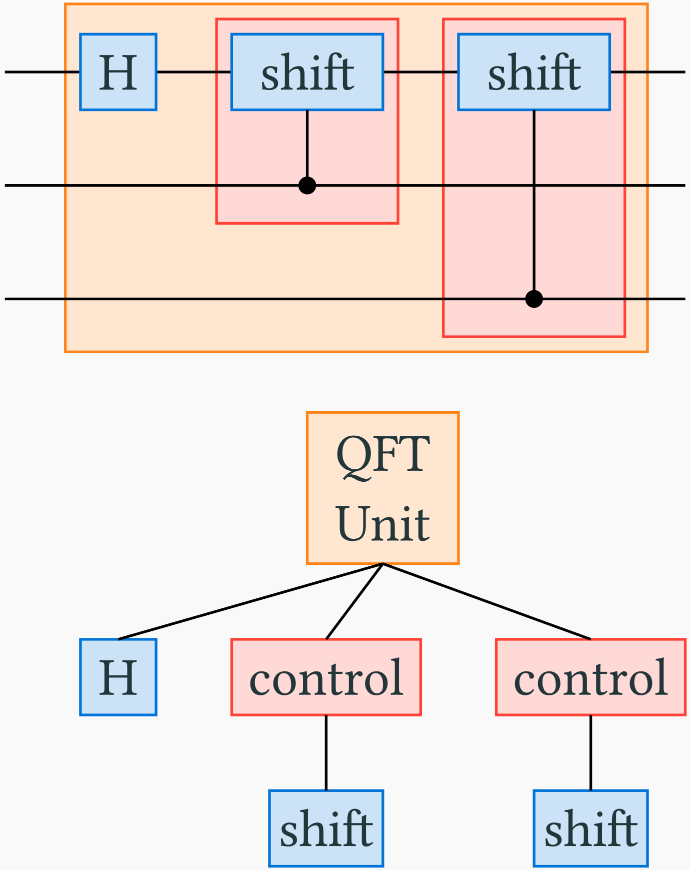
Introduction of Selected Packages

The Circuit Expression in Yao

A differentiable, efficient & extensible framework for quantum algorithm design. Top performance in exact simulation.

Features

- Ability to compose circuits



Xiuzhe Luo, Jinguo Liu, Pan Zhang and Lei Wang, Quantum, 2019

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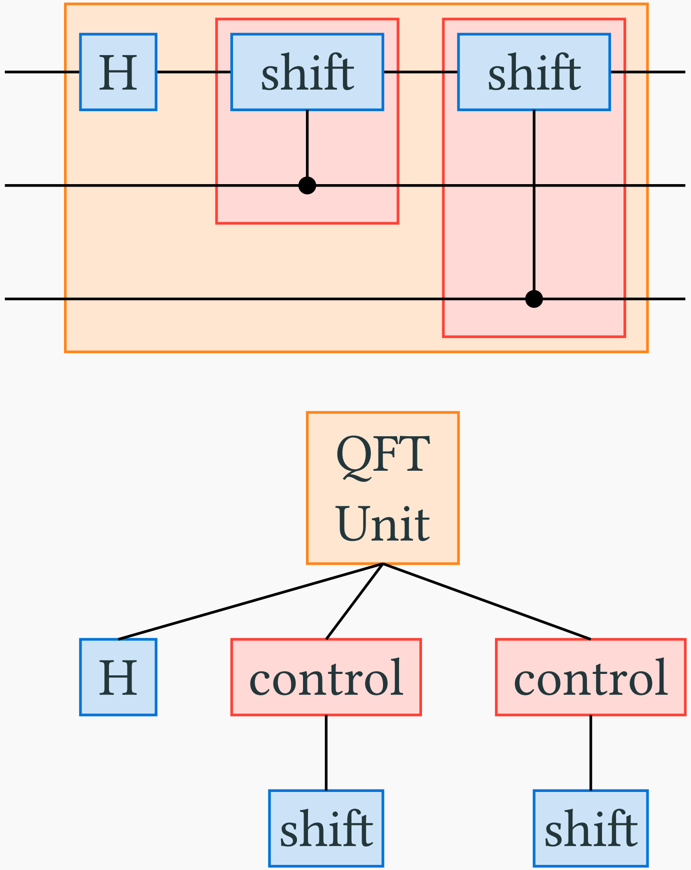

