Julia in action – An HPC application from the field of particle physics

Anton Reinhard[1,2], Simeon Ehrig[1,2], Dr. Michael Bussmann[1, 2], Uwe Hernandez Acosta[1,2]

[1] Helmholtz-Zentrum Dresden-Rossendorf, [2] Center for Advanced Systems Understanding

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whoami

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HZDR
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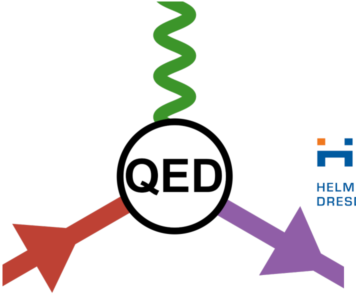
CASUS
CENTER FOR ADVANCED SYSTEMS UNDERSTANDING

whoami

- Diploma in computer science from TU Dresden in 2024 with Uwe as supervisor
- Previous background in C++, currently mostly Julia
- Scientist at CASUS/HZDR
- Currently working on QED in an HPC context in Julia



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CASUS
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CASUS and Computational Radiation Physics

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- Focus on modelling, simulating, visualizing laser-matter interaction

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CASUS and Computational Radiation Physics

Center for Advanced Systems Understanding

- Focus on modelling, simulating, visualizing laser-matter interaction
- Open-source project PIConGPU
- Aim at laser particle acceleration and models for compact radiation sources
- Further development into laser-driven fusion

PIConGPU Simulation Example

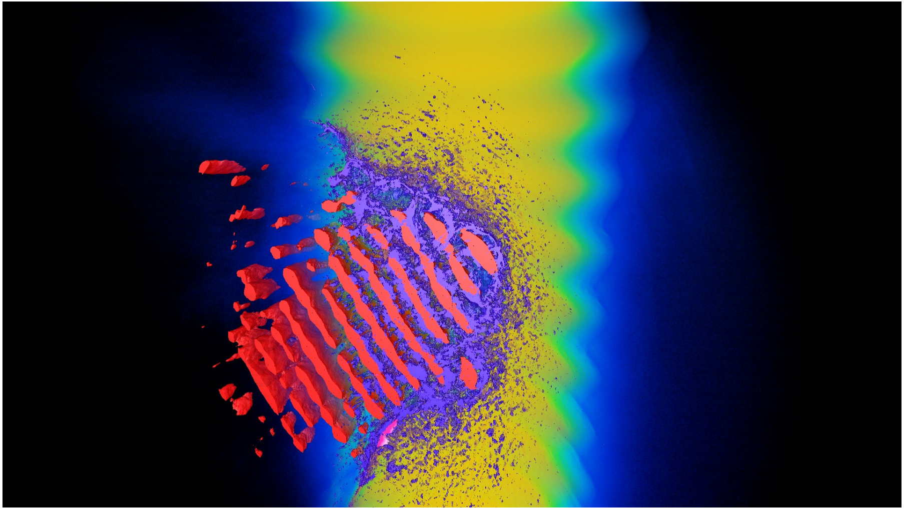

Figure: Laser (red) hitting cryogenic hydrogen (blue-yellow-pink for increasing electron energy density)

Multiple Dispatch

Multiple Dispatch

```
abstract type Particle end
```

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struct Electron <: Particle end
struct Positron <: Particle end
struct Photon <: Particle end
```

Multiple Dispatch

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abstract type Particle end


struct Electron <: Particle end
struct Positron <: Particle end
struct Photon <: Particle end

can_interact(p1::T, p2::T) where {T<:Particle} = false
can_interact(p1::T1, p2::T2) where {T1<:Particle, T2<:Particle} = true
```

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abstract type Particle end


struct Electron <: Particle end
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abstract type Particle end


struct Electron <: Particle end
struct Positron <: Particle end
struct Photon <: Particle end

can_interact(p1::T, p2::T) where {T<:Particle} = false
can_interact(p1::T1, p2::T2) where {T1<:Particle, T2<:Particle} = true

using Test
@test can_interact(Photon(), Electron()) == true
@test can_interact(Electron(), Positron()) == true
@test can_interact(Electron(), Electron()) == false

# Done? What if we want to add more particles?
```

Multiple Dispatch

```julia
abstract type Particle end
abstract type Boson <: Particle end
abstract type Fermion <: Particle end
struct Electron <: Fermion end
struct Positron <: Fermion end
struct Photon <: Boson end

can_interact(p1::T, p2::T) where {T<:Fermion} = false
can_interact(p1::Photon, p2::Photon) = false
can_interact(p1::Photon, p2::Fermion) = true
can_interact(p1::Fermion, p2::Photon) = true
can_interact(p1::Electron, p2::Positron)  = true
can_interact(p1::Positron, p2::Electron)  = true
```

Multiple Dispatch - Reusability

```
struct Muon <: Fermion end
struct AntiMuon <: Fermion end
```

Multiple Dispatch - Reusability

```julia
struct Muon <: Fermion end
struct AntiMuon <: Fermion end

can_interact(p1::Muon, p2::AntiMuon) = true
can_interact(p1::AntiMuon, p2::Muon) = true

@test can_interact(Muon(), Photon()) == true
@test can_interact(Muon(), AntiMuon()) == true
@test can_interact(AntiMuon(), AntiMuon()) == false
```

Multiple Dispatch - Reusability

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can_interact(p1::Muon, p2::AntiMuon) = true
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@test can_interact(Muon(), Photon()) == true
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```

We can reuse existing functions for new types

Multiple Dispatch - Reusability

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```

We can reuse existing functions for new types

Without owning the functions

Multiple Dispatch - Reusability

```julia
interaction_result(::T, ::T) where {T<:Fermion}          = nothing
interaction_result(::Photon, ::Photon)                   = nothing
interaction_result(::Photon, ::T) where {T<:Fermion}  = T()
interaction_result(::T, ::Photon) where {T<:Fermion}  = T()
interaction_result(::Electron, ::Positron)               = Photon()
interaction_result(::Positron, ::Electron)               = Photon()
```

Multiple Dispatch - Reusability

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interaction_result(::Electron, ::Positron)                = Photon()
interaction_result(::Positron, ::Electron)                = Photon()

@test interaction_result(Positron(), Photon()) == Positron()
@test interaction_result(Photon(), Electron()) == Electron()
@test interaction_result(Positron(), Electron()) == Photon()
@test isnothing(interaction_result(Muon(), Muon()))
```

Multiple Dispatch - Reusability

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@test interaction_result(Positron(), Photon()) == Positron()
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@test isnothing(interaction_result(Muon(), Muon()))
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We can reuse existing *types* for new *functions*

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We can reuse existing *types* for new *functions*

Without owning the types

Multiple Dispatch

But how is this different from function overloading?

Multiple Dispatch

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```
particles1 = [rand([Photon(), Electron(), Positron()]) for _ in 1:10]
particles2 = [rand([Photon(), Electron(), Positron()]) for _ in 1:10]

for (p1, p2) in Iterators.zip(particles1, particles2)
      if can_interact(p1, p2)
            println("$p1 and $p2 can interact")
      else
            println("$p1 and $p2 can not interact")
      end
end
```

Multiple Dispatch

But how is this different from function overloading?

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particles1 = [rand([Photon(), Electron(), Positron()]) for _ in 1:10]
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- C++ can do static multiple dispatch → function overloading

Multiple Dispatch

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```

- C++ can do static multiple dispatch → function overloading
- C++ can do single dynamic dispatch → polymorphism

Multiple Dispatch

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- C++ can do static multiple dispatch → function overloading
- C++ can do single dynamic dispatch → polymorphism
- C++ **cannot** do multiple dynamic dispatch

Multiple Dispatch

But how is this different from function overloading?

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particles1 = [rand([Photon(), Electron(), Positron()]) for _ in 1:10]
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      end
end
```

- C++ can do static multiple dispatch → function overloading
- C++ can do single dynamic dispatch → polymorphism
- C++ **cannot** do multiple dynamic dispatch[1]

[1] C++ can of course *functionally* do this, as can every language that is turing-complete

Code Generation

Julia understands its own code

```
julia> Meta.parse("1 + 2")
:(1 + 2)

julia> dump(ans)
Expr
  head: Symbol call
  args: Array{Any}((3,))
    1: Symbol +
    2: Int64 1
    3: Int64 2
```

Code Generation

Julia understands its own code

```
julia> expr = Meta.parse("x + 3")
:(x + 3)

julia> x = 5
5

julia> eval(expr)
8
```


DRESDEN concept HZDR

Code Generation

Julia understands its own code

```
julia> expr = Meta.parse("x + 3")
:(x + 3)

julia> eval(Meta.parse("add3(x) = $expr"))
add3 (generic function with 1 method)

julia> add3(5)
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Code Generation

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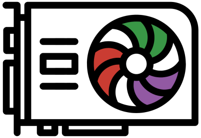
```
julia> expr = Meta.parse("x + 3")
:(x + 3)

julia> eval(Meta.parse("add3(x) = $expr"))
add3 (generic function with 1 method)

julia> add3(5)
8
```

→ We can generate functions at runtime

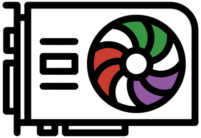
Many more capabilities, see the Julia Docs on Metaprogramming

GPU Usage



- JuliaGPU with
  - CUDA.jl (NVIDIA GPUs)
  - AMDGPU.jl (AMD GPUs)
  - oneAPI.jl (Intel GPUs)
  - Metal.jl (Apple GPUs)
  - KernelAbstractions.jl for writing kernels that run on any of the above

GPU Usage



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- Varying degrees of support

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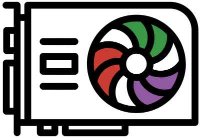

- JuliaGPU with
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  - oneAPI.jl (Intel GPUs)
  - Metal.jl (Apple GPUs)
  - KernelAbstractions.jl for writing kernels that run on any of the above
- Varying degrees of support
- Array-driven programming via broadcast

GPU Usage - Example

```
julia> using oneAPI

julia> heavy_compute(x) = begin for _ in 1:100 x = sin(sqrt(x))^2 end; return x end
heavy_compute (generic function with 1 method)

julia> gpu_vec = oneVector([rand(Float32) for _ in 1:10_000])
10000-element oneArray{Float32, 1, oneAPI.oneL0.DeviceBuffer}:
 0.50362855
 ...
 0.042337418