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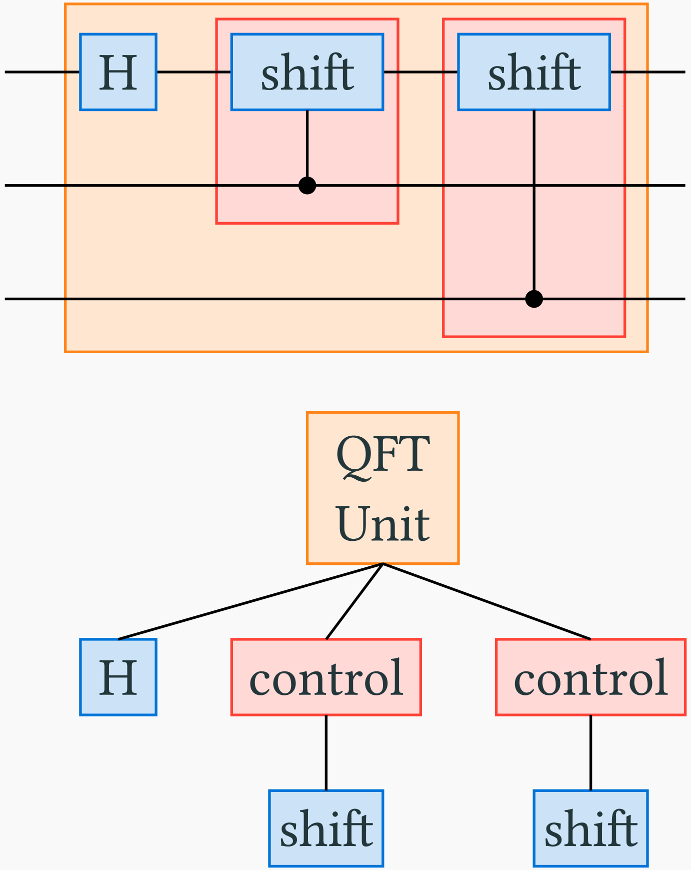

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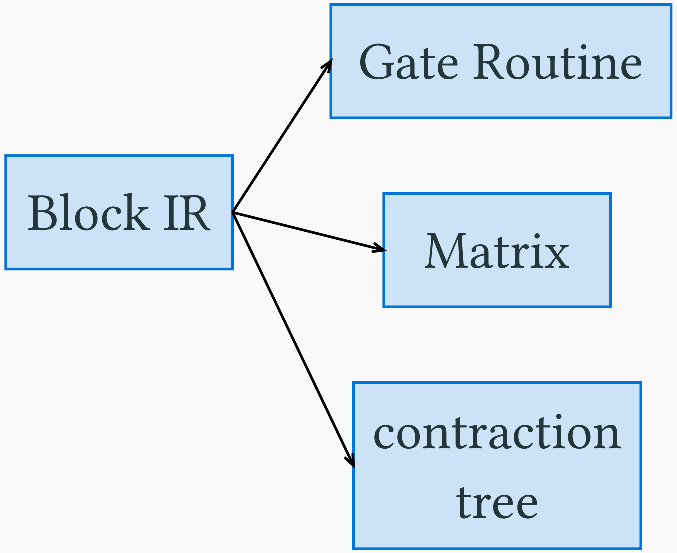
Use cases

- Varitional quanutm algorithms (VQA)
- Tensor network circuits
- Matrix representation construction for general operators



Xiuzhe Luo, Jinguo Liu, Pan Zhang and Lei Wang, Quantum, 2019

Ecosystem

Addon Packages

- OpenQASM, YaoBlocksQASM: support for OpenQASM 2.0

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- FLOYao: A fermionic linear optics simulator backend for Yao.jl

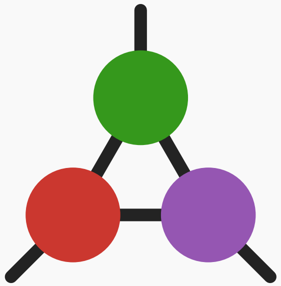
Tensor Networks

Tensor Networks

Tensor networks has a long history in Julia community.