julia> heavy_compute.(gpu_vec)
10000-element oneArray{Float32, 1, oneAPI.oneL0.DeviceBuffer}:
 0.027846681
 ...
 0.01750382
```


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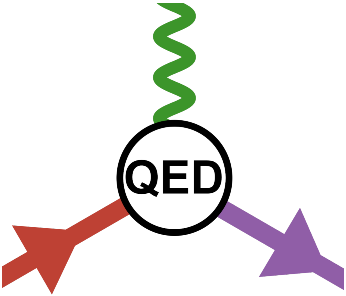
Goal

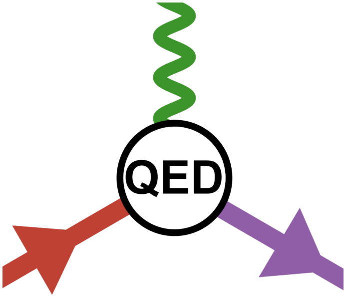
Event Generation



Goal

Event Generation

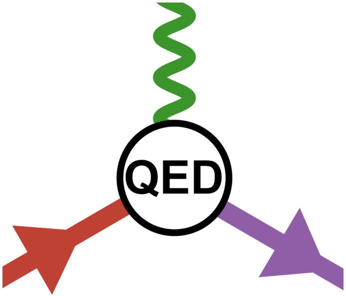
- Subgoal: Computation of matrix elements



Goal

Event Generation

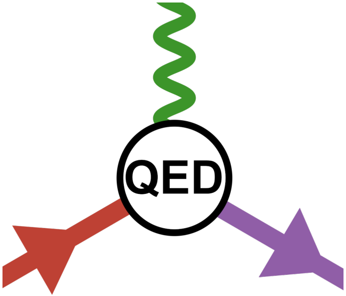
- Subgoal: Computation of matrix elements (for arbitrary scattering processes, in QED, at tree-level, for any/all spin and polarization combinations)



Goal

Event Generation

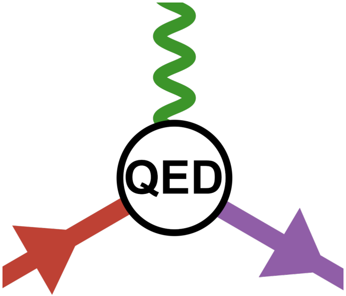
- Subgoal: Computation of matrix elements
- Where to start?



Goal

Event Generation

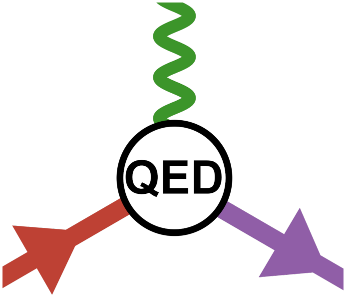
- Subgoal: Computation of matrix elements
- Where to start?
- Simpler model than QED → ABC toy model



Goal

Event Generation

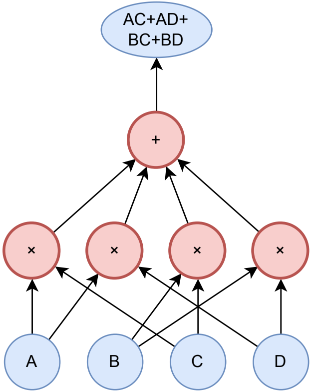
- Subgoal: Computation of matrix elements
- Where to start?
- Simpler model than QED $\rightarrow$ ABC toy model
- Generate code per particle process



DRESDEN concept HZDR

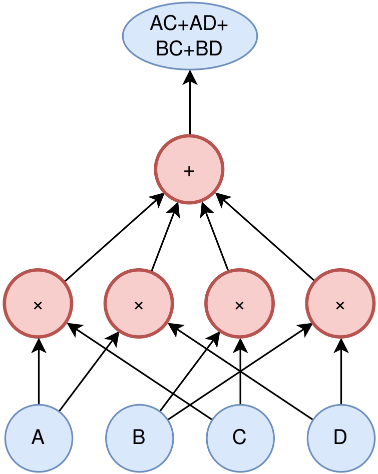
ComputableDAGs.jl

- Represent computation as a directed acyclic graph (DAG) of function calls
- Allows dynamic construction, analysis, scheduling, and execution (threaded, GPU, etc.)
- ~ 2000 lines of code, ~ 700 lines of comments

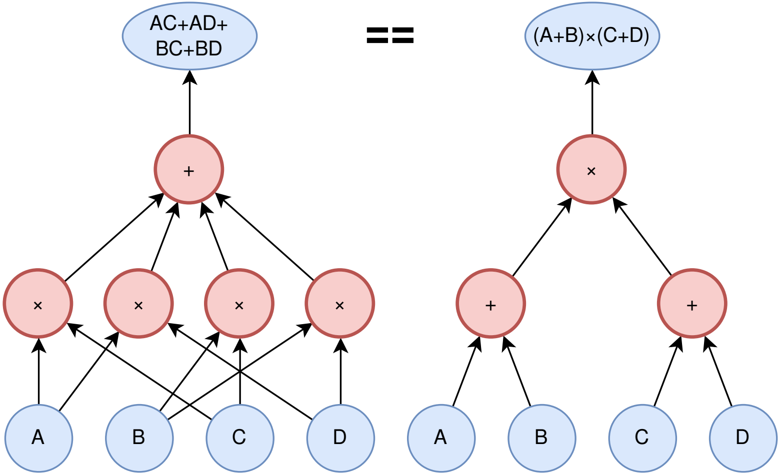


ComputableDAGs.jl

ComputableDAGs.jl - Distributivity



ComputableDAGs.jl - Distributivity



ComputableDAGs.jl - Outline

- Get graph, a scheduler, and machine information

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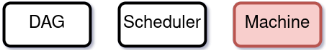
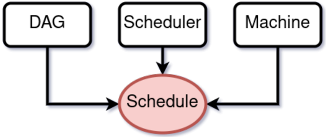
ComputableDAGs.jl - Outline



- Get graph, a scheduler, and machine information

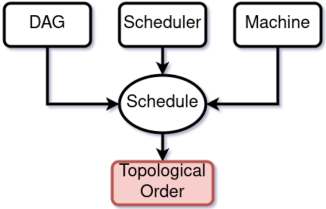
ComputableDAGs.jl - Outline

- Get graph, a scheduler, and machine information
- Use scheduler interface



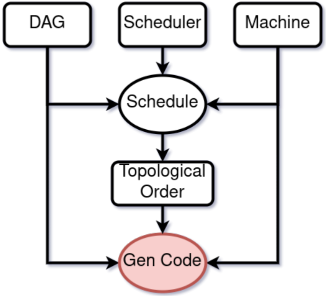
ComputableDAGs.jl - Outline

- Get graph, a scheduler, and machine information
- Use scheduler interface to create a topological ordering of tasks for each device



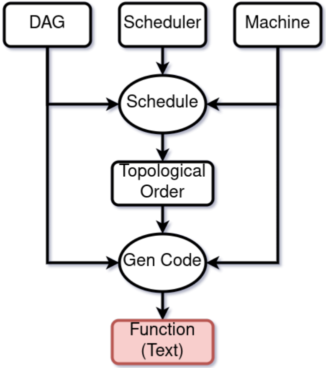
ComputableDAGs.jl - Outline

- Get graph, a scheduler, and machine information
- Use scheduler interface to create a topological ordering of tasks for each device
- For each task in the ordering, generate code using the scheduled device



ComputableDAGs.jl - Outline

- Get graph, a scheduler, and machine information
- Use scheduler interface to create a topological ordering of tasks for each device
- For each task in the ordering, generate code using the scheduled device
- Evaluate the function code



ComputableDAGs.jl - Outline

- Get graph, a scheduler, and machine information
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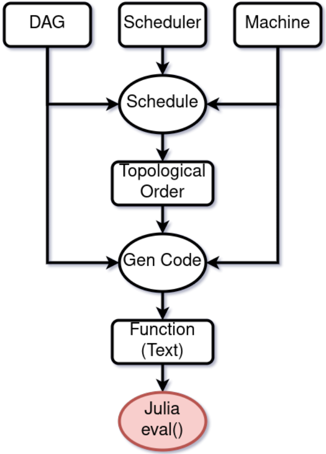

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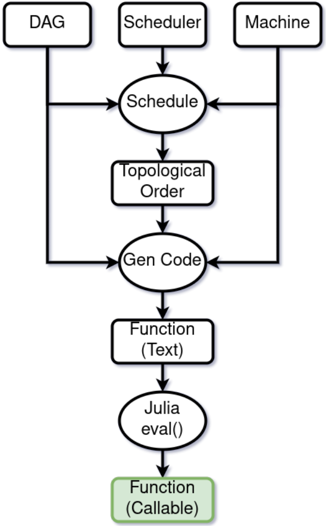

Code Generation in Detail (Simplified)

```
struct FunctionCall
    func::Function
    arguments::Vector{Symbol}
    return_symbol::Symbol
    return_types::Type
end
```

Code Generation in Detail (Simplified)

```julia
struct FunctionCall
    func::Function
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end

function expr_from_fc(fc::FunctionCall)
    func_call = Expr(:call, fc.func, fc.arguments...)
    return Expr(:(=), fc.return_symbol, func_call)
end
```

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end

function function_body(function_calls::Vector{FunctionCall})
    return Expr(:block, expr_from_fc.(function_calls)...)
end
```

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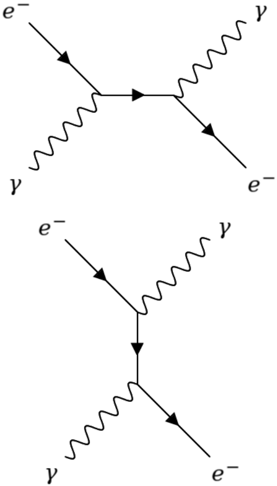
end
```

Not a lot of Code!

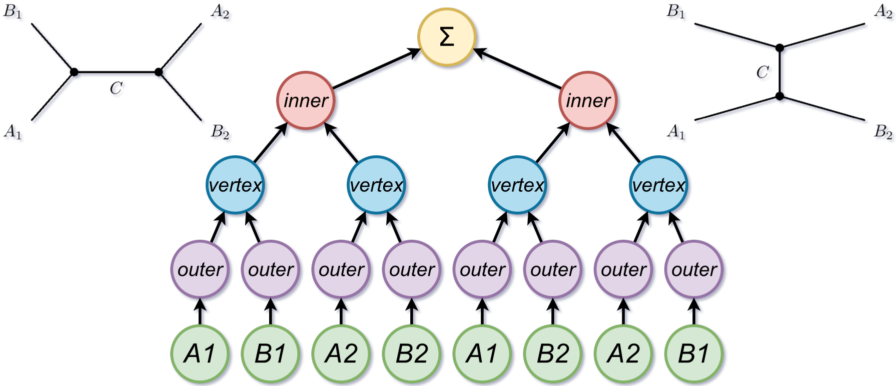
QEDFeynmanDiagrams.jl

- From a given particle process, e.g., $e^- + \gamma \to e^- + \gamma$, generate a function for its squared matrix element, given the particle momenta
- Built on top of ComputableDAGs.jl
- ~ 1700 lines of code, ~ 270 lines of comments

QEDFeynmanDiagrams.jl



From Process to Function



Code Adventure: Fun with Multiple Dispatch

Problem: We want a process object that contains external particles and their respective spins or polarizations.