TensorOperations

static & basic contraction order optimization, with good performance and syntax.



TensorOperations.jl

```julia
using TensorOperations
α = randn()
A = randn(5, 5, 5, 5, 5, 5)
B = randn(5, 5, 5)
C = randn(5, 5, 5)
D = zeros(5, 5, 5)
@tensor begin
    D[a, b, c] = A[a, e, f, c, f, g] * B[g, b, e] + α * C[c, a, b]
    E[a, b, c] := A[a, e, f, c, f, g] * B[g, b, e] + α * C[c, a, b]
end
```

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ITensors

long established, with good performance and a strong DMRG related algorithm implementation.

ITensors.jl

```
using ITensors
N = 100
sites = siteinds("S=1",N)

os = OpSum()
for j=1:N-1
  os += "Sz",j,"Sz",j+1
  os += 1/2,"S+",j,"S-",j+1
  os += 1/2,"S-",j,"S+",j+1
end
H = MPO(os,sites)
```

```
psi0 = randomMPS(sites,10)

nsweeps = 5
maxdim = [10,20,100,100,200]
cutoff = [1E-10]

energy, psi = dmrg(H,psi0; nsweeps, maxdim, cutoff)
```

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OMEinsum

a new package, with a focus on contraction optimization and automatic differentiation.

OMEinsum.jl

```
julia> optcode = optimize_code(code, uniformsize(code, 3), TreeSA())
SlicedEinsum{Char, DynamicNestedEinsum{Char}}(Char[], ago, goa ->
├─ ago
└─ gcojl, cjal -> goa
   ├─ bgck, bojlk -> gcojl
   ⋮  ⋮  ⋮
   └─ cjf, afl -> cjal
       ├─ cjf
       └─ afl
)
julia> contraction_complexity(optcode, uniformsize(optcode, 3))
Time complexity: 2^12.737881076857779
Space complexity: 2^7.92481250360578
Read-write complexity: 2^11.247334178028728

julia> optcode(fill(s, 10)...)[]
0
```

And More …

QuantumOptics: exact simulation of general quantum system

QuantumInformation

A Julia package for numerical computation in quantum information theory

QuantumSavory

Clifford circuits, graph states, and other quantum Stabilizer formalism tools.