```
struct ScatteringProcess{INT,OUTT,INSP,OUTSP}
        where {INT<:Tuple,OUTT<:Tuple,INSP<:Tuple,OUTSP<:Tuple}
    incoming_particles::INT
    outgoing_particles::OUTT

    incoming_spin_pols::INSP
    outgoing_spin_pols::OUTSP
end
```

Code Adventure: Fun with Multiple Dispatch

Problem: We want a process object that contains external particles and their respective spins or polarizations.

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How do we make sure that fermions have a spin and bosons have a polarization?

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    outgoing_particles::OUTT

    incoming_spin_pols::INSP
    outgoing_spin_pols::OUTSP
end
```

How do we make sure that fermions have a spin and bosons have a polarization?
→ Input validation!

Code Adventure: Input Validation

```
function ScatteringProcess(
    in_particles::NTuple{I,AbstractParticleType},
    out_particles::NTuple{O,AbstractParticleType},
    in_spin_pols::NTuple{I,AbstractSpinOrPolarization},
    out_spin_pols::NTuple{O,AbstractSpinOrPolarization},
) where {I,O}
    _assert_spin_pol_particle_compatibility(in_particles, in_spin_pols)
    _assert_spin_pol_particle_compatibility(out_particles, out_spin_pols)

    return new{
        typeof(in_particles),
        typeof(out_particles),
        typeof(in_spin_pols),
        typeof(out_spin_pols),
    }(
        in_particles, out_particles, in_spin_pols, out_spin_pols
    )
end
```

Code Adventure: Input Validation

```
_assert_spin_pol_particle_compatibility(::Tuple{}, ::Tuple{}) = nothing
```

Code Adventure: Input Validation

```
_assert_spin_pol_particle_compatibility(::Tuple{}, ::Tuple{}) = nothing

function _assert_spin_pol_particle_compatibility(
    particles::Tuple{AbstractParticleType,Vararg},
    spin_pols::Tuple{AbstractSpinOrPolarization,Vararg},
)
    if is_fermion(particles[1]) && !(spin_pols[1] isa AbstractSpin)
        throw("invalid combination")
    end
    if is_boson(particles[1]) && !(spin_pols[1] isa AbstractPolarization)
        throw("invalid combination")
    end
    return _assert_spin_pol_particle_compatibility(
        particles[2:end],
        spin_pols[2:end],
    )
end
```

Code Adventure: Input Validation

Okay, but why so complicated? Why not just loop it?

```julia
function _assert_spin_pol_particle_compatibility_loop(
    particles::Tuple{AbstractParticleType,Vararg},
    spin_pols::Tuple{AbstractSpinOrPolarization,Vararg},
)
    for (p, s) in Iterators.zip(particles, spin_pols)
        if is_fermion(p) && !(s isa AbstractSpin)
            throw("invalid combination")
        end
        if is_boson(p) && !(s isa AbstractPolarization)
            throw("invalid combination")
        end
    end
    return nothing
end
```

Code Adventure: Comparison

```
julia> using BenchmarkTools, QEDcore

julia> # define functions from above...

julia> @btime _assert_spin_pol_particle_compatibility(
           (Electron(), Photon()),
           (SpinUp(), PolX()),
       )
  1.021 ns (0 allocations: 0 bytes)
```

Code Adventure: Comparison

```
julia> using BenchmarkTools, QEDcore

julia> # define functions from above...

julia> @btime _assert_spin_pol_particle_compatibility(
           (Electron(), Photon()),
           (SpinUp(), PolX()),
       )
  1.021 ns (0 allocations: 0 bytes)

julia> @btime _assert_spin_pol_particle_compatibility_loop(
           (Electron(), Photon()),
           (SpinUp(), PolX()),
       )
  12.256 ns (0 allocations: 0 bytes)
```

What gives?

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Code Adventure: Code Inspection

- Generate with `@code_native <call>`
- The blue lines are assembly instructions
- It compiles the loop into code

Native code of the looped version

Code Adventure: Code Inspection

Native code of the recursive version

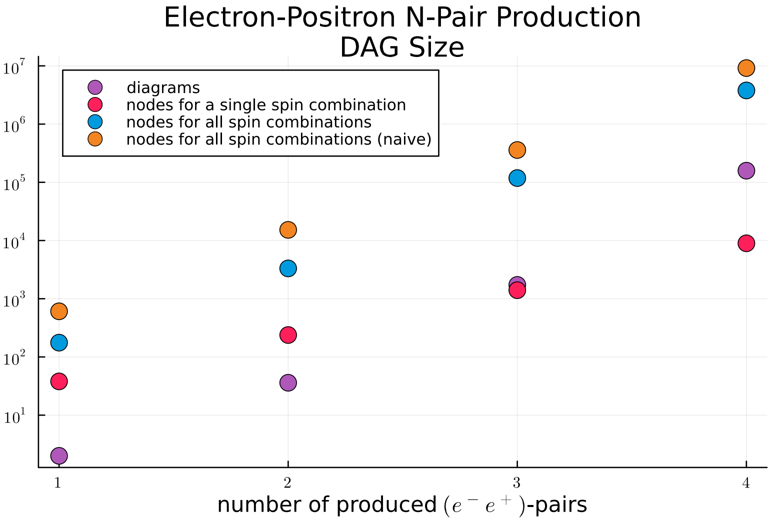
```
julia> @code_native _assert_spin_pol_particle_compatibility((Electron(), Photon()), (SpinUp(), PolX()))
        .text
        .file   "_assert_spin_pol_particle_compatibility"
        .globl  julia__assert_spin_pol_particle_compatibility_2920 # -- Begin function julia__assert_spin_pol_particle_compatibility_2920
        .p2align        4, 0x90
        .type   julia__assert_spin_pol_particle_compatibility_2920,@function
julia__assert_spin_pol_particle_compatibility_2920: # @julia__assert_spin_pol_particle_compatibility_2920
; Function Signature: _assert_spin_pol_particle_compatibility(Tuple{QEDcore.Electron, QEDcore.Photon}, Tuple{QEDbase.SpinUp, QEDbase.PolarizationX})
; ┌ @ REPL[3]:1 within `_assert_spin_pol_particle_compatibility`
# %bb.0:                                # %top
        push    rbp
        mov     rbp, rsp
        pop     rbp
        ret
.Lfunc_end0:
        .size   julia__assert_spin_pol_particle_compatibility_2920, .Lfunc_end0-julia__assert_spin_pol_particle_compatibility_2920
; └
                                        # -- End function
        .section        ".note.GNU-stack","",@progbits
```

Results - Reproducibility

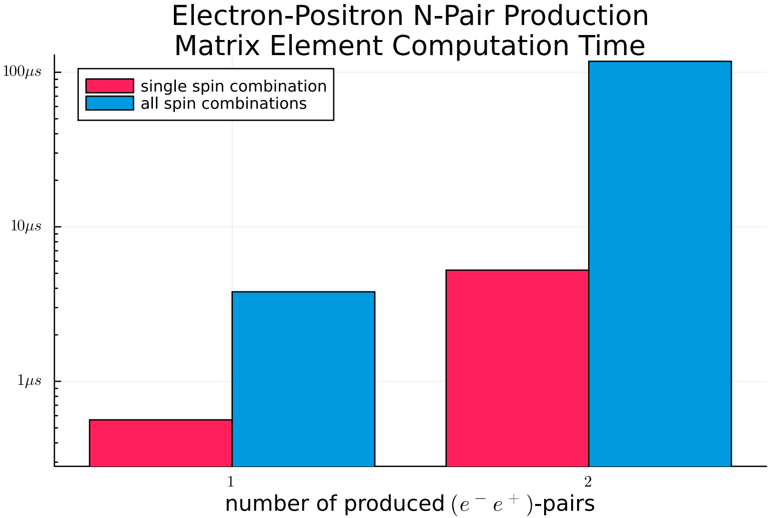
The following results can be reproduced using the Jupyter notebooks at this URL:

https://github.com/AntonReinhard/QEDFeynmanDiagrams.jl/tree/profiling/profiling

Results - $e^- + e^+ \to n(e^- + e^+)$ - DAG Sizes



Results - $e^- + e^+ \rightarrow n(e^- + e^+)$ - DAG Computation Time



Results - Profiling Flamegraph

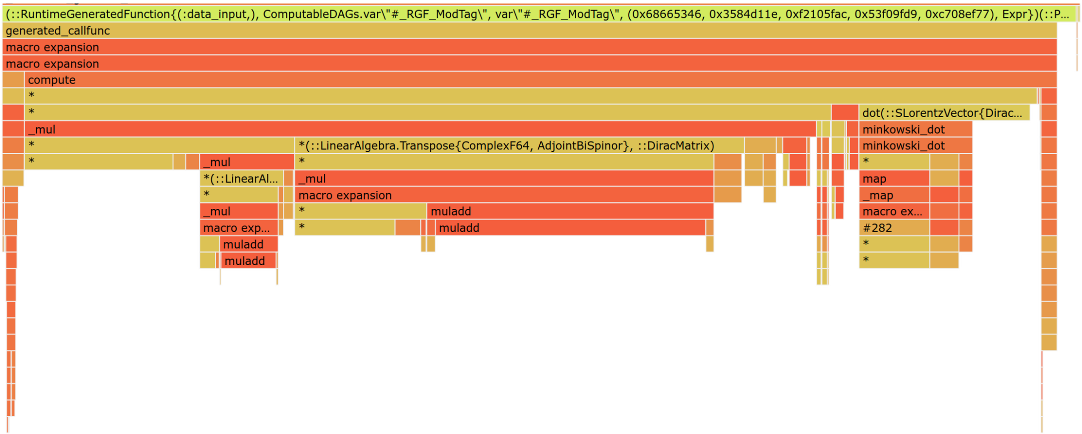


Figure: Created with PProf.jl

Results - $e^- + n\gamma \to e^- + \gamma$ - 4 GPU HPC Node heterogeneous

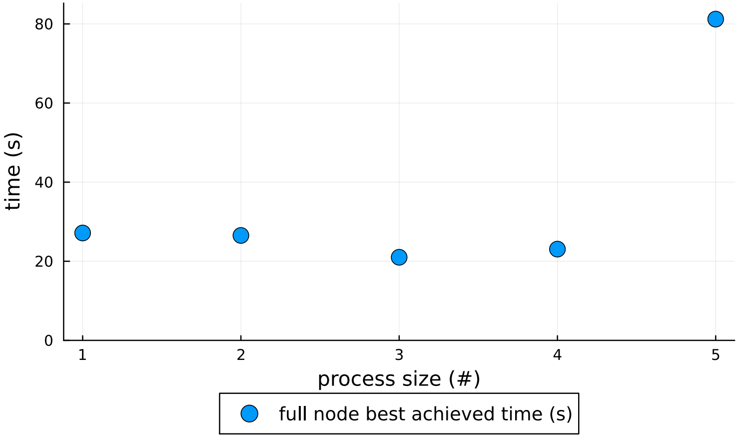


Figure: Time taken for $2^{30} \approx 10^9$ squared matrix elements for n-photon Compton events