QuantumCircuitOpt

A Julia/JuMP Package for Optimal Quantum Circuit Design

DFTK

DFTK: Density-functional toolkit

…

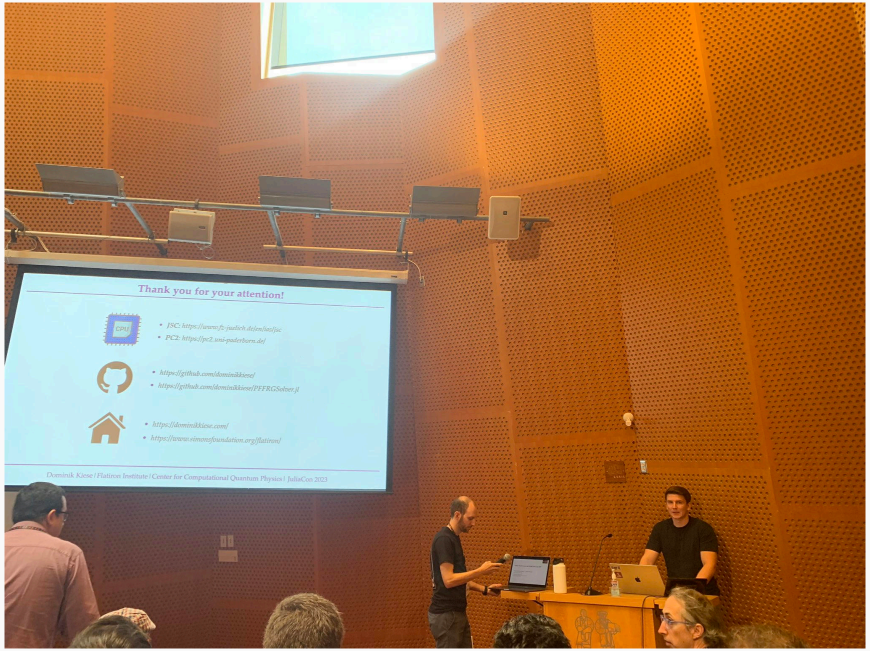
The Quantum "Gang" in Julia Community

The Quantum "Gang" in Julia

The Quantum Track at JuliaCon 2023

Organizers

- Xiuzhe (Roger) Luo, Perimeter Institute
- Katharine Hyatt, AWS Braket
- Ashley Milsted, AWS Braket
- Matthew Fishman, Flatiron Institute
- Miles Stoudenmire, Flatiron Institute
- Michael F. Herbst, EPFL



Thank you for your attention!

- JSC: https://www.fz-juelich.de/en/ias/jsc
- PC2: https://pc2.uni-paderborn.de/

- https://github.com/dominikkiese/
- https://github.com/dominikkiese/PFFRGSolver.jl

- https://dominikkiese.com/
- https://www.simonsfoundation.org/flatiron/

Dominik Kiese | Flatiron Institute | Center for Computational Quantum Physics | JuliaCon 2023

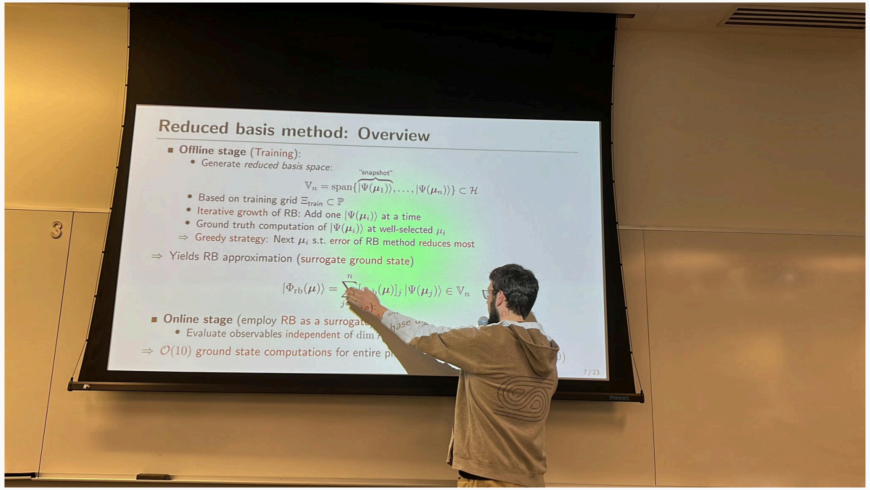
ITensor presentation

The Quantum "Gang" in Julia

The Quantum Track at JuliaCon 2023

over 14 talks including (online not included):

- Quantum Information
- Tensor Networks
- Quantum Chemistry
- Quanutm Control
- ...


Reduced basis method: Overview
Offline stage (Training):
Generate reduced basis space:
"snapshot"
$\mathbb{V}_n = \mathrm{span}\{|\Psi(\mu_1)\rangle, \ldots, |\Psi(\mu_n)\rangle\} \subset \mathcal{H}$
Based on training grid $\Xi_{\text{train}} \subset \mathbb{P}$
Iterative growth of RB: Add one $|\Psi(\mu_i)\rangle$ at a time
Ground truth computation of $|\Psi(\mu_i)\rangle$ at well-selected μ_i
⇒ Greedy strategy: Next μ_i s.t. error of RB method reduces most
⇒ Yields RB approximation (surrogate ground state)
$|\Phi_{\text{rb}}(\mu)\rangle = \sum^{n}$ $(\mu)]_j |\Psi(\mu_j)\rangle \in \mathbb{V}_n$
Online stage (employ RB as a surrogat
Evaluate observables independent of dim
⇒ $\mathcal{O}(10)$ ground state computations for entire p
7 / 23
3

DFTK talk by Michael Herbst

The Quantum "Gang" in Julia

The Quantum Track at JuliaCon 2023

1-day mini-symposium within JuliaCon

- chat with package developers and users
- learn about the latest developments
- discuss the future of quantum software in Julia

JuliaCon 2024 is coming to Eindhoven, Netherlands!

QuantumSymbolics by Stefan Krastanov