Outlook

- Ongoing development
- Compare to existing solutions (MadGraph5 [1], O'Mega [2], SHERPA [3])
- Extension for other quantum field theories through generalized diagram generation
- Consider vectorization inside the graph

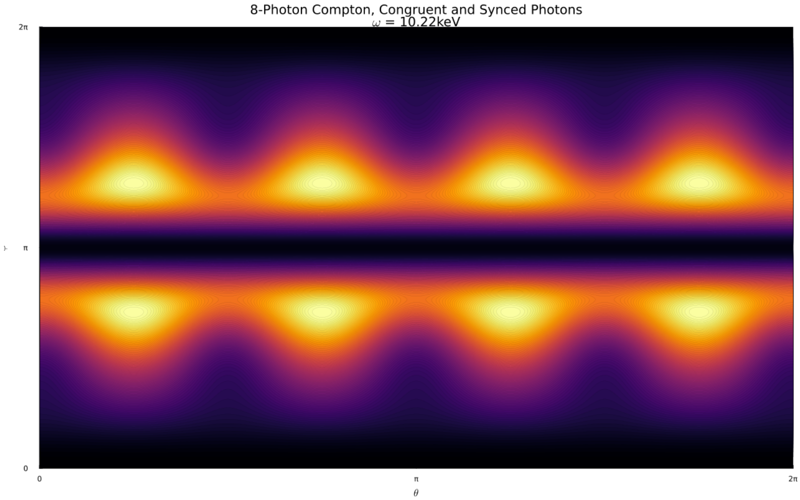
Acknowledgements

Collaborators:

- **Dr. Uwe Hernandez Acosta**[1,2]
- **Simeon Ehrig**[1,2]
- **Dr. Klaus Steiniger**[1,2]
- **Dr. Michael Bussmann**[1,2]

[1] Center for Advanced Systems Understanding (CASUS)
[2] Helmholtz-Zentrum Dresden-Rossendorf (HZDR)

Discussion


8-Photon Compton, Congruent and Synced Photons
ω = 10.22keV
2π
π
0
0
π
2π
θ

References

[1] Johan Alwall et al. "The automated computation of tree-level and next-to-leading order differential cross sections, and their matching to parton shower simulations". In: *Journal of High Energy Physics* 2014.7 (2014), pp. 1–157.

[2] Mauro Moretti, Thorsten Ohl, and Jürgen Reuter. *O'Mega: An Optimizing Matrix Element Generator*. 2001. arXiv: hep-ph/0102195 [hep-ph]. URL: https://arxiv.org/abs/hep-ph/0102195.

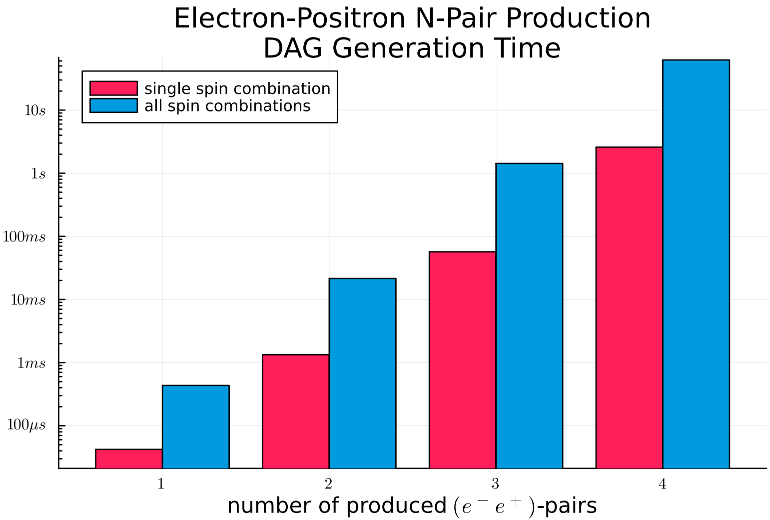
[3] Tanju Gleisberg et al. "Event generation with SHERPA 1.1". In: *Journal of High Energy Physics* 2009.02 (2009), p. 007.

[4] Tim Besard, Christophe Foket, and Bjorn De Sutter. "Effective extensible programming: unleashing Julia on GPUs". In: *IEEE Transactions on Parallel and Distributed Systems* 30.4 (2018), pp. 827–841.

[5] Stefan Karpinski et al. *Why we created julia*. Feb. 2012. URL: https://julialang.org/blog/2012/02/why-we-created-julia/.

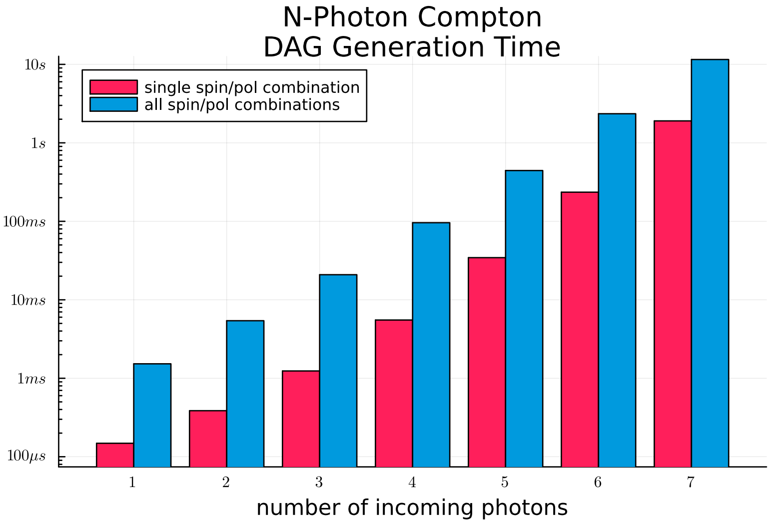
[6] Valentin Churavy et al. "Bridging HPC Communities through the Julia Programming Language". In: *arXiv preprint arXiv:2211.02740* (2022).

Results - $e^- + e^+ \rightarrow n(e^- + e^+)$ - DAG Generation Time

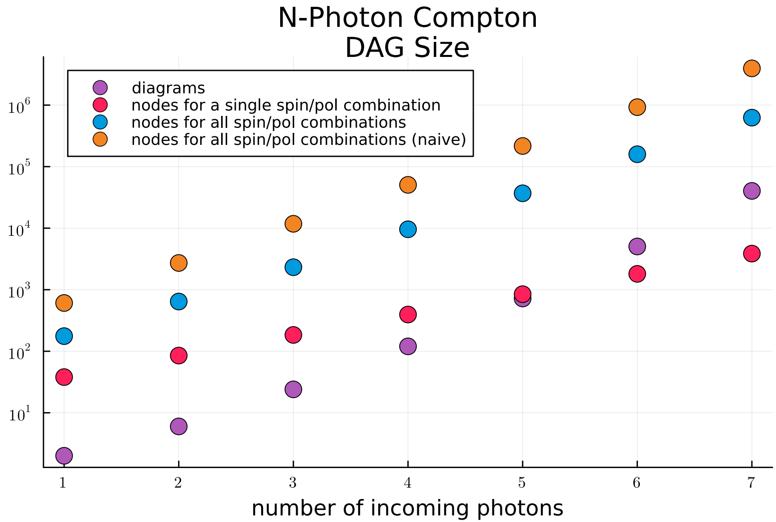


DRESDEN concept HZDR

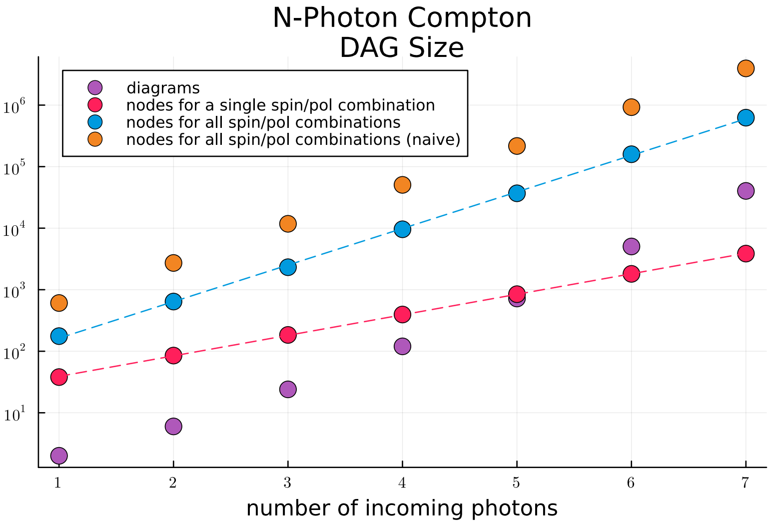
Results - $e^- + k\gamma \to e^- + \gamma$ - DAG Generation Time



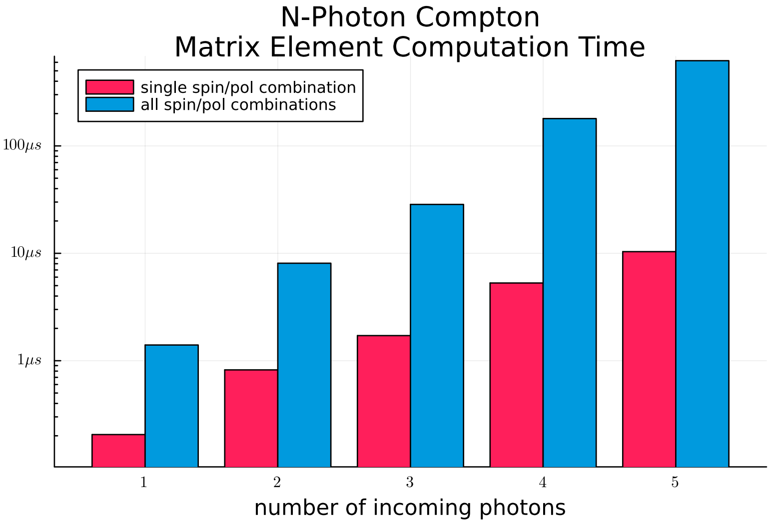
Results - $e^- + k\gamma \to e^- + \gamma$ - DAG Sizes



Results - $e^- + k\gamma \to e^- + \gamma$ - DAG Sizes



Results - $e^- + k\gamma \to e^- + \gamma$ - DAG Computation Time



Benchmarking Machine

Home PC with

- Ryzen 7900X3D
- 2×32GB DDR5 RAM @ 6000MHz
- Julia v1.